CFD Investigation of an Air Cooled Microstructured Water Gas Shift Reactor

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Highlights

- Water-gas shift reaction is modeled in wash-coated microchannel reactor.
- Single channel model predicts experimental data with 4% error.
- Enabling cooling function increases CO conversion by ~10%.

1. Introduction

Hydrogen is considered as a clean energy carrier for fuel cells, however, is not readily available, and should be produced from either fossil or renewable hydrocarbons via fuel processing. This process involves H_2 production and purification sections. Purification is crucial since CO is poisonous to fuel cell catalysts and water-gas shift reaction (WGS) plays a critical role in reducing CO concentrations down to ~1-2%. Considering that WGS converter is the bulkiest unit in fuel processors, its size should be reduced without compromising from performance. Running WGS in microchannel reactors is promising as these units are capable of delivering high conversions in small volumes. Although there are studies investigating WGS in microchannel reactors, the literature lacks a comprehensive study of a microchannel WGS converter which also functions as a heat exchanger (HEX). In this respect, the aims of this study are to carry out parametric investigation of heat exchange function integrated microchannel WGS reactor by using computational fluid dynamics (CFD) based techniques and to understand the effect of structural and operating parameters of the intensified reactor on regulation of WGS temperature and CO conversion.

2. Methods

Two different geometries, namely single and heat exchange integrated microchannels, are constructed in GAMBIT platform. Dimensions for the single microchannel are selected according to the study of Germani and Schuurman [1] as 4×10^{-4} m for height, 6×10^{-4} m for width, and 5×10^{-2} m for length. The single channel is operated adiabatically with a volumetric flow rate 5.67×10^{-9} $Nm^3\ s^{-1}$ composed of H_2 (30%), CO (10%), CO_2 (10%), H_2O (20%) and balancing gas Ar (30%) in accordance with the reported experimental conditions [1]. Heat exchange integrated microchannel reactor is composed of parallel cooling and reaction channels in which coolant (air) and reactive mixture flow counter-currently. Dimensions for the cooling and reaction channels are the same, both being equal to those of the single microchannel. The channels are separated by a solid wall with a default thickness value of 6×10^{-4} m. In both geometries, WGS is catalyzed by Pt-CeO_2/Al_2O_3 that is waschoated as a 5×10^{-5} m thick layer to the inner walls of the reaction channels [1]. Operation of the single microchannel is modeled in two-dimensions by means of finite volume method via ANSYS 16.0 platform in which simultaneous solution of steady-state transport of momentum, heat and mass in gas and porous catalyst phases are obtained via a HP Z620 series workstation equipped with 12×2 GHz Intel Xeon™ processors and 32 GB of memory. Reaction is assumed to take place only within the catalyst layer, and gas phase reactions are neglected. Upon comparison and validation of its outcomes with the experimental data provided in the literature [1], the reactor model is adapted to simulate the heat exchange integrated microchannel reactor. In this context, parametric study is made on reactant and coolant inlet temperatures, and wall thickness which are selected in the range 290-340 °C, 215-325 °C and 4×10^{-4}-8×10^{-4} m, respectively. Wall materials are selected as aluminum, cordierite and stainless steel.

3. Results and discussion

Solution of the single adiabatic microchannel model show that WGS is kinetically controlled until ~315 °C, above which thermodynamics starts to suppress CO conversions. This peculiar feature of WGS calls for the

need of cooling to relax the opposing impact of thermodynamics over the reaction. The model is found to be capable of predicting experimental data [1] in the range of 200-320 °C with maximum error below 4% (Figure 1). This validation allows the single channel model to be used in exploring the operating and design characteristics of an intensified, air-cooled microchannel WGS unit. In this context, presence of neighboring air-cooled channels is simulated to provide almost isothermal conditions in the reaction channel (Figure 2) and improved CO conversions from 67.4% to 77.6% and the effluent H_2/CO ratio from 11.2 to 16.8.

Reactant inlet temperature has a notable impact on CO conversion whereas the effect of coolant inlet temperature is found to be negligible. The highest CO conversion of ~78% is achieved at reactant and coolant feed temperatures of 320 °C and 275 °C, respectively. The equilibrium conversion at the same operation conditions is 80%. Effect of cooling is investigated by selecting the inlet temperature of the coolant either 10, 15, or 20 °C lower than reactant inlet temperature. Higher CO conversions are obtained with a temperature difference of 10 °C. This trend is valid in cases where the reactant inlet temperature is below 300 °C, and indicates the domination of kinetics over thermodynamic effects. On the other hand, above 300 °C, higher CO conversions are achieved when the gap between reaction and coolant inlet temperatures increase. In other words, role of cooling becomes critical when the thermodynamic effects become notable.

Cooling function of the HEX integrated microchannel is dictated by the properties of the wall between the coolant and reactant channels. Heat transfer rate within the wall of the microreactor is affected by its thickness and material of construction. Although its effects on CO conversion are negligible when compared with the reactant temperature effect, thermal conductivity of the wall material is positively correlated with the rate of heat removal from the reaction channel and favors isothermal conditions. A similar effect is observed in cases involving thicker walls, which favors heat conduction in the axial coordinate of the reactor and, in turn, allows faster heat removal rates.

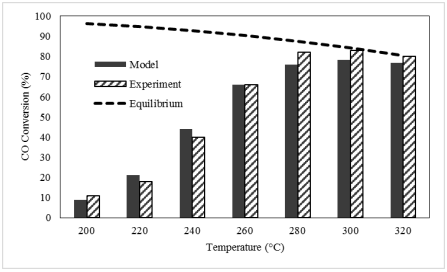

Figure 1. Comparison of CO conversions obtained from experiments [1] and mathematical model.

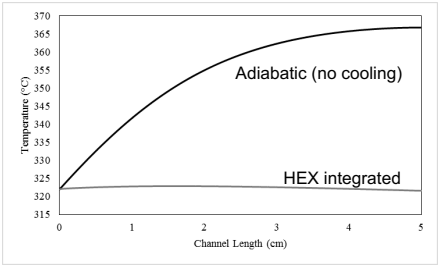

Figure 2. Temperature distribution along the centerline of the reaction channel in case of absence and presence of cooling.

4. Conclusions

Experimental data is validated with the single channel model and extensive parameter investigation is made on heat exchange function integrated microchannel reactor model. Introduction of cooling function increased CO conversion by 10.2% and uniform temperature distribution due to this function allowed efficient utilization of the catalyst. Through an extensive parameter investigation, microchannel reactor is found to be most sensitive to reactant inlet temperature and effects of wall material type and its thickness together with coolant feed temperature are found negligible.

References

[1] Germani G, Schuurman Y. Water-gas shift reaction kinetics over m-structured Pt/CeO_2/Al_2O_3 catalysts. AlChE J 2006;52:1806-13.

Keywords
Hydrogen, water-gas shift, microchannel reactor, process intensification