Model Coupling in thermochemical Heat Storage

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Why store heat?
- Energy storage bridges the gap between fluctuating sources of renewable energy and energy consumption.
- Energy storage enhances energy efficiency and process optimization.
- Heat is the major part of the end consumption: 56.3 %
- Decentralized technologies avoid transportation and conversion losses.

End energy consumption in Germany, see [1]

Storage concept
The heat is stored in the conversion of calcium hydroxide Ca(OH)₂ into calcium oxide CaO.

\[ \text{CaO}_n + \text{H}_2\text{O} \rightarrow \text{Ca(OH)}_{2n} + \Delta H_R \]
with \( \Delta H_R = 112 \text{kJ/mol} \)

Main Processes
- The reaction kinetics depend on the temperature and the partial water pressure. The equilibrium temperature is determined by the Van’t Hoff equation [3].

\[ T_{eq} = \frac{H^0}{R} \left( \frac{\Delta S^0}{R} + \ln \frac{p_H}{p_0} \right)^{-1} \]
with \( p_0 = 1.013 \text{bar} \)

\( T > T_{eq} \) : charge
\( T < T_{eq} \) : discharge

- Equilibrium temperature, see [4]
- Volume change of about 50% of the solid particles during the reaction [5]

Fixed-bed Reactor Concepts of

Direct reactor concept [5]: A mixture of reaction fluid and heat transfer fluid is injected directly into the reactor.

Indirect Reactor Concept [6]: Heat transfer and reaction fluid are decoupled. Heat is conducted into the heat transfer channel and transported by a gas flow.

Model concept
The numerical model is implemented in DuMu* [2]. For the direct reactor concept the thermochemical reaction model is sufficient. The indirect reactor concept necessitates coupling between two domains: the thermochemical reaction model and the channel flow.

Thermochemical reaction model solves for the porous medium:
- mass and momentum balance equations for water vapor
- mass balance equations for the solid phases CaO and Ca(OH)₂
- an overall energy balance assuming local thermodynamic equilibrium

using linear reaction kinetics according to [7]

accounting for a porosity atteration due to the porosity change [8].

Channel flow model solves for the heat-exchanger gas-flux:
- the Navier-Stokes equations
- an energy balance equation

Coupling accounts for:
- heat conduction between the two domains assuming a continuous temperature distribution at the interface

Model Setup

First Results

Temperature distribution after 5 seconds

Reaction rate in the porous medium domain after 5 seconds

Pressure distribution after 5 seconds

Outlook
- study the importance of turbulence for the heat convection
- reduce computational effort by simplifying the channel flow model
- investigate the assumption of a continuous temperature distribution at the interface
- verify model results with experimental data

Literature

www.hydrosys.uni-stuttgart.de

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