MODELLING OF CO_2 METHANATION IN PACKED BED REACTOR USING DUAL FUNCTION MATERIALS

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ABSTRACT

Greenhouse gas emissions are massive concern for scientists to minimize the effect of global warming. The development of carbon capture and utilisation (CCU) technologies attempts to reduce the release of CO_2 emissions in the atmosphere [1]. CO_2 conversion to an energy carrier, CH_4, is creating a power-to-gas platform and a circular economy [2]. Dual function materials (DFMs) can couple the processes of the capture and conversion of CO_2 into a two-step process [3]. In this work, we aimed to develop a model to validate experimental results according to the hydrogenation phase where CO_2 is already adsorbed on the surface of the catalyst and H_2 is injected. 1D model was designed to determine the transport phenomena of heterogeneous flows within the reactor, coupling all the boundary conditions, mass balances and conservation equations.

A packed bed reactor with length of 30 cm was used for the modelling with a total flow rate of 50 mL/min (10% H_2). A monometallic and a bimetallic DFMs were used where a good validation between the experimental and simulated results was obtained, and the kinetic model can be used for further studies to optimize the performance of the reaction. Optimisation studies investigating the effect of H_2 content in the flow showed that the CH_4 conversion is increased with the H_2 % in the inlet flow. Additional studies were occurred to assess the effect of the inlet flow rate revealing that a reduction of the flow rate leads to higher concentrations of CH_4 due to larger fluid residence time inside the reactor. The reactor's inertial diameter on the CH_4 generation was another parameter that was investigated showing an enhancement on the production of CH_4 by increasing the inertial diameter of the reactor as velocity field inside the reactor is influenced at constant flow rates whereas this affects the residence time.

KEYWORDS: Modelling, CO_2 methanation, DFM, Packed Bed Reactor.

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