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Entitled

MODELLING AND SIMULATION OF HYDROGEN PRODUCTION VIA MEMBRANE REACTOR

by

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Abstract

A membrane reactor is a promising device to produce pure hydrogen and enrich CO2 from syngas. A simulation study of a double tubular catalytic membrane reactor for the water–gas shift reaction (WGS) under steady-state operation is presented in this work. The membrane consists of a dense Pd layer (selective to H2) deposited on a porous glass cylinder support. The reaction side was filled with a commercial iron-chromium oxide catalyst, designed as Girdler G-3. The mass of the catalyst was 12.1 g and the height of the catalyst bed was 8 cm. The WGS model was carried out with and without the membrane at a temperature of 673 K, pressure of 2 atm, argon flow rate of 400 cm3 (STP) min−1, and steam-to-carbon (S/C) ratio of 1. The membrane reactor could achieve a CO conversion efficiency of up to 93.7%, whereas a maximum value of only 77.5% was attained without using a membrane under the same operating conditions. The WGS membrane model was tested under different operating conditions. In order to find the optimum operating conditions, the response surface method was used at a temperature of 673 K and sweep gas (argon) flow rate of 3200 cm3/min in the Minitab software package. It was found that a nearly complete CO conversion could be achieved under the following conditions: S/C ratio = 4, total retentate pressure = 12 atm, and membrane thickness = 5 µm. Under these conditions, the S/C ratio obtained is satisfactory and a nearly complete conversion of CO was achieved. The developed model results were verified with available experimental results in the literature. It was found that the model results are in complete agreement with the experimental results.

Keywords: Membrane reactor, palladium (Pd) composite membrane, water–gas shift reaction (WGSR), H_2 production, carbon monoxide (CO) conversion, mathematical model, simulation, response surface method (RSM).