ID: 12.1c

Title: Modelling of solar energy storage using chemical heat pumps

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A growing interest has recently developed on the possibility to exploit reversible exothermic chemisorption to efficiently store solar thermal energy for long, inter-seasonal periods of time. In particular, the chemisorption of water on inorganic salts proved to be especially suited to such applications. In the framework of a collaborative project involving several universities, research centers and industries, we built a model for this kind of systems by using the Maxwell-Stefan relations applied to the Dusty Gas Model for mass transport, and different kinetic models for chemisorption. The numerical simulations show that the coupling between mass transport and reaction can occur in a very similar fashion for both advective (1-component system) and diffusive (2-component system) motion. This coupling generates a propagating wave-like front of adsorbed product. This occurrence has important consequences on the kinetics of the global process, whose timescale can strongly depend on quantities like the total amount of reactive solid and on the geometrical properties of the reactor. Those are key features in the design of any engineering applications, and they should therefore be carefully tuned after the physico-chemical dynamics of the system. We used these results to explain and rationalize some intriguing effects observed during adsorption experiments, performed by our collaborators within the framework of the project. The reaction/transport coupling seems to be the dominant process, and the surprising experimental results can be explained without the need to invoke spatial heterogeneities or more exotic phenomena. Our analysis however proves that special attention must be paid to the microscopic details of the adsorption process in the grains. I will also discuss how we plan to integrate such a microscopic description inside the macroscopic one, while keeping the possibility to perform upper-level tasks, such as a stability analysis of the wave.