Effects of Geometry and Operating Conditions on Membrane Reactor for Water Gas Shift Reaction

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Abstract

Recently, hydrogen is widely used as environmental energy and high energy content. The hydrogen is mainly produced by water gas shift reaction(WGSR) from coal to hydrogen process in Integrated Gasification Combined Cycle(IGCC) plant. WGSR, well known for hydrogen production, is a considerable exothermic reaction with equilibrium as temperature. The traditional WGSR process are composed of high temperature(300℃-500℃) reactor and low temperature(200℃-250℃) reactor. The high temperature reactor is used to operate for high reaction rate, and the low temperature reactor is used to operate for high conversion for carbon monoxide. However, to enhance the overall coal to hydrogen thermal efficiency and cost effective design, the water gas shift reaction in membrane reactor(WGSR-MR) has been developed. This reactor can get high purity hydrogen to remove hydrogen using a Pd-based membrane that is selectively permeable to hydrogen, and the WGSR is further reacted and the sweep gas removes the heat due to the reaction, so that the process can be operated very efficiently.

In this study, to simulate water gas shift reaction in membrane reactor, COMSOL Multiphysics® software is used to analysis internal physical phenomenon and evaluate the reactor performance as various operating conditions and geometry. In the Chemical Reaction Engineering Module of COMSOL Multiphysics® software, the Transport of Concentrated Species interface is used to study mass balance for mixture of gas, the Free and Porous Media Flow interface is used to study momentum balance in free flow and porous media flow, and the Heat Transfer in Fluid interface is used to study heat balance in overall system. The used physics interfaces are coupled with each other, so that physical phenomena are simulated in WGSR-MR. In this study, the model is referred from Chein[1]. This model is validated from reference paper, and extended to calculate as various conditions. The performance of WGSR-MR is evaluated from CO conversion and hydrogen fraction at outlet of sweep gas.

Reference

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Figures used in the abstract

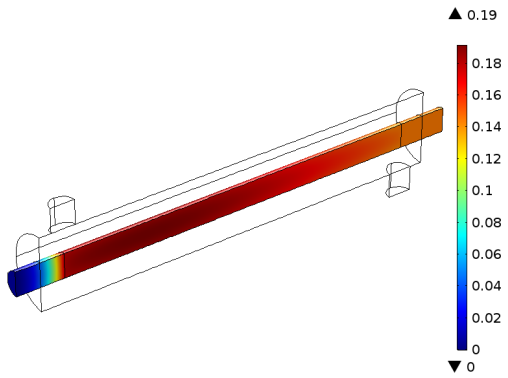

Figure 1: Hydrogen molar fraction in WGSR-MR.