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Model Coupling in thermochemical Heat Storage

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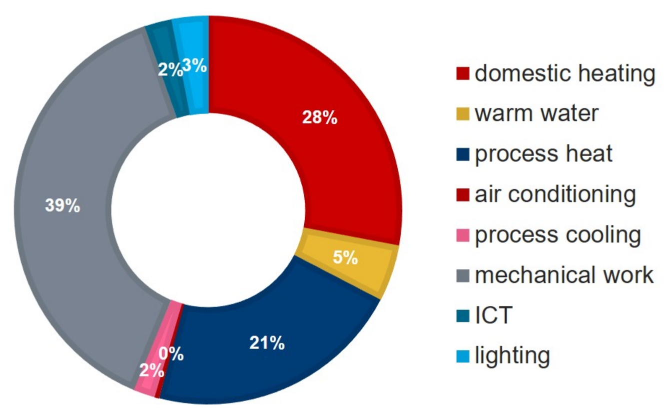
Why store heat?

- 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 energy 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 $Ca(OH)_2$ to calcium oxide CaO.

$$\boxed{CaO_s + H_2O_g \rightleftharpoons Ca(OH)_{2,s} + \Delta H_R}$$

with $\Delta H_R = 112\,\mathrm{kJ/mol}$

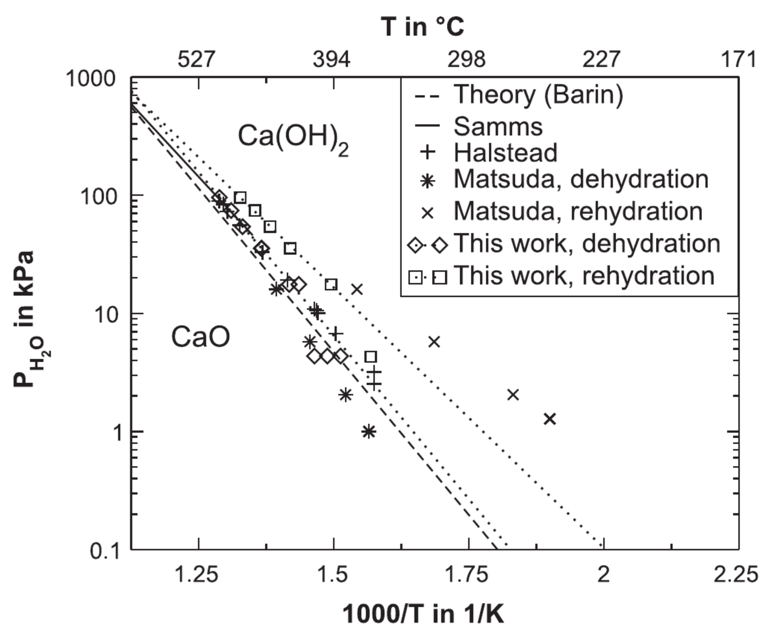
Main Processes

- The reaction kinetics depends on the temperature and the partial water pressure. The equilibrium temperature is determined by the Van't Hoff equation [3].

$$T_{eq} = \frac{H^0}{R}\left(\frac{\Delta S^0}{R} + \ln\frac{p_v}{p_0}\right)^{-1}$$

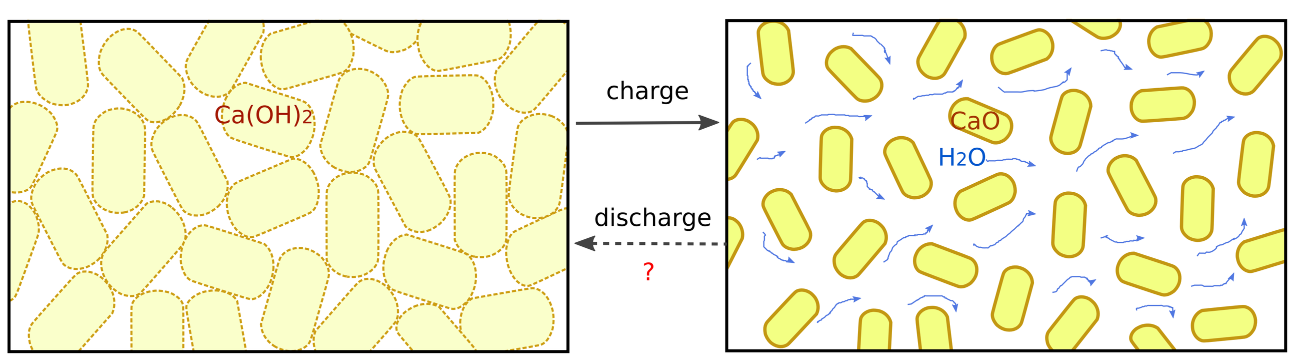
with $p_0 = 1.013 bar$

$T > T_{eq}$: charge
$T < T_{eq}$: discharge

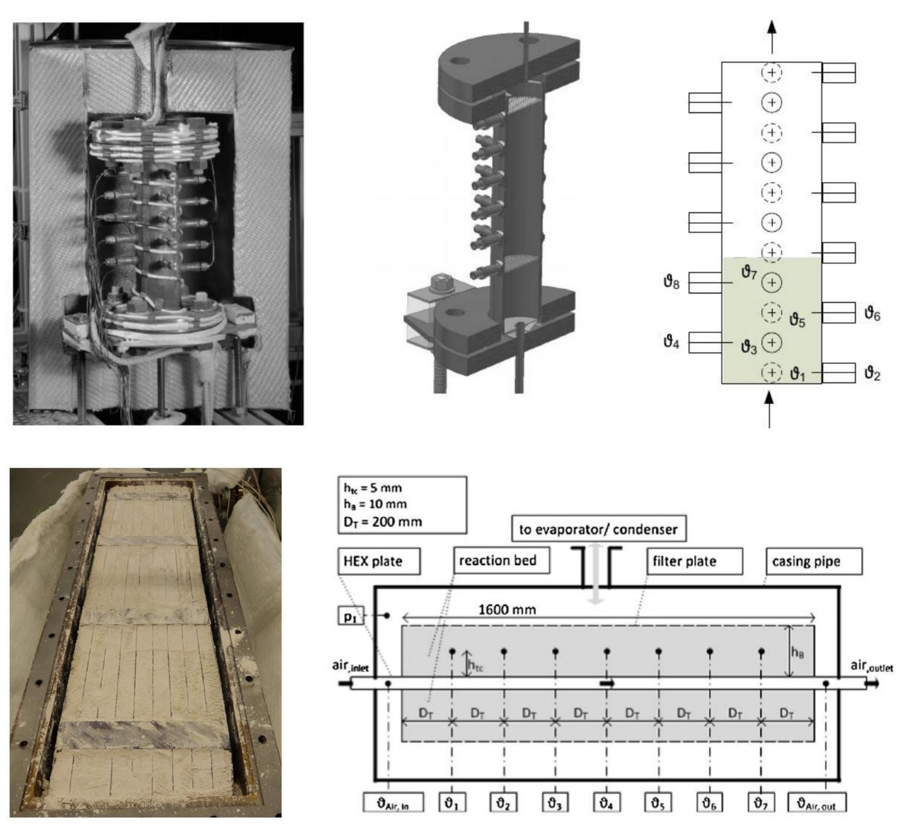


equilibrium temperature, see [4]

- Volume change of about 50% of the solid particles during the reaction [5]



Fixed-bed Reactor Concepts of DLR



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

Advantages

- $Ca(OH)_2$ / CaO has high storage densities : 430 kWh/m^3
- $Ca(OH)_2$ / CaO is a cheap, abundant and environmentally friendly material
- $Ca(OH)_2$ / CaO can be operated as chemical heat pump

Model concept

The numerical model is implemented in DuMu^x [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 permeability aterlation due to the porosity change [8].

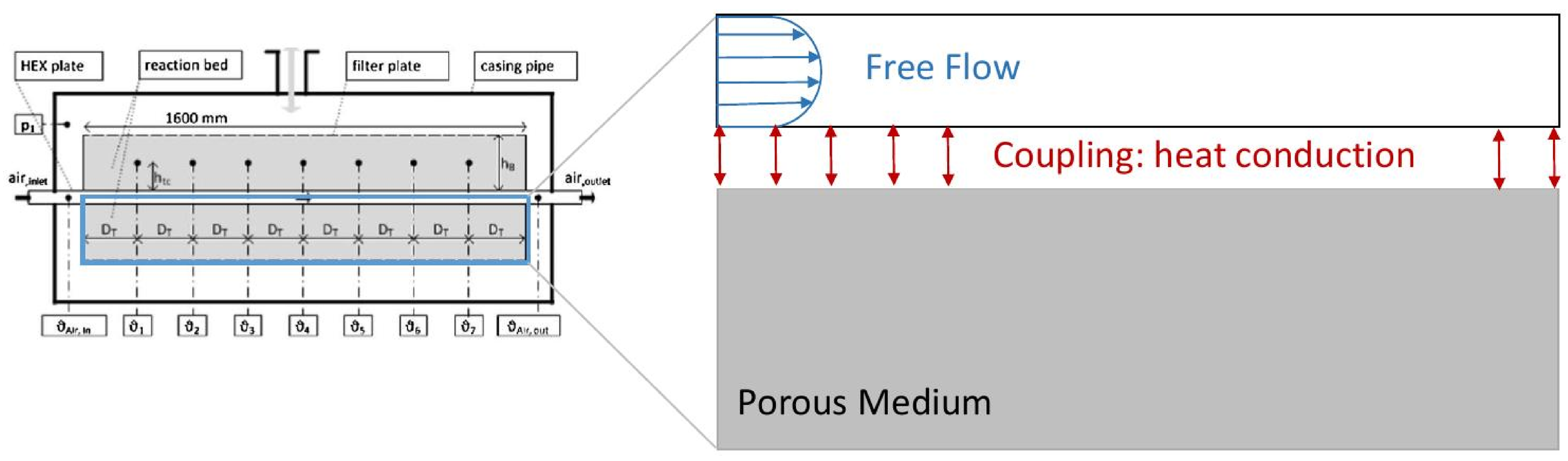
Channel flow model solves for the heat-exchanger gas-flux

- the Navier-Stokes equations
- an energy balance equation

Coupling accounts for

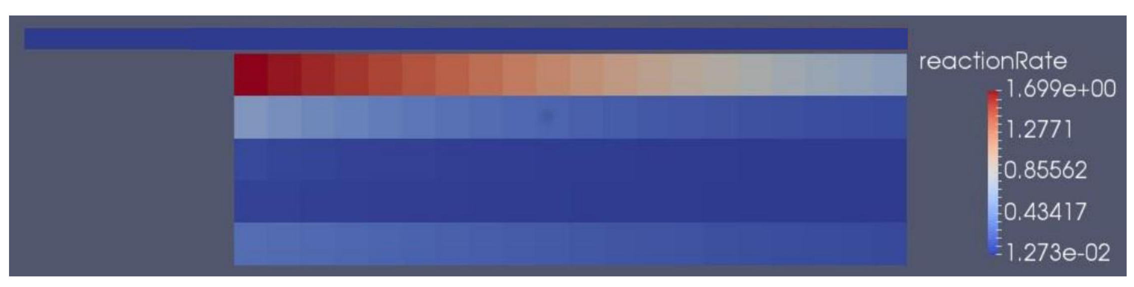
- heat conduction between the two domains assuming a continuous temperature distribution at the interface

Model Setup

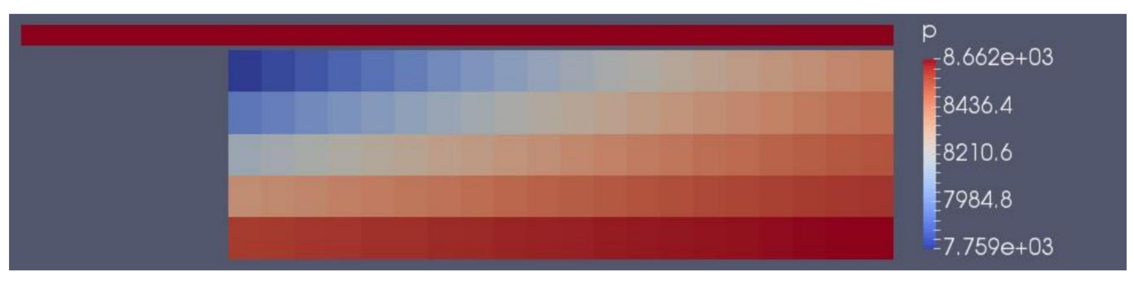


First Results

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 simplfying the channel flow model
- investigate the assumption of a continuous temperature distribution at the interface
- verify model results with experimental data

Literature

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