# HIGH-PERFORMANCE COMPUTING TECHNIQUES APPLIED TO THE CHARACTERIZATION AND OPTIMIZATION OF A THERMOCHEMICAL HEAT STORAGE SYSTEM FOR CONCENTRATED THERMAL SOLAR POWER

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As a carbon-free energy supply technology, the operation time and final energy output of thermal solar power plants can be greatly extended if efficient thermal storage systems are applied. One of the proposed design of such system is to utilize reversible thermochemical reactions and its embedded reaction enthalpy, e.g. the Ca(OH)2/CaO hydration circle, in a fixed-bed gas-solid reactor (Schaube et al. 2011)

The modeling of such a storage system involves multiple strongly-coupled physical and chemical processes. Seepage velocity is calculated by the nonlinear Forchheimer law. Gas phase density and viscosity are temperature, pressure and composition dependent. Also, heat transfer between gas and solid phases is largely influenced by the exothermal heat produced by the hydration of calcium oxide. Numerical solution of four governing PDEs include the mass balance, reactive transport, heat balance equations for gas and solid phases, which are implemented into the open source scientific software OpenGeoSys in a monolithic way. Based on it, a 2D numerical model, considering the boundary heat loss of the system, was set up to simulate the energy-storage and release circle.

The high performance computing techniques were employed in two stages. First, the dynamic behavior of the heat storage system is simulated on a parallel platform. Second, a large number of processors are employed to perform Mont-Carlo simulations, whereas the reaction rates and efficiency factor of heat transfer are parameterized so that the measured and simulated temperature profile fit with each other. The model showed that heat loss on the device surface, grain size of the material and the geometry of the system will influence the final performance. By varying these factors, the calibrated model will be further applied to optimize the design of such energy storage system.