

Modelling of a Fluidized Bed Reactor for Thermochemical Energy Storage Applications

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Motivation

The rapid increase of the global energy demand along with the heightened awareness for climate change and the shift towards sustainable energy systems demand the development of novel thermal energy storage concepts. Due to the volatile nature of renewable energy resources, especially wind and solar sources, as well as the discontinuous waste heat flows from industrial processes, the interest in storage methods in order to match intermittent output with consumer demand has increased rapidly. Amongst the existing thermal energy storage mechanisms, thermochemical heat storage shows great promise compared to sensible or latent heat storage.

Thermochemical Energy Storage (TCES)

Thermochemical energy systems utilize reversible chemical reactions to store and release heat. During the charging process the heat is absorbed while decomposing the material A into the products B and C. Discharge occurs when the materials B and C are brought to contact again, releasing the stored heat.

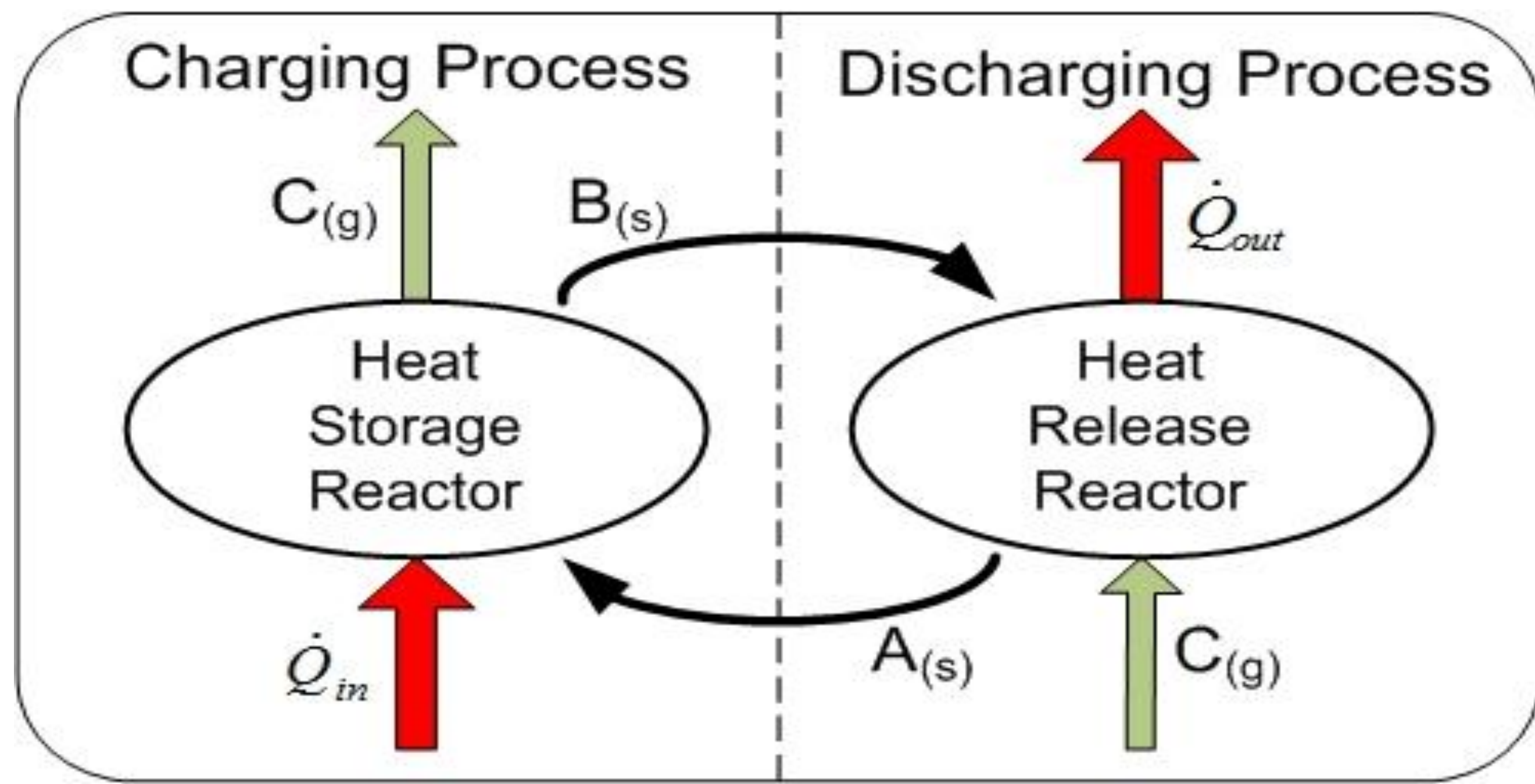
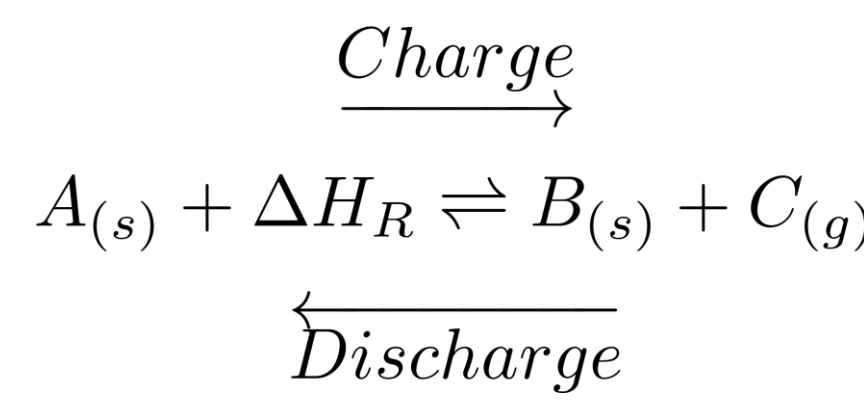


Figure 1: Schematic principle of thermochemical energy storage

Thermochemical energy storage has considerable advantages compared to sensible and latent heat storage:

- Loss-free storage at ambient temperature
- Theoretically unlimited storage time
- Transportability
- High gravimetric and volumetric energy density (see Fig. 2)

Potential applications of TCES:

- Household heating and cooling
- Waste heat recovery
- Concentrating solar power plants
- Chemical heat pumps

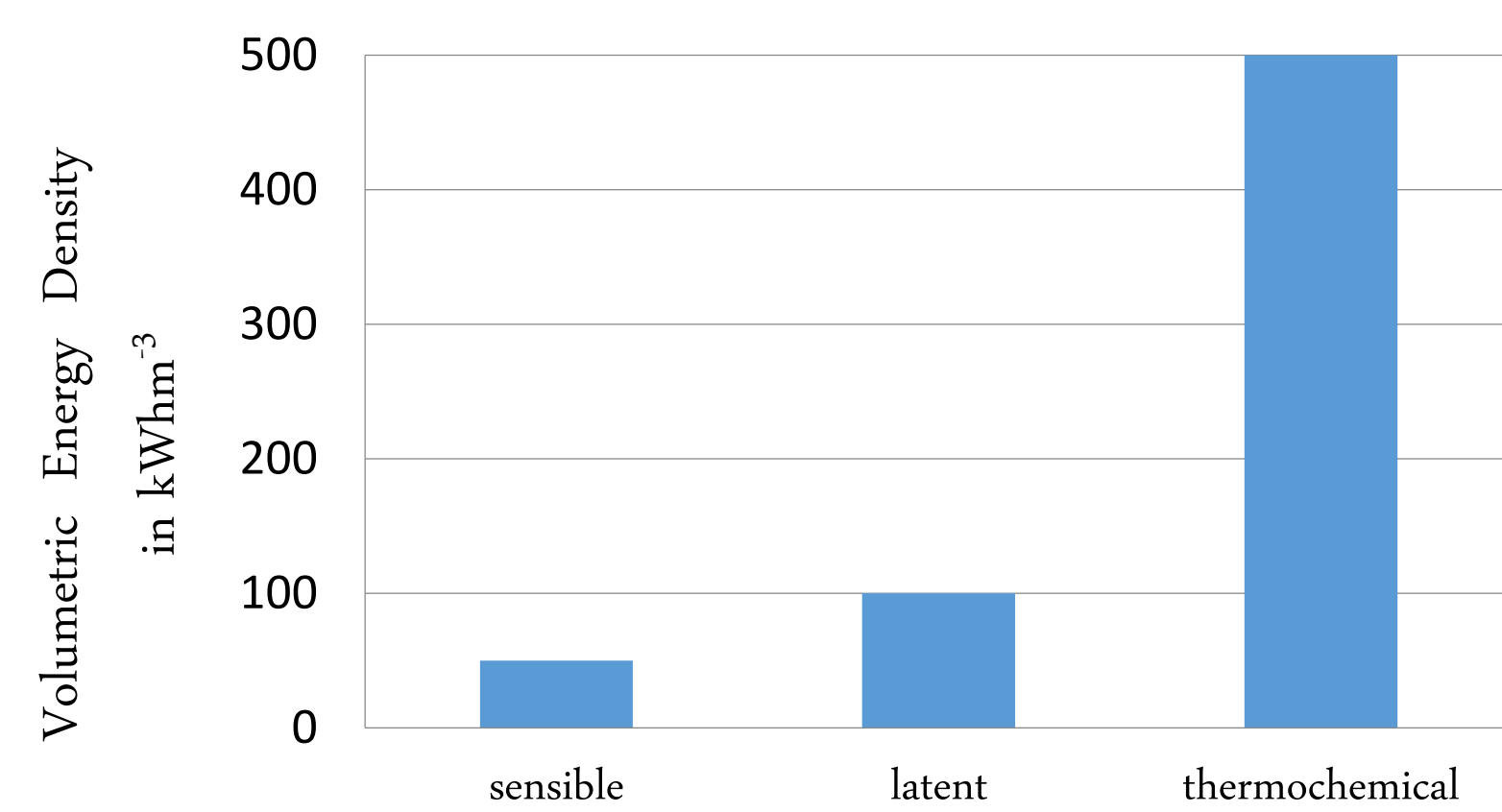


Figure 2: Theoretical volumetric energy density of sensible latent and thermochemical heat storage [1]

Kinetics of Solid-Gas Reactions

The conversion rate of solid-gas reactions is described on the basis of three major variables. The temperature at which the reaction occurs, the extent of conversion α , and the partial pressure of the gaseous reactant as follows:

$$\frac{d\alpha}{dt} = k(T)f(\alpha)h(p)$$

The temperature dependency is described by the Arrhenius equation and the pressure dependency is expressed in relation to the equilibrium pressure.

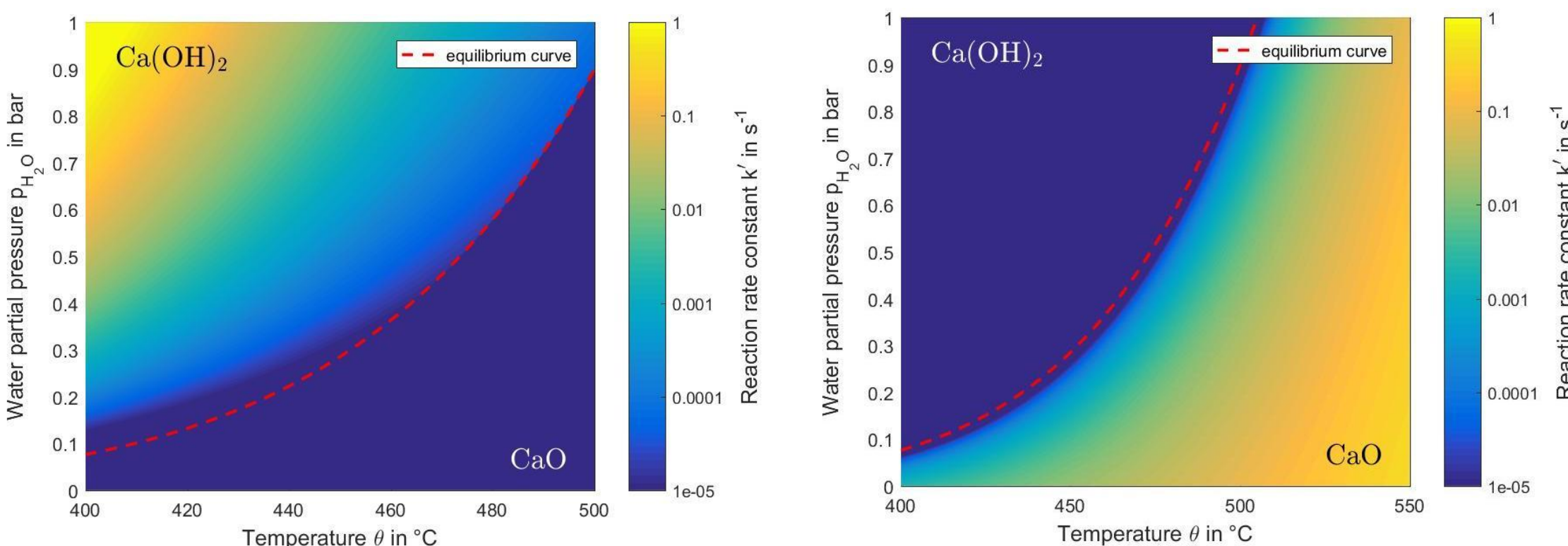
$$k(T) = A \exp\left(-\frac{E_a}{RT}\right)$$

$$h(p) = \left(\left|\frac{p}{p_{eq}} - 1\right|\right)^\nu$$

The conversion dependence $f(\alpha)$ of the process rate is described by reaction models that are based on rate control mechanism. Fig. 3 shows the rate constant and the equilibrium curve of the hydration (left) and dehydration (right) reaction of the CaO/Ca(OH)₂ system according to the kinetic expressions provided by Schaube et al. [2].

Figure 3: Rate constant

k' as the product of $k(T)$ and $h(p)$ along with the equilibrium curve of the hydration (left) and dehydration (right) reaction of the CaO/Ca(OH)₂ system



Modelling of the Fluidized Bed Reactor

The model combines solid-state reaction kinetics and fluidized bed reactor technology (Kunii Levenspiel [3] model). Integration of the conversion rate assuming isothermal conditions within the reactor as well as an initial conversion level yields:

$$\int_{\alpha_{in}}^{\alpha_{out}} \frac{d\alpha}{f(\alpha)} = A \int_0^\tau \exp\left(\frac{-E_a}{RT}\right) h(p) dt \Rightarrow g(\alpha_{out}) - g(\alpha_{in}) = A \exp\left(\frac{-E_a}{RT}\right) h(p) \tau$$

In an continuously operating fluidized bed reactor the individual particles do not have the same residence time hence the conversion level varies from particle to particle. Taking into account the residence time distribution $E(t)$ of the particles the final conversion of the solids is:

$$1 - \alpha_{FBR} = \int_0^\infty (1 - \alpha) E(t) dt$$

The heat flux released or stored by the reaction is given by:

$$\dot{Q}_R = \Delta H_R \alpha_{FBR} \dot{n}_{s,in}$$

Taking into account the stoichiometry of the reaction (coefficient b), the concentration of the gaseous reactant in the fluidization gas (C_g), the cross section of the reactor (A_{FBR}) and the fluidization velocity (u_o), the relation of the conversion of the gaseous reactant with that of the solid reactant is expressed as:

$$\frac{\dot{n}_{s,in}}{M_r} \alpha_{FBR} = b A_{FBR} u_o C_{g,in} \alpha_g$$

Also bubble growth and splitting at the internal heat exchanger tubes and the transfer of gas between the bubble and emulsion phase were investigated in order to optimize the parameters relevant for reaction.

Cascaded Process for Heat Recovery

Fluidized bed reactors in general operate isothermally. This property is desired for thermochemical energy storage applications in order for the reaction to occur at optimal conditions. On the other hand when utilizing a heat source for waste heat recovery the goal is to cool the source as much as possible to achieve high heat recovery effectiveness. This means that the utilization of only one reaction system, would either not allow the effective utilization of the heat source if the system reacts at high temperature values, or that the high temperature heat is downgraded if a system reacting at low temperature levels is used.

Three variants of a concept that utilizes three reaction systems in a cascaded arrangement in order to efficiently utilize the sources for thermochemical energy storage were investigated. The variants differ in terms of complexity and efficiency.

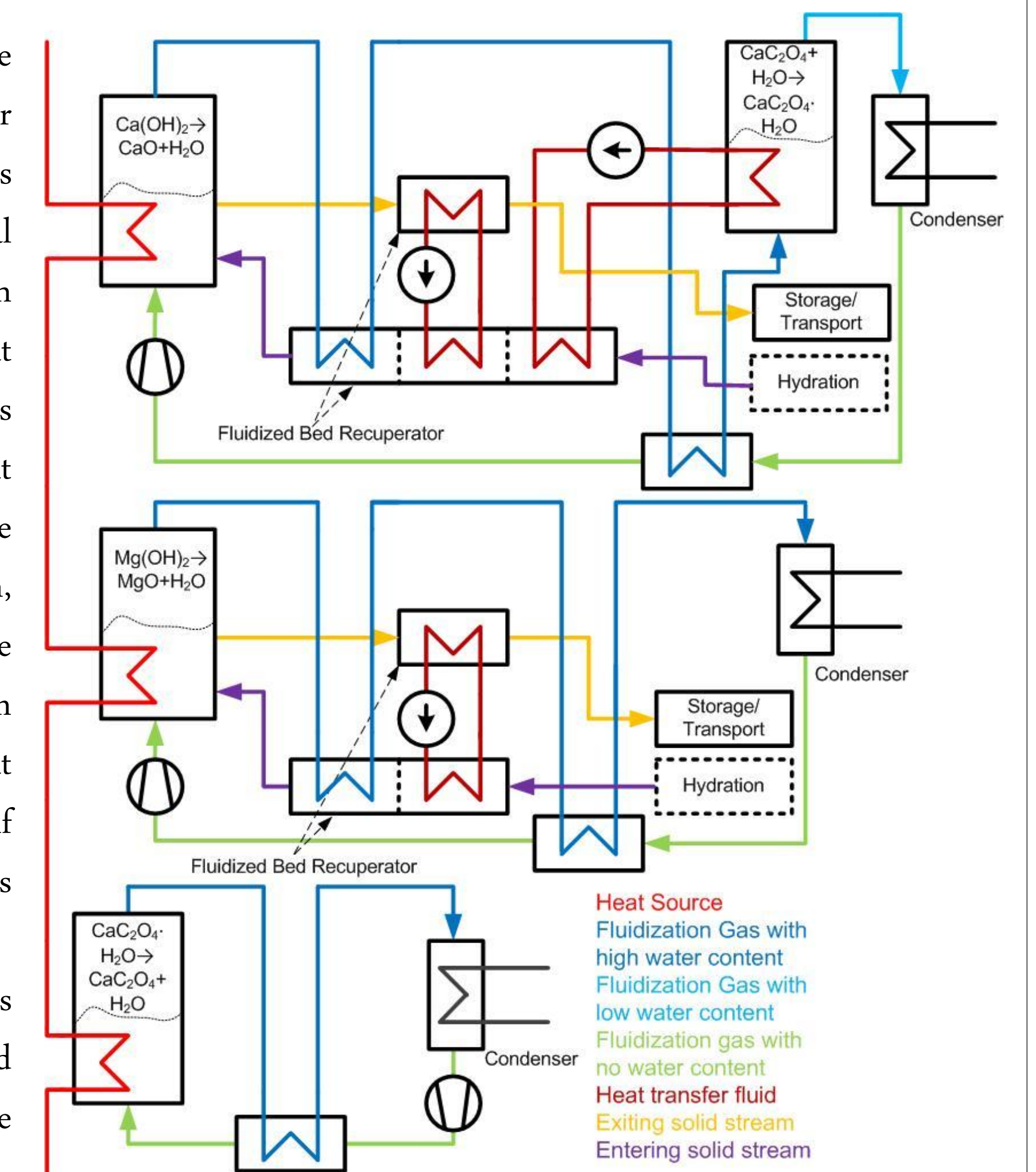
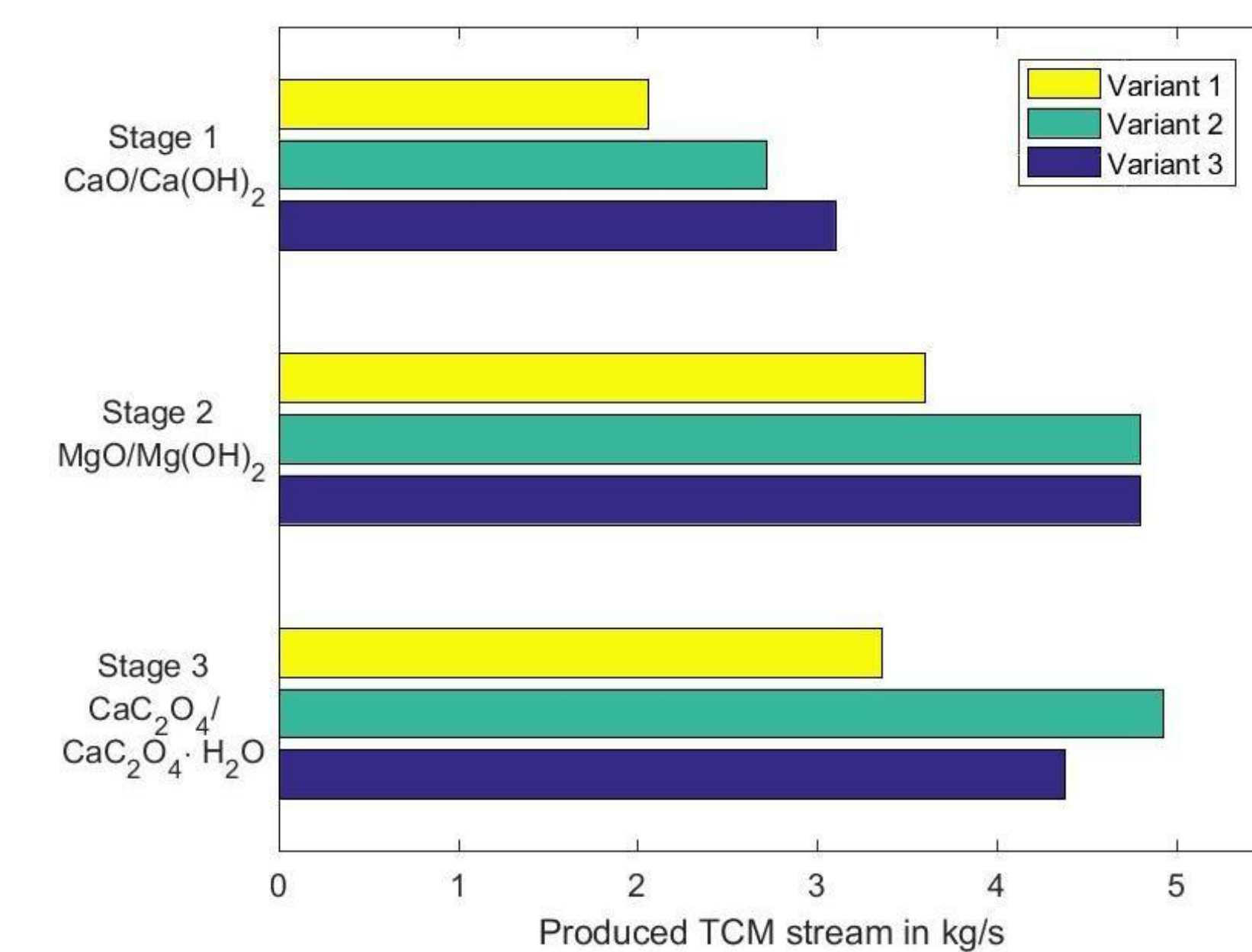


Figure 4: Illustration of a heat storage concept utilizing three fluidized bed reactors with different thermochemical materials

Each stage of the first configuration consists of the fluidized bed reactor, a gas recuperator and a condenser. Variant 2 also utilizes the sensible heat of the outgoing solid mass stream in a fluidized bed recuperator, to pre-heat the entering solid stream. The schematic of the third variant is shown in Fig. 4.



In order to reach higher pre-heating temperature levels, in the first reactor stage a portion of the produced material of the third stage is used to provide the necessary additional heat increasing the efficiency further. A comparison of the produced solid stream is provided in Fig. 5.

Figure 5: Comparison of the produced thermochemical material streams of the three different variants.

Outlook

- Further reaction-kinetic investigations necessary to obtain more precise results.
- Model validation planned by means of a fluidized bed test rig at the TU Vienna.

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[1] P. Pardo et al., "A review on high temperature thermochemical heat energy storage," *Renewable and Sustainable Energy Reviews*, vol. 32, pp. 591–610, 2014.

[2] F. Schaube et al., "A thermodynamic and kinetic study of de- and rehydration of Ca(OH)₂ at high H₂O partial pressures for thermo-chemical heat storage," *Thermochimica Acta*, vol. 538, pp. 9–20, 2012.

[3] Kunii D. and Levenspiel O., "Fluidization Engineering," Butterworth-Heinemann, Boston, Massachusetts, USA, 1991.