Numerical analysis of glycerol-to-H_2 conversion in a microstructured reformer with integrated heating

Numerical Analysis of Glycerol-to-H_2 conversion in a Microstructured Reformer with Integrated Heating

Amin Delparish, Ahmet K. Avci*

Department of Chemical Engineering, Bogazici University, Bebek 34342, Istanbul, Turkey

**Corresponding author: avciahme@boun.edu.tr*

Highlights

- Glycerol conversion is modeled in a microstructured reformer with integrated heating.
- Reactor model is successfully validated by the experimental data.
- Presence of heating function improves glycerol conversion by 9%.

1. Introduction

Production of biodiesel, a renewable fuel, is carried out by transesterification of animal-based or vegetable oils with methanol (or ethanol). In this process, one mole of glycerol is produced for every three moles of biodiesel. This stoichiometry, however, causes undesirably high supply of glycerol. Solution of this problem is possible by efficient conversion of glycerol into value-added products such as H_2 [1]. Glycerol-to-H_2 conversion requires high temperatures and external energy demand, both of which depend strongly on the catalyst type and reactor geometry. Microchannel reactors are known to enable high heat transfer rates, and fast and homogeneous distribution of external heat to the catalyst bed, favoring its efficient utilization. These reactors can also be configured to exchange heat between two separate streams in the same volume. Previous studies showed that temperature distribution in the reaction channels can be improved by fast heat exchange between the adjacent channels [2,3]. The aim of this study is to investigate glycerol steam reforming in a heat exchange integrated microchannel reactor by means of detailed mathematical modeling techniques.

2. Methods

Microstructured reformer is presented in Figure 1. Inner walls of the reaction channels, each of which having dimensions of 6.5×10^{-4} m height, 1×10^{-2} m width and 2×10^{-1} m length, are coated with 5×10^{-5} m thick layers of porous Co-Ni/Al_2O_3 catalyst. The heating channels, having the same dimensions with the reaction channels, carry the hot fluid (steam) flowing in the opposite direction of the reactive stream. Simultaneous reaction and heat exchange within the unit cell (Figure 1), the representative and repeating unit of the multichannel reactor, are modeled by 2D Navier-Stokes equations describing the steady-state conservation of mass, momentum and energy. Kinetic model used to describe glycerol steam reforming over Co-Ni/Al_2O_3 catalyst is adapted from the literature [4]. The resulting model, solved by finite volume method on ANSYS 16.0 platform, is used to study the effects of operational parameters (inlet flow rate, inlet temperature and flow direction of the hot fluid) and structural parameters (reactor wall material, thickness of the wall between the reaction and heating channels) on temperature distribution and glycerol conversion. In all simulations, temperature of the reactive mixture involving 1.25×10^{-5} mol/s of glycerol vapor, 1.5×10^{-4} mol/s of steam and 7.75×10^{-5} mol/s of nitrogen flow is taken as 450 °C. Temperature and linear flow rate of steam is varied in the ranges of 390-510 °C and 2-8 m/s, respectively. Thickness of the separating wall is taken in the 4-12$\times 10^{-4}$ m range, while its material is simulated as cordierite, AISI steel and silicon carbide (SiC). The base case simulations involved 450 °C and 5 m/s as the inlet temperature and flow rate of steam, respectively, wall thickness of 6×10^{-4} m, AISI steel as the wall material and counter-current flow of the reactive and hot fluids.

3. Results and discussion

Prior to the parametric investigation of the intensified reformer unit (Figure 1), outcomes of the reactor model are compared with the experimental counterparts reported in the literature. Comparison is carried out on the basis of per cent mole fraction defined as the ratio of the molar flow rate of the particular product to the to the sum of molar flow rates of H_2, CO, CO_2 and CH_4. Comparisons given in the form of a parity plot in

Figure 2 reveal good agreement between the model outcomes and experimental results [4]. The reactor model is then used in the simulation of the microstructured reformer with integrated heating.

The results show that temperature control in the reforming channel can be improved by fast heat transfer rates offered by the microchannel architecture. Heating by steam has an obvious contribution to glycerol conversion, which is found to be 73% and 64% in the presence and absence of steam heating, respectively. Increasing the steam inlet temperature from 390 to 510 °C is found to have a significant impact on glycerol conversion, which increased by 10%. Similarly, changing feed temperature of the reactive mixture from 400 to 500 °C improved conversion by ~12%. Steam inlet velocity, however, did not cause a notable effect on temperature distribution and conversion within the reaction channel, since higher sensible heat flow of steam at increased velocities, which offers the potential of efficient heating of the reaction channel, is counterbalanced by its shortened residence within the reactor. In addition to these outcomes, almost the same reactor response is obtained at counter- and co-current flow of reactive mixture and steam.

The results also reveal that reactor configuration can slightly affect heat flow between the channels. Glycerol conversion is observed to improve when thicker separating walls made of thermally conductive materials are used. It is reported that axial component of the heat flux along the separating wall increases with wall thickness [5]. This effect is also observed in the present study and allowed ~1.5 % increase in glycerol conversion upon changing the wall thickness from $4x10^{-4}$ to $1.2x10^{-3}$ m. A similar response, ~2.5% increase in conversion, is obtained upon using SiC instead of AISI steel. This trend is associated with the difference in thermal conductivity of the materials and can be explained by the reduced conductive resistance to heat flow between channels. Degree of uniformity of reaction channel temperature, that can be adjusted by the extent of integrated heating, favors H_2 production and dampens formation of undesired CH_4.

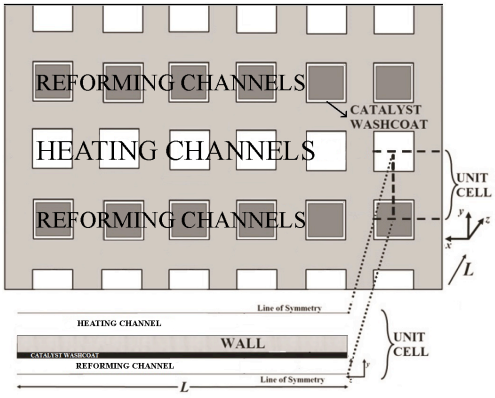

Figure 1. Microstructured reformer with integrated heating

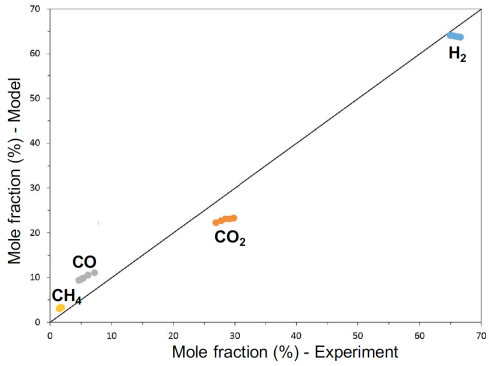

Figure 2. Comparison of molar compositions of products obtained from experiments [4] and mathematical model

4. Conclusions

Catalytic steam reforming of glycerol is simulated in a microstructured reformer in which reaction and heating functions are integrated. The mathematical model used to simulate the intensified reformer is successfully verified with the experimental data. Simultaneous heating by steam improved glycerol conversion by 9%. Inlet temperatures of steam and reactive stream lead to the most significant changes in reactor response, which, however, remains limited upon changing structural parameters.

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Keywords
Glycerol; Hydrogen; Microchannel; Modeling; Simulation