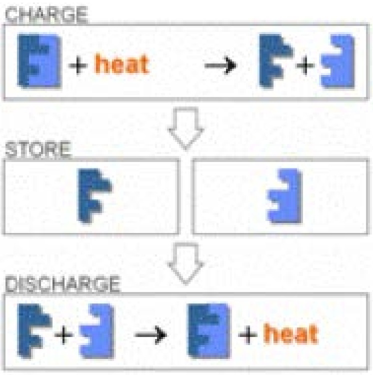
Modelling salt hydrate particles in Open Foam – establishing inter-particle thermodynamic and hydrodynamic transport properties

Introduction

Solar energy is one of the most promising sources of energy, especially since tap water and space heating account for 64% of the total energy consumption in Dutch households. However, there is a mismatch between supply and demand. During summer, solar energy is abundant but the demand for heating is low, while in winter the demand is high but the supply is low. This mismatch between supply and demand could potentially be resolved by seasonal thermal energy storage. The principle of thermochemical heat storage is based on a reversible hydration / dehydration reaction of a thermochemical material (TCM) with water vapor. When a TCM is dehydrated, energy is stored and when the TCM is hydrated, energy is released again (see reaction equation below). The ability to store and release heat using a TCM allows one to create a "heat battery".



$$TCM \cdot xH_2O_{(s)} + heat \leftrightarrow TCM_{(s)} + xH_2O(g)$$

Problem definition

Modelling TCM reactors is frequently done by using analytical models for the solid particles. However, less attention is paid to the fluid surrounding the particles. The overall kinetics of the reactions depend largely on the particle environment. To take the influence of the particle environment into account, heat and mass transport processes in the void spaced between the packed particles have to be investigated. In general, there are two approaches to describe hydrodynamics and reactive transport properties of packed beds. In the first method, packed beds are treated as a continuum at macroscopic scale without any structure. Flow is assumed to obey phenomenological laws like for example Darcy's law, with macroscopic parameters such as permeability and reactive rates. These macroscopic variables are commonly defined by the volume average of microscopic variables over a representative elementary volume (REV). In the second approach, packed beds are simulated based on the actual packed bed geometry. This yields detailed descriptions of the fluid flow and mass and heat transfer processes in between particles. This method requires no additional empirical correlation. A model describing the transport properties in between particles is established and to be extended.

Project description

The aim of this project is to model TCM particles using the simulation software Open Foam, and establish flow and heat transfer characteristics in between the TCM particles. These characteristics are to be extrapolated to a continuum scale model that describes the TCM used in a reactor vessel. In addition, TGA/DSC experiments can be performed as input for the model and to further characterize the TCM. The focused tasks in this project are:

- Modelling of the hydration and dehydration reaction of TCM particles in Open Foam.
- Establish the inter-particle heat and flow characteristics by modelling.
- Characterization of the TCM by TGA/DSC experiments which serve as input for the numerical model.
- Extending an existing continuum model with the found inter-particle heat and flow characteristics.

Required characteristics

- Affinity with and interest in the numerical modelling of heat and flow problems.
- Experience with Comsol and/or Open Foam is a plus.

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