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Design and modeling of large-scale cross-current multichannel Fischer–Tropsch reactor using channel decomposition and cell-coupling method

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HIGHLIGHTS

- We build a distributed parameter model for the micro channel FT reactor.
- The model was validated against the operating data of industrial scale reactor.
- The model could handle more than 13,000 channels with 6 reaction kinetics.
- Safety and productivity could be achieved by adjustment of catalyst loading.
- Increasing channel size will reduce the core volume, but increase max temperature.

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ABSTRACT

Design and modeling of a micro channel Fischer–Tropsch reactor was considered in this study. A cross-current heat-exchange reactor was modeled using a new method, in which all the process and cooling channels are decomposed into a number of unit cells. Each neighboring process and cooling channel unit cells are coupled to set up material and energy balance equations, including heat-transfer equations for the entire reactor domain, which are then solved simultaneously. The model results were compared with the experimental data for a pilot-scale reactor described in the literature, and were found to be in good agreement. Several case studies were performed to see the effect of variables such as catalyst loading ratio, coolant flow rate, and channel layout on design of a reactor with state-of-the-art Fischer–Tropsch catalyst. The developed model could handle more than 5800 process channels, 7500 cooling channels, and 130 layers, with implementation of six complex reaction kinetics.

1. Introduction

Gas-to-liquid (GTL) processes have been identified as promising processes for converting abundant natural gas (NG) to a clean synthetic fuel (Bao et al., 2010; Cao et al., 2009; Deshmukh et al., 2010; Kim et al., 2009; Knochen et al., 2010; Lee et al., 2008). The NG is first converted to syngas, which consists mainly of carbon monoxide (CO) and hydrogen, through a reforming process, and then the synthetic liquid fuel is chemically synthesized via a Fischer–Tropsch (FT) reaction. FT synfuel is almost sulfur and nitrogen free, and is therefore considered to be a clean energy fuel.

Recently, the GTL-FPSO (floating, production, storage, and off-loading) process has been considered as an alternative process for exploiting NG from stranded gas reserves or for using associated gases in conventional oil fields (Lee et al., 2011; Park et al., 2013). The design of compact, but highly productive, FT reactors will play a central role in the commercialization of GTL-FPSO. The large amount of heat generated during the FT reaction, ca. 165 kJ/mol, must be removed to achieve isothermal operation of the reactor and prevent runaway situations. Novel microchannel heat-exchange FT reactors have received much attention because of their high heat-transfer efficiencies and high production rates per unit volume of reactor (Cao et al., 2009, 2004; Chin et al., 2005;

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Deshmukh et al., 2011). A microchannel FT reactor was studied by Chin et al., using a novel engineered catalyst (Chin et al., 2005), which improved mass- and heat-transfers and enabled safe operation of the reactor without increasing undesired methane formation. Cao et al. (2009) evaluated the FT reaction performance of a supported cobalt catalyst in a microchannel catalytic reactor. Heat was effectively removed, enabling the reaction to be performed at a high gas hourly space velocity (GHSV).

Many variables such as channel layout, reactant inlet temperature, coolant flow rate, catalyst loading ratio, and space velocity are involved in multichannel FT reactor design. For successful reactor design, the effect of each important variable should be estimated and analyzed in the design step, and computational fluid dynamics (CFD) is widely used for detailed evaluation of reaction systems (Arzamendi et al., 2010, 2009; Jeon et al., 2013; Mohammadi et al., 2013; Shin et al., 2013; Troshko and Zdravistch, 2009; Uriz et al., 2011). However, when many process and coolant channels are involved, for large-scale reactors, CFD is highly computationally intensive and time consuming. CFD therefore may not be able to handle all the channels; the problem is unrealistically large, because it deals with rigorous physics such as flow patterns over the entire domain, the shear stress and viscous effects of the flowing entity, and material and energy balances, rather than using simple empirical equations. The current research trend in FT reaction design in a CFD environment is towards reduction of the problem size and analysis of the effects of key variables in the newly defined reduced domain (Arzamendi et al., 2010; Gumuslu and Avci, 2012).

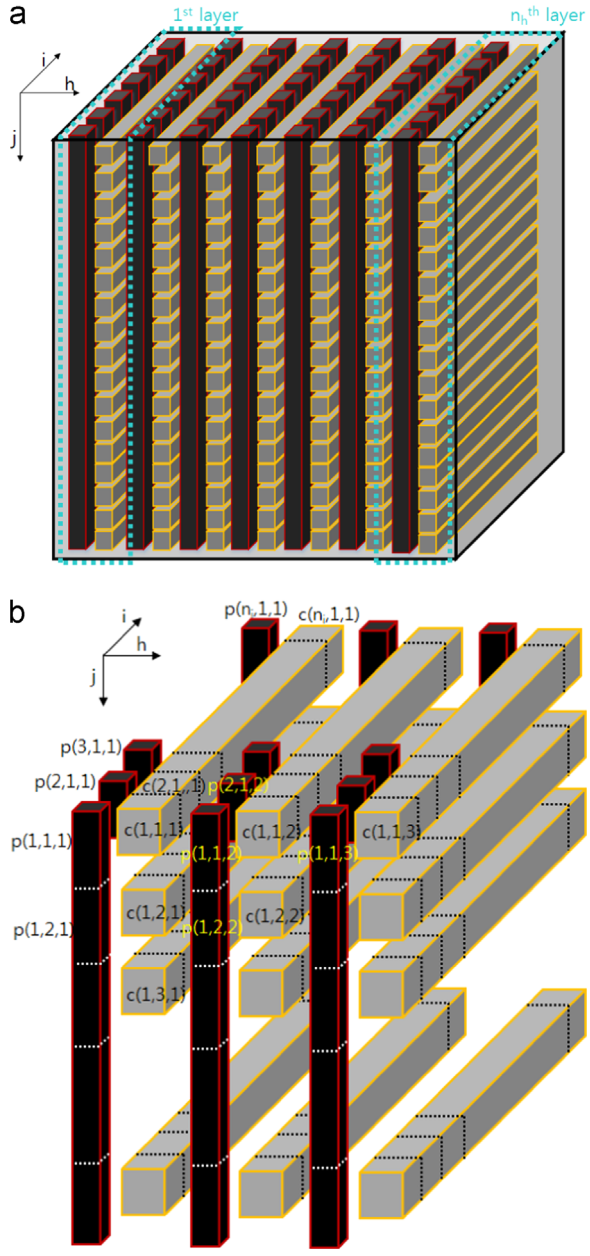

Fig. 1. Conceptual diagrams of cross-current heat-exchange reactor, and channel decomposition and cell-coupling method. (a) Cross-current reactor domain. (b) Channel decomposition and cell-coupling schemes for arbitrary sub domain.

A quick check of the effect of some variable changes is essential for decision making in the preliminary design phase. Sensitivity analyses of the channel layout such as channel width and height, gaps between channels, and wall thickness should be conducted to determine the feasible range of the channel size before the detailed design phase. The influences of some important variables such as reactant inlet temperature, coolant velocity, and feed composition on other related variables, e.g., heat generation, heat removal rate, reaction kinetics, and heat-transfer coefficient, should be rapidly estimated throughout the entire channel.

In this study, a new method for modeling large-scale cross-current microchannel FT reactors using a channel decomposition and cell-coupling method was developed. External models such as the channel layout model, kinetic model, single-channel model, and empirical heat-transfer model were used to constitute an integrated multichannel distributed model. First, the method and algorithm for model construction were developed, and then the developed model was validated against literature data. Several case studies of the design of cross-current FT reactors with use of the state-of-the-art FT catalyst (Deshmukh et al., 2011) were performed to determine design criteria, analyses, and strategies.

2. Model description

As will be described in the following sections, a distributed model for the cross-current FT reactor was developed to handle all the channels in the system. It is supported by four external models: a channel layout model that defines channel geometries, a kinetic model that provides kinetic information on the catalytic FT reaction, an empirical heat-transfer model that calculates the heat removal rate, and a single-channel model that evaluates the heat and mass balances for the reaction system in one dimension. Especially, in the channel layout model, structural information such as the number of both process and cooling channels, and the overall size of the reactor core is obtained by specifying the width, height, length, and wall thickness of the process and cooling channels, target wax production rate, space velocity of the reactant, and the catalyst loading amount.

Fig. 1 shows a diagram of channel decomposition and cell coupling in the cross-current heat-exchange reactor. From the channel configuration, which was predefined based on the channel layout model, all the process and cooling channels are decomposed in the i, j, and h directions. All the decomposed channel cells are then matched not only to the adjacent cells, but also to the distant cells that interact each other: A process cell located at an arbitrary position (j, i, h) is first coupled to every neighboring cells located at the position e.g., (j, $i \pm 1$, h), (j, $i \pm 2$, h), (j, i, $h \pm 1$), (j, i, $h \pm 2$), etc., to set up heat and material balance equations, which are then solved to obtain the solution. It is assumed that the heat transfer rate is in inverse relationship with the distance between each cell. Fig. 1(b) illustrates this pairing concept over an arbitrary cell domain.

Fig. 2 shows the algorithm for computing the mass and energy balance and heat-transfer equations involved in the model. First, it