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Hydrogen by sorption enhanced methane reforming: A grain model to study the behavior of bi-functional sorbent-catalyst particles

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ABSTRACT:

This work utilizes a previously developed particle grain model (PGM) for carbon dioxide CaO-based sorbents, properly integrated to describe numerically the behavior of a single particle where some catalytic activity is combined to the sorption function. In this way, the model capability is extended to the investigation of a bi-functional sorbent-catalyst particle for sorption enhanced steam methane reforming (SE-SMR) processes to produce hydrogen. The kinetic description of carbon dioxide capture by calcium oxide is assumed to be that successfully validated in a previous work bymeans of dynamic carbonation data obtained with calcined dolomite particles ofdifferentsize fluidized by a N2/CO2 gas mixture. Further simulations presented here show the ability of the sorption model to describe faithfully the additional influence of temperature, carbon dioxide concentration in the gas phase and number of solid carbonation cycles. A state of the art methane and water gas shift kinetic model is utilized to predict the particle catalytic activity in the sorption enhanced reaction process. A numerical

procedure is developed in MATLAB to integrate over time and particle radius the model equations, assuming that small particles, of the order of those of interest for fluidized bed reactors (dp ¼500 μm), are in contact with different gas phases of constant composition. The results show that conversion of the sorbent grain sand the increasing thickness of the calcium carbonate layer around them make carbon dioxide sorption and methane reforming rate strong functions of residence time of particle in the reacting atmosphere, with different scenarios for the interaction between catalytic steam reforming and CO2 sorption. The model predicts that, with sufficient amount of calcium oxide inside the particle, conditions exist where the time averaged rates of carbon dioxide sorption, methane reforming and water gas shift, respectively, are such that a perfect balance exists between carbon dioxide captured by the solid phase and CO + CO2 produced by the reforming reactions.