International Journal of Chemical, Materials and Biomolecular Sciences
ISSN: 2415-6620
Vol:3, No:9, 2009

Hydrodynamic Simulation of Fixed Bed GTL Reactor Using CFD

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Abstract**—**In this work, axisymetric CFD simulation of fixed bed GTL reactor has been conducted, using computational fluid dynamics (CFD). In fixed bed CFD modeling, when N (tube-to-particle diameter ratio) has a large value, it is common to consider the packed bed as a porous media. Synthesis gas (a mixture of predominantly carbon monoxide and hydrogen) was fed to the reactor. The reactor length was 20 cm, divided to three sections. The porous zone was in the middle section of the reactor. The model equations were solved employing finite volume method. The effects of particle diameter, bed voidage, fluid velocity and bed length on pressure drop have been investigated. Simulation results showed these parameters could have remarkable impacts on the reactor pressure drop.

Keywords**—**GTL Process, Fixed bed reactor, Pressure drop, CFD simulation.

I. INTRODUCTION

GAS-TO-LIQUID (GTL) is the conversion of natural gas to liquid fuels, mainly diesel. The GTL 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, and (4) hydrocracking.The Fischer Tropsch synthesis is rather new to large-scale production plants, it was developed 80 years ago in Germany [1]-[2].

In the Fischer Tropsch synthesis, which was invented in Germany in 1923, synthesis gas reacts over some metal-based catalyst to produce liquid hydrocarbons (mainly paraffins). The main conversion reaction is given by:

Mainly iron and cobalt are used as catalysts at 200-300 °C and 10-60 bar pressure. The temperature, pressure and catalyst determine whether light or heavy hydrocarbons are produced. For example, high temperature process using iron catalyst at about 340 °C mainly produces gasoline and chemicals like alpha olefins and the low temperature process using either iron or cobalt based catalyst at about 230 °C mainly produces waxes.

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For economic and logistic reasons, up-scaling of F-T reactors (such as energy conversion) and strong exothermic of F-T Reactions are two important considerations while selecting a reactor for commercial scale GTL plant [3]. Keeping in mind these two aspects, different configurations of reactor had been used at different times. Recent developments have shown that three major types of F-T reactors used for commercial GTL production are: (a) fluidized bed reactor, (b) fixed bed tubular reactor, and (c) bubble column slurry reactor [3]-[4].

In a fixed bed reactor, gas phase reactions are generally carried out using a stationary bed of solid catalyst. In a typical reactor, suitable screens support the bed of catalyst particles, through which the gas phase flows.

The choice of reactor type depends on several issues including intrinsic reaction rate, heat of reaction, influence of external transport resistance on selectivity, molar change during the reaction, and so on. Several commercially important processes such as steam reforming (of methane or naptha), water gas shift reaction, methanol from synthesis gas, oxidation of sulfur dioxide, isomerization of xylenes, ammonia synthesis, alkylation of benzene, hydro de-waxing, reduction of nitrobenzene to aniline, manufacture of tetra-hydrofuran and butanediol from maleic anhydride, butadiene from ethanol, and so on, are carried out in fixed bed reactor [5].

Energy loss as characterised by a pressure drop of the process fluid, is an important consideration in the design and operation of fixed-bed systems and has consequently been a subject great interest for few decades.a wast amount of information in the form of empirical and semi-emprical correlations which relate the pressure drop to the hydrodynamic conditions of the packed beds is available. The Ergun correlation, as given by equation (1), accounts for viscous and inertial energy losses and relates them to the dynamic variable, velocity of the fluid, a well as the structure of the bed, as characterised by the bed voidage [6].

$$\frac{|\Delta P|}{L} = \frac{150\mu}{D_P^2}\frac{(1-\varepsilon)^2}{\varepsilon^3}\ V\infty + \frac{1.75\rho}{D_p}\frac{(1-\varepsilon)}{\varepsilon^3}V_\infty^2 \tag{1}$$

When modeling laminar flow through a packed bed, the second term in the above equation may be dropped, resulting in the Blake-Kozeny equation [6]:

$$\frac{|\Delta P|}{L} = \frac{150\mu}{D_P^2}\frac{(1-\varepsilon)^2}{\varepsilon^3}\ V\infty \tag{2}$$

In these equations, "μ is the viscosity (Kg/m.s)", "D_P is the particle diameter (m)", "L is the bed length (m)", and"ε is the bed voidage".

II. Governing Equations

For steady state laminar flow, the conservation equations of continuity and momentum can be simplified respectively:

$$\nabla.(\rho U) = 0 \tag{3}$$

$$\nabla.(\rho UU) = -\nabla P + Si \tag{4}$$

"ρ is density (Kg/m^3)", "U is velocity vector" and "∇P is pressure gradient".

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 (5), and an inertial loss term (the second term on the right-hand side of Equation (5)).

$$Si = -\left(\sum_{j=1}^{3} D_{ij}\mu v_j + \sum_{j=1}^{3} Cij\ \frac{1}{2}\rho|v|v_j\right) \tag{5}$$

Where S_i is the source term for the i^th (x, y, or z) momentum equation $|v|$ is the magnitude of the velocity 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:

$$Si = -\left(\frac{\mu}{\alpha}v_i + C_2\frac{1}{2}S|v|v_i\right) \tag{6}$$

"α (m^2) is permeability" and "C_2(1/m) is inertial loss coefficient" in each component direction may be identified as:

$$\alpha = \frac{D_p^2}{150}\frac{\varepsilon^3}{(1-\varepsilon)^2} \tag{7}$$

$$C_2 = \frac{3.5}{D_p}\frac{(1-\varepsilon)}{\varepsilon^3} \tag{8}$$

III. Geometry and Analysis

A. Geometrical Model

Three zones were considered in the reactor as: 1) fluid top, 2) porous zone and 3) fluid bottom.

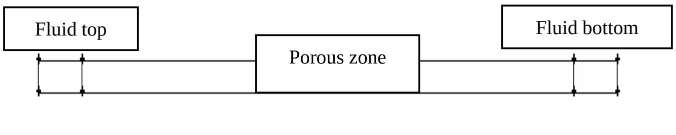

Fig. 1 Reactor is devided in three sections

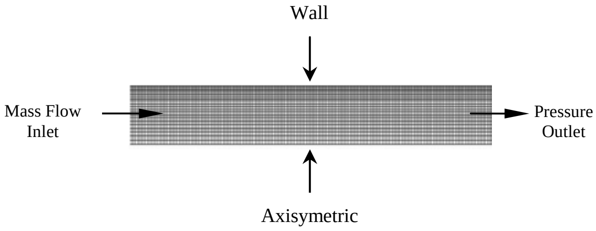

Fig. 2 Grid configuration with boundary conditions

B. Model Analysis

The fluid was taken in a laminar flow regime. Synthesis gas was chosen as the emulation fluid. First order upwind (for momentum) was used in all emulations. The pressure-velocity coupling algorithm was the SIMPLE scheme.

IV. Result and Discussion

A. Effect of Particle Diameter (Bed voidage) On Pressure Drop

For evaluating the effect of particle diameter (bed voidage) on pressure drop, three different catalyst diameters of 274 (micrometer), 374 (micrometer), and 474 (micrometer) were applied. Other parameters are listed in Table I. Pressure drop through the bed length in three different bed voidage are shown in Fig. 3. Equation "2" shows pressure drop is inversely related to the bed voidage. Due to this fact, an increase in the bed voidage causes a reduction in pressure drop.

TABLE I
Axisymmetric Simulation Parameters

No. of simulation	Molar ratio of H2/CO in feed	Particle Diameter (micrometer)	Bed voidage	Length of bed(m)
1	1	274	0.3865172	0.18
2	1	374	0.3885407	0.18
3	1	474	0.3908562	0.18

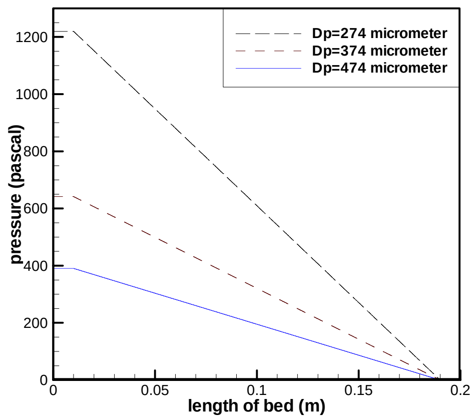

Fig. 3 Pressure drop through the simulated bed

B. The Effect of Length of the Bed on Pressure Drop

In order to determine the effect of length of the bed on pressure drop, three bed lengths of 0.17 (m), 0.18 (m), and 0.19 (m) were used.

Other process parameters are listed in Table II.

Pressure drop through the bed length in three different length of the bed are illustrated in Fig. 4. Equation "2" implies that the pressure drop is directly related to the bed length. Therefore, an increase in the length of the bed causes an increase in pressure drop.

TABLE II
AXISYMMETRIC SIMULATION PARAMETERS

No. of simulation	Molar ratio of H2/CO in feed	Particle Diameter (micrometer)	Bed voidage	Length of bed(m)
1	1	274	0.3865172	0.17
2	1	274	0.3865172	0.18
3	1	274	0.3865172	0.19

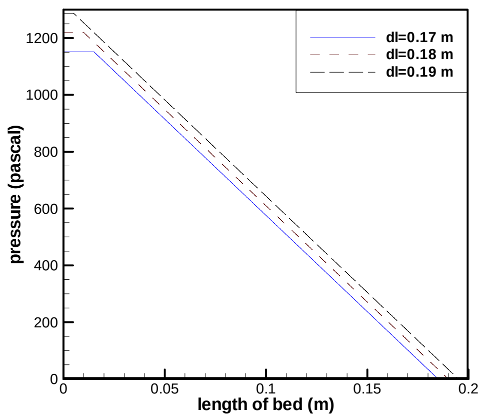

Fig. 4 Pressure drop through the simulated bed

C. The Effect of Fluid Velocity on Pressure Drop

In order to evaluate the effects of fluid velocity on pressure drop, three different flow rates of feed 2.0320e-04 (Kg/s), 2.4372e-04 (Kg/s), and 3.0465e-04 (Kg/s) were applied in the simulations.

Other parameter values are presented in Table III.

Pressure drop through the bed length in three different flow rates of feed are shown in Fig. 5. According to equation "2", pressure drop is directly related to fluid velocity. Therefore, an increase in the fluid velocity leads to an increase in pressure drop.

TABLE III
AXISYMMETRIC SIMULATION PARAMETERS

No. of simulation	Molar ratio of H2/CO in feed	Particle Diameter (micrometer)	Mass flow rate of feed (Kg/s)	Length of bed(m)
1	1	274	2.0320e-04	0.18
2	1	274	2.4372e-04	0.18
3	1	274	3.0465e-04	0.18

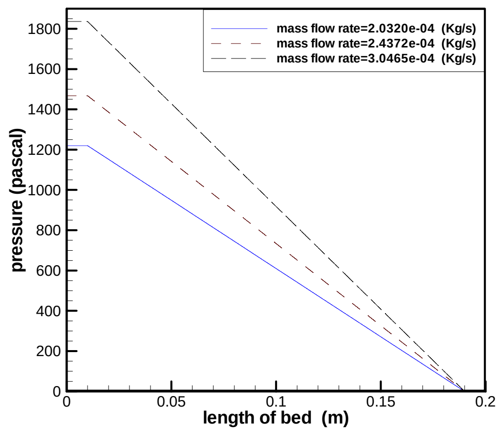

Fig. 5 Pressure drop through the simulated bed

V. CONCLUSION

In this research, the effects of different parameters of GTL reactor on its pressure drop were investigated applying the CFD technique. The simulation results showed an increase in particle diameter or bed voidage lead to lower bed pressure drop. In addition, raising the length of the bed reduced pressure drop in the fixed bed reactor. Moreover, increasing fluid velocity resulted in lower pressure drop in the fixed bed reactor.

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