



Modeling a channel-type reactor with a plate heat exchanger for cobalt-based Fischer–Tropsch synthesis



Min-Sol Shin^{a,b}, Nonam Park^{a,b}, Myung-June Park^{a,b,*}, Joo-Young Cheon^c, Jin Kyu Kang^a,
Ki-Won Jun^c, Kyoung-Su Ha^{c,*}

^a Department of Chemical Engineering, Ajou University, Suwon 443-749, Republic of Korea

^b Department of Energy Systems Research, Ajou University, Suwon 443-749, Republic of Korea

^c Research Center for Green Catalysis, Korea Research Institute of Chemical Technology (KRICT), Daejeon 305-600, Republic of Korea

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ABSTRACT

A channel-type reactor for the cobalt-based Fischer–Tropsch synthesis reaction was considered and a commercial software package (COMSOL Multiphysics) was used to simulate the profiles of conversion and temperature in the reactor under a variety of conditions. The CO consumption rate was calculated using a lumped kinetic model, and kinetic parameters and the heat transfer coefficient between the reaction module and the atmosphere were estimated to reduce deviations from the experimental measurements. Comparison between simulation results and experimental data corroborated the validity of the developed model with errors lower than 7.00% and 0.15% for CO conversion and temperature in the catalytic bed, respectively. Further examination showed that the increased heat transfer rate in the channel-type reactor resulted in nearly isothermal operation in the catalytic bed, and the temperature was satisfactorily controlled even when the modules were numbered-up for high capacity. In addition, the effect of coolant flow-rate was evaluated to determine operating conditions in the case of numbering-up of reaction modules.

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1. Introduction

Fischer–Tropsch synthesis (FTS) is a commercial pathway for the conversion of synthesis gas (CO and H₂) to transportation fuels, and is applied to gas-to-liquid (GTL), biomass-to-liquid (BTL), and coal-to-liquid (CTL) processes. FT-derived products are considered to be high-performance and clean diesel fuels owing to their high cetane number, as well as low content of sulfur and aromatic compounds. In addition, the GTL process plays an important role in reducing CO₂ emission when dry (CO₂) reforming is combined with steam reforming [1]; thus, the development of an efficient FTS reactor is one of the key factors for successful commercial GTL processes.

Although iron-based catalysts remain the preferred choice in commercial plants owing to their low cost and propensity to yield high olefinic content in the hydrocarbon distribution [2], catalysts based on cobalt have been commercially used because they show high activity and selectivity for heavy hydrocarbons. Other benefits of cobalt-based catalysts include low oxygenate selectivity when using H₂-rich syngas obtained from natural gas [3], low CO₂ emission resulting from a low water–gas shift reaction rate [4], and high sensitivity of product selectivity to H₂/CO ratio, pressure, and temperature compared to iron-

based catalysts [5]. Cobalt-based FTS is further favored since water has little effect on the reaction [6–8].

The FTS reaction is a hydrogenation reaction followed by an exothermic ($\Delta H^R = -165$ kJ/mol) surface polymerization reaction and it is highly selective with respect to the carbon length of the hydrocarbon. The rate of catalyst deactivation is temperature sensitive. Therefore, the removal of heat and its transfer rate from the reaction system plays dominant roles in the overall reactor performance, influencing the capital and operational cost of the entire XTL process [9,10]. In order to control the temperature, various reactors such as slurry bubble column reactors, fluidized reactors, and microscale fixed-bed reactors are used for FTS. Microscale reactors have a large number of small, parallel channels with enhanced mass transfer properties and intensified heat transfer, enabling isothermal operation of the highly exothermic Fischer–Tropsch reactions [11]. Although the basic concept of the microscale reactor sounds simple, its performance strongly relies on the channel design, wall properties, and interplay between adjacent channels for either exothermic or endothermic reactions. Therefore, understanding the operational performance and its dependence on the structure parameters is of great importance [12].

In this study, a detailed three-dimensional modeling of a channel-type reactor with a plate heat exchanger for cobalt-based FTS was conducted using COMSOL Multiphysics 4.0a (COMSOL, Inc.) for the purpose of providing useful information on the design of channel structure and the determination of operating conditions in the case of numbering-up. Although a detailed mechanistic model was developed in our

* Correspondence to: M.-J. Park, Department of Chemical Engineering, Ajou University, Suwon 443-749, Republic of Korea. Tel.: +82 31 219 2383; fax: +82 31 219 2395.

** Corresponding author. Tel.: +82 42 860 7286; fax: +82 42 860 7388.

E-mail addresses: mjpark@ajou.ac.kr (M.-J. Park), filouseus@kRICT.re.kr (K.-S. Ha).

previous work [13], lumped reaction rate is newly suggested in the present study since the main objective of using COMSOL Multiphysics is to obtain information regarding CO conversion and temperature profile under various operating conditions.

2. Experimental

The FTS catalyst with 23 wt.% cobalt and 0.05 wt.% platinum on a Si-coated Al_2O_3 support (surface area $170 \text{ m}^2/\text{g}$, Puralox®) was prepared by the impregnation method using cobalt nitrate and platinum nitrate as precursors. The 23 wt.% cobalt and 0.05 wt.% Pt were co-impregnated into the Al_2O_3 support using cobalt nitrate (II) hexahydrate and tetraamine platinum (II) nitrate, and dried at 110°C , then calcined at 400°C for 5 h. The catalyst powders were adhered to each other with boehmite sol solution (10 wt.%) to prepare porous catalyst granules of approximately 1 mm in size to enhance the heat and mass transfer capabilities, and they were calcined at 450°C for 1 h. The finished granular catalysts were tested in a channel-type reactor ($\sim 1.0 \times 10^{-4}$ bbl/day with 1 g catalyst). The reactor had a catalyst bed that was 1 mL or 2 mL in volume. Plane figures for channels A and B are provided in Fig. 1b, and the catalyst bed was sandwiched with two plate-type

microchannel heat exchangers, as shown in Fig. 1c. The channel-type reactor was situated inside an oven with no forced convection and the oven temperature was set at 70°C . Prior to the FTS activity test, the catalyst was activated at 400°C for 12 h under 5% H_2/He flow. The activity test was conducted for ca. 75 h at the reaction temperature of $220\text{--}250^\circ\text{C}$, pressure of 2.0 MPa, space velocity of $10,000\text{--}20,000 \text{ mL}/(\text{g}_{\text{cat}} \cdot \text{h})$, and mole ratio of $\text{H}_2/\text{CO} = 2$. The detailed syngas composition was $\text{H}_2/\text{CO}/\text{CO}_2/\text{Ar} = 57.3:28.4:9.3:5.0$ (mol%). Ar was used as an internal standard for GC analysis. Effluent gas from the channel-type reactor was analyzed by an online gas chromatograph (Young Lin Acme 6000 GC) employing a GS-GasPRO capillary column connected to a flame ionization detector (FID) for the analysis of hydrocarbons, and a Porapak Q/molecular sieve packed column connected to a thermal conductivity detector (TCD) for the analysis of carbon oxides and the internal standard gas Ar.

3. Mathematical model

The main reaction for FTS can be schematically written as $n\text{CO} + 2n\text{H}_2 \rightarrow -(\text{CH}_2)_n- + n\text{H}_2\text{O}$, where $-(\text{CH}_2)_n-$ is the methylene group polymerizing into a hydrocarbon chain. Various kinetic equations of

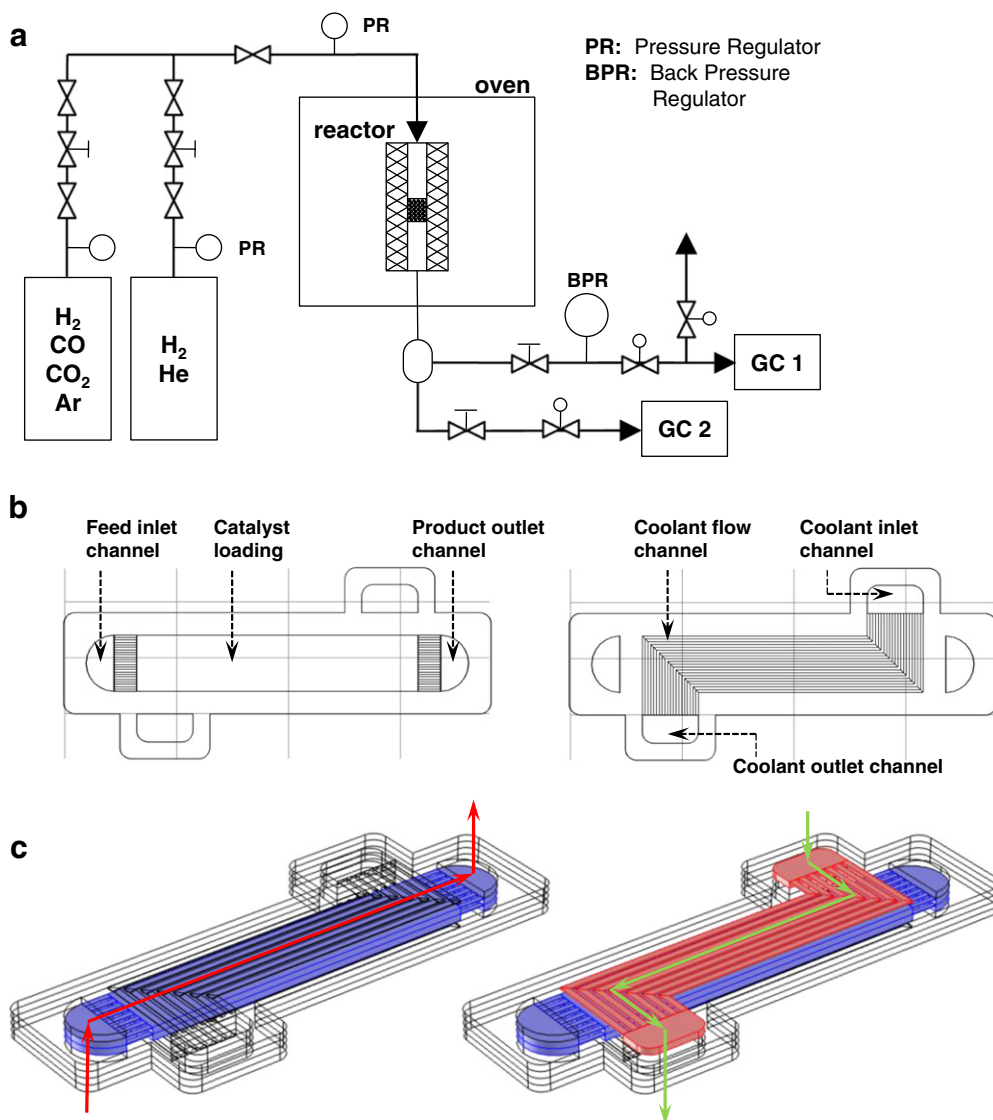


Fig. 1. (a) Experimental setup, (b) top view of the reactant flow channel (left, channel A) and coolant flow channel (right, channel B), and (c) scheme of flows in each channel.

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