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Sorption enhanced catalytic Steam Methane Reforming: Experimental data and simulations describing the behaviour of bi-functional particles

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ABSTRACT:

Steam Methane Reforming (SMR) combined with simultaneous CO2 sorption is a convenient reaction path to enhance H2 yield, leading to more favourable thermodynamic conditions and reducing environmental footprint. In order to obtain an efficient integration of exothermic and endothermic reactions and minimize physical resistances, bi-functional catalyst-sorbent materials are under development, containing both CaO sorbent grains and nickel catalytic sites. Solo-sorbent, solo-catalyst and bi-functional materials were synthetized at laboratory scale. In this work, they are studied by means of thermo-gravimetric and packed bed micro-reactor tests, to highlight both catalytic and sorption functions, and their mutual interactions. Experimental results are simulated by a Particle Grain Model (PGM), conceived by Stendardo and Foscolo (2009) for solo-sorbent particles, and more recently extended to Sorption Enhanced SMR (SESMR) processes by Aloisi et al. (2016). For micro-reactor simulations, PGM is supplemented

by molar balances of gaseous components surrounding the granular bed, assuming an Axial Dispersion Plug Flow Reactor approach. The sorption and catalytic behaviour of synthesized materials is successfully described by this model, for the first time. Initial decline and subsequent stabilization of CO2 sorption capacity as a function of repeated carbonation cycles, as well as the whole dynamic sorption behaviour in each cycle, is simulated by varying just one model parameter, the sorbent grain size. SMR Numaguchi and Kikuchi (1988) kinetics, plugged in PGM, predicts accurately H2 yield, CH4 conversion, and weight hourly space velocities allowing thermodynamic equilibrium or kinetic regime at the micro-reactor exit. In SE-SMR tests, the breakthrough characterizing outlet gas concentrations as functions of time, exhibited by fresh samples of bifunctional materials, is well described by model calculations, spanning the whole range between SESMR and SMR equilibria.