SORPTION ENHANCED-CHEMICAL LOOPING REFORMING FOR HIGH-PURITY H₂ PRODUCTION WITH LOW ENERGY DEMANDS: DYNAMIC MODELING OF REGENERATION STAGE IN A PACKED BED REACTOR

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ABSTRACT

Hydrogen is recognized as a primary industrial gas and a promising energy carrier for the transition to a cleaner and sustainable future. Nowadays however, hydrogen is produced on industrial scale mainly via Steam Methane Reforming (SMR), an energy-intensive process with high carbon footprint. High-purity H_2 can be produced in a single step with in-situ capture of the generated CO_2 via the intensified, low-energy Sorption Enhanced Chemical Looping Steam Methane Reforming process. This novel process consists of two stages. In the first stage, steam reforming of methane is carried out in the presence of a CaO-based CO_2 capture material and a Ni-based oxygen carrier/reforming catalyst. During reforming, NiO is reduced to metallic Ni by the CH_4 feedstock, serving as the reforming catalyst, while the produced CO_2 is captured in-situ via the strongly exothermic carbonation reaction of CaO, which covers also the energy demands of this stage. Since CaO is gradually consumed, the operation is inherently dynamic, requiring a second step for periodic regeneration of the CO_2 capture material. Calcination of the formed $CaCO_3$ however is strongly endothermic, with the required energy being supplied in-situ by the reoxidation of the NiO-based oxygen carrier [1]. The type of oxidant used and the residence time of the feed in the reactor can generate conditions in favor of the calcination reaction and lead to an efficient coupling of the two reactions. This work focuses on the dynamic modeling of the regeneration reactor to predict the degree of autothermicity that can be achieved. In a packed bed reactor experiment over an OTM/sorbent mechanical mixture with NiO/CaO ratio of 0.5, it was shown that 47% of the calcination thermal requirements can be provided from nickel oxidation using pure oxygen as oxidant [2], which corresponds to 82% of the maximum theoretical degree under those conditions. The reactor was simulated by a heterogeneous, non-isothermal, one-dimensional model with the reaction front moving in the axial direction of the reactor. The model, accounting for intraparticle diffusion and reaction by employing the Shrinking Core Model (SCM), is solved using Runge-Kutta methods implemented in MATLAB and validated with experimental results.

KEYWORDS: Sorption Enhanced-Chemical Looping Steam Methane Reforming, Ca – Ni looping, Autothermal sorbent regeneration, Heat coupling, Computational modeling

REFERENCES

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