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CFD Simulation of Fixed Bed Reactor in Fischer-Tropsch Synthesis of GTL Technology

Sh. Shahhosseini, S. Alinia, and M. Irani

***Abstract*—**In this paper 2D Simulation of catalytic Fixed Bed Reactor in Fischer-Tropsch Synthesis of GTL technology has been performed utilizing computational fluid dynamics (CFD). Synthesis gas (a mixture of carbon monoxide and hydrogen) has been used as feedstock. The reactor was modeled and the model equations were solved employing finite volume method. The model was validated against the experimental data reported in literature. The comparison showed a good agreement between simulation results and the experimental data. In addition, the model was applied to predict the concentration contours of the reactants and products along the length of reactor.

***Keywords*—**GTL, Fischer–Tropsch synthesis, Fixed Bed Reactor, CFD simulation.

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I. INTRODUCTION

GAS-TO-LIQUID (GTL) is the process of natural gas conversion to liquid fuels, mainly diesel. The process consists of four steps that all require catalysts: 1) Gas cleaning. 2) Reforming of the gas into a mixture of carbon monoxide and hydrogen (Syngas). 3) Fischer Tropsch (FT) synthesis. 4) Hydrocracking. The Fischer Tropsch synthesis is rather new to large-scale production plants. It was developed 80 years ago in Germany [1]-[2].

The Fischer–Tropsch synthesis (FTS) has become a subject of renewed interest in recent years due to an escalation in the price of oil and the discovery of several gas reserves. Parts of the world gas reserves are located in remote areas and several of them are offshore, and in these cases the transport of natural gas can become expensive and uneconomical. The FTS can be used to convert natural gas into liquid hydrocarbons.

Furthermore, a great part of the world energy source is based in liquid hydrocarbons such as gasoline, kerosene, and diesel, so the conversion of natural gas into liquid .

Transportation fuels are interesting to many countries and oil companies [3]. Due to the high demand on gasoline in the World and its higher price relative to that of diesel, production of gasoline from the FT process, becomes more favorable. The octane number of FT gasoline is lower than that of the gasoline obtained from crude oil processing, since the FT gasoline mainly consists of n-paraffin. To promote the yield and quality of the gasoline from Fischer–Tropsch synthesis, bifunctional catalysts have received extensive attention in the recent years [4].

The various types of reactors, including multi-tubular fixed-bed reactor; bubble column slurry reactor; bubbling fluidized-bed reactor; three-phase fluidized bed reactor; and circulating fluidized-bed reactor, have been considered in the history of FTS process development. It is now widely accepted that because of good mixing and heat transfer characteristics, the bubble column slurry reactor is an appropriate reactor type for large-scale plants. FT synthesis is either low temperature FT process (LTFT) or high temperature FT process (HTFT) depending on the product required. High temperature process operates at 300–350 °C and Fe-based catalysts and is mainly used for the production of gasoline and linear olefins while low temperature process operates at 200–240 °C and either Fe or Co-based catalyst and is applied for the production of waxy material [5].At the higher temperatures used in the HTFT process, the WGS reaction is rapid and goes to equilibrium, which allows CO2 to be converted to FT products as well. This is accomplished by the reverse WGS followed by the FT reaction [5].

In this work 2D simulation of catalytic fixed bed reactor in Fischer-Tropsch Synthesis of GTL technology has been performed using CFD technique. Furthermore, the simulation results were compared with the experimental data that have been reported by Ahmadi [6]. The results show acceptable predictions versus the experimental data. Concentration contours of some species in the length of reactor were simulated.

II. GOVERNING EQUATIONS

A. The Mass Conservation Equation

The equation for conservation of mass, or continuity equation, can be written as follows. [7]

$$\frac{\partial \rho}{\partial t}+\nabla.(\rho \vec{v})=0 \quad (1)$$

B. Momentum Conservation Equations

$$\frac{\partial}{\partial t}(\rho \vec{v})+\nabla.(\rho \vec{v}\vec{v})=-\nabla.p+S_i \quad (2)$$

Where " p is the static pressure (Pascal)", " ρ is the density (Kg/m^3)", " $\vec{v}$ is velocity vector (m/s) " and " S_i is the model-dependent source term from porous-media".

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Porous media are modeled by the addition of a momentum source term to the standard fluid flow equations. The source term is composed of two parts: a viscous loss term (Darcy, the first term on the right-hand side of Equation "3", and an inertial loss term (the second term on the right-hand side of Equation "3".

$$Si=-\left(\sum_{j=1}^{3}D_{ij}\mu v_j+\sum_{j=1}^{3}C_{ij}\frac{1}{2}\rho|v|v_j\right) \quad (3)$$

Where" Si is the source term for the i[th] (x, y, or z) momentum equation", "$|v|$ is the magnitude of the velocity (m/s) " and "D and C are prescribed matrices". This momentum sink contributes to the pressure gradient in the porous cell, creating a pressure drop that is proportional to the fluid velocity (or velocity squared) in the cell.

To recover the case of simple homogeneous porous media:

$$S_i=-\left(\frac{\mu}{\alpha}v_i+C_2\frac{1}{2}\rho|v|v_i\right) \quad (4)$$

Where "α (m^2) is permeability" and "C_2 (1/m) is the inertial resistance factor". [7]

C. Species Transport Equations

A conservation equation for chemical species takes the following general form:

$$\frac{\partial}{\partial t}(\rho Y_i)+\nabla.(\rho\vec{v}Y_i)=-\nabla.\vec{J}_i+R_i \quad (5)$$

Where "R_i is the net rate of production of species i by chemical reaction", "Yi is the local mass fraction of each species" and "$\vec{J}_i$ is the diffusion flux of species i". [8]

D. Energy Equation in Porous Media

Equation "6" is the standard energy transport equation in porous media regions with modifications to the conduction flux and the transient terms. In the porous medium, the conduction flux uses an effective conductivity and the transient term includes the thermal inertia of the solid region on the medium:

$$\frac{\partial}{\partial t}(\varepsilon\rho_f E_f+(1-\varepsilon)\rho_s E_s)+\nabla.(\vec{v}(\rho_f E_f+p))=\nabla.\left[k_{eff}\nabla T-\left(\sum_i h_i J_i\right)\right]+S_f^h \quad (6)$$

Where "E_f is the total fluid energy", "E_s is the total solid medium energy", "ε is the porosity of the medium", "k_{eff} is the effective thermal conductivity of the medium " and "S_f^h is the fluid enthalpy source term".[9]

E. Effective Conductivity in the Porous Medium

The effective thermal conductivity in the porous medium, k_{eff} , is computed as the volume average of the fluid conductivity and the solid conductivity:

$$k_{eff}=\varepsilon k_f+(1-\varepsilon)k_s \quad (7)$$

Where" ε is the porosity of the medium", "k_f is the fluid phase thermal conductivity" and "k_s is the solid medium thermal conductivity".[9]

III. Grid and Simulation Boundary Conditions

The simulated fixed bed reactor is illustrated in Figure 1. The two dimensional system (20 cm * 1.27 cm) which is feeded with synthesis gas (a mixture of predominantly carbon monoxide and hydrogen). Furthermore, the reactor is divided in three sections:1) fluid top, 2) porous zone, and 3) fluid bottom. Porous media is used as packed bed due to the large value of N (tube-to-particle diameter ratio). Moreover, the porous zone in the middle section of the reactor and reactions were occurred in this zone.

The mass-flow-inlet boundary condition is used to introduce gas flow to the reactor. The pressure-outlet boundary condition is specified at the bottom of the reactor. The finite volume method has been used to discrete the partial differential equations of the model using the SIMPLE method for pressure–velocity coupling.

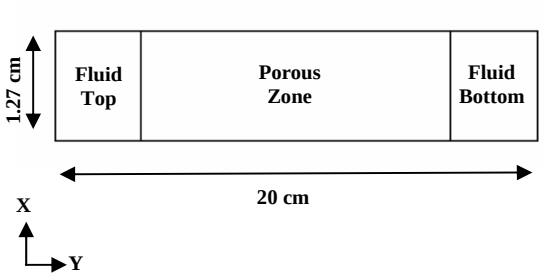


Fig.1 Schematic diagram of geometry

IV. Simulation and Discussion

A. Reaction network

The Fischer–Tropsch components Include H_2 , CO , CO_2 , H_2O , CH_4 , C_2H_4 , C_2H_6 , C_3H_8 , $n-C_4H_{10}$, $i-C_4H_{10}$ and C_{5^+}. The following reactions are listed in table 1 as leading Fischer–Tropsch reactions [10]:

TABLE 1
FTS REACTIONS [10]

$$CO+3H_2\xrightarrow{R_1}CH_4+H_2O$$
$$2CO+4H_2\xrightarrow{R_2}C_2H_4+2H_2O$$
$$2CO+5H_2\xrightarrow{R_3}C_2H_6+2H_2O$$
$$3CO+7H_2\xrightarrow{R_4}C_3H_8+3H_2O$$

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$$4CO+9H_2 \xrightarrow{R_5} n_C_4H_{10}+4H_2O$$

$$4CO+9H_2 \xrightarrow{R_6} i_C_4H_{10}+4H_2O$$

$$8.96CO+18.05H_2 \xrightarrow{R_7} C_{8.96}H_{18.18}(C_5^+)+8.96H_2O$$

$$CO+H_2O \overset{R_8}{\leftrightarrow} CO_2+H_2$$

The reaction rate equation is as follows and the kinetic parameters are given in table2: [11]

$$R_i(mol\ /\ hr\ gr_{cat}) = k_i \exp(-\frac{E_i}{R_g T}) P_{CO}^{m} \cdot P_{H2}^{n} \quad (8)$$

TABLE II
KINETIC PARAMETERS DATA [11]

Reaction Number	m	n	k_i	E_i
1	-1.0889	1.5662	142583.8	83423.9
2	0.7622	0.0728	51.556	65018
3	-0.5645	1.3155	24.717	49782
4	0.4051	0.6635	0.4632	34885.5
5	0.4728	1.1389	0.00474	27728.9
6	0.8204	0.5026	0.00832	25730.1
7	0.5850	0.5982	0.02316	23564.3
8	0.5742	0.710	410.667	58826.3

B. Model Validation

The model predictions were validated against the experimental data as reported in the literature [6]. The data were obtained using a pilot plant with the characteristics given in table 3 [6].

Table 4 exhibits the model results and the corresponding observed data of the pilot plant. [6] The estimated results are in good agreement with the pilot plant data.

TABLE III
FTS PILOT PLANT CHARACTERISTICS [6]

Tube Dimension (mm)	0.127 × 0.015 × 2
Number of Tubes	1
Molar Ratio of H_2/CO in Feed	1
Feed Temperature (K)	563.15
Catalyst Size (mm)	273.5e-03
Bed Density (Kg/m^3)	84.65
Reactor Pressure (kPa)	1700
GHSV((hr^{-1})	3000
Bed Voidage	0.4

TABLE IV
COMPARISON BETWEEN MEASURED AND PREDICTED VALUES FOR THE PILOT PLANT FTS PROCESS [6]

Parameter	pilot plant	Model	Relative Error (%)
X_{CO}(%)	81.94	70.11	14.44
X_{H2}(%)	56.01	59.06	-5.45
X_{CO+H2}(%)	68.97	64.585	9.945

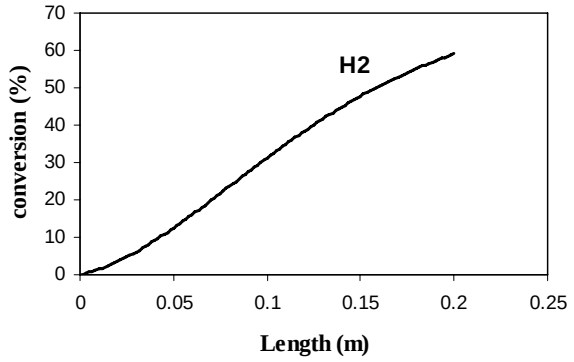


Fig. 2 Conversion of H_2 through the reactor length

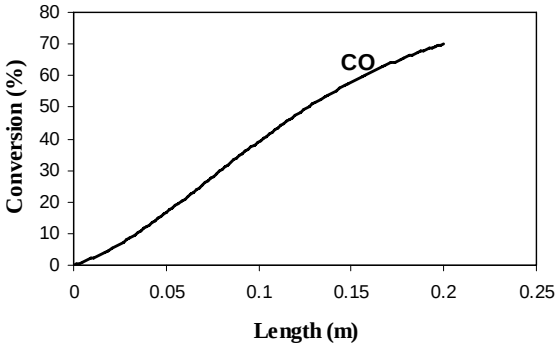
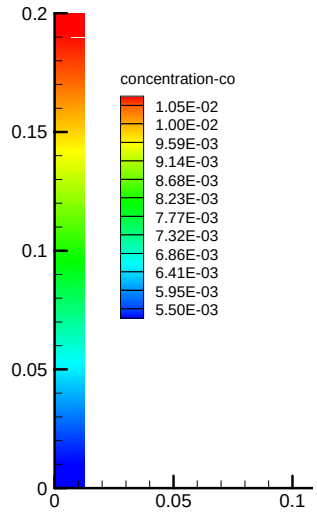


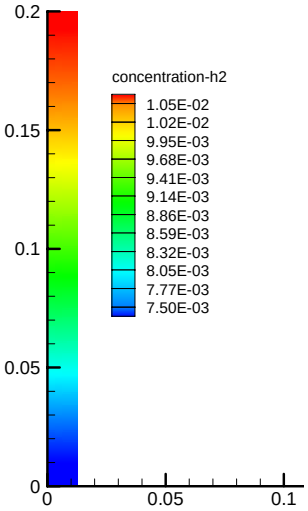
Fig. 3 Conversion of CO through the reactor length

C. Concentration Contours

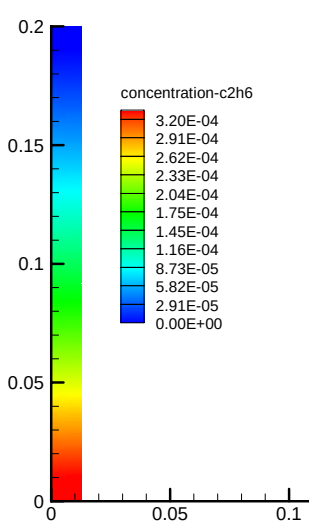
Concentration contours of some species along the length of reactor are shown in Figure 4. This figure indicates that as the reactions progress the concentrations of CO and H_2 decrease along the length of the reactor and the concentrations of the products such as: CH_4 , C_2H_4 , C_2H_6 , C_3H_8, $n\text{–}C_4H_{10}$, C_5^+ increase.

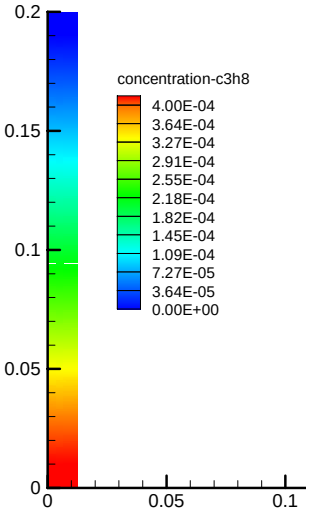
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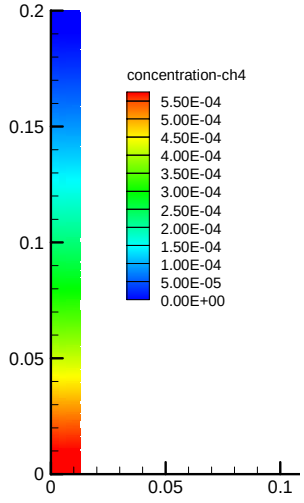


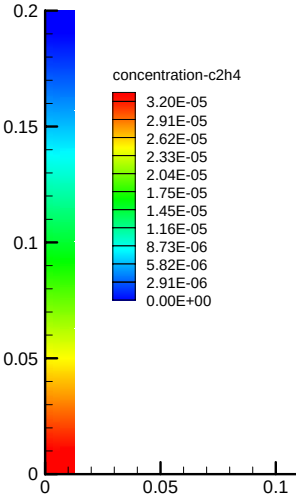
(a)



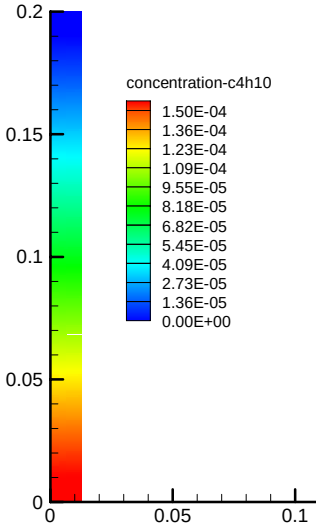


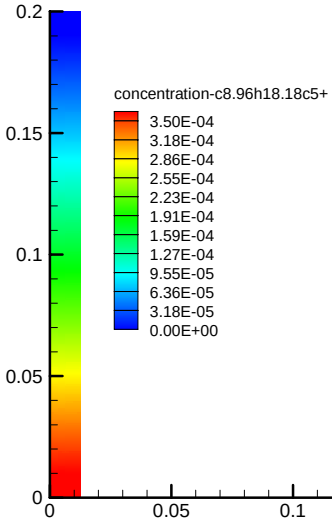
(c)





(b)





(d)

Fig. 4 Molar Concentration Contours (a) Reactants (b), (c), (d) Products

V. Conclusion

Simulation results of species concentrations were compared with those of experimental data reported in the literature. There was a good agreement between the simulation values and the experimental data. Simulation results indicated that of CO and H_2 concentrations decreased due to the reactions occurred along the length of the reactor and the concentrations of the product species (CH_4, C_2H_4, C_2H_6, C_3H_8, $n\text{–}C_4H_{10}$, C_5^+) increased.

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