



CFD Analysis for Fixed Bed Fischer-Tropsch Process

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ABSTRACT

In this study a 3D simulation of Fixed Bed Fischer-Tropsch Synthesis (FTS) of GTL technology has been performed using Computational Fluid Dynamics (CFD). This simulation was performed to numerically demonstrate the conversion of synthesis gas (a mixture of carbon monoxide and hydrogen) to higher hydrocarbons over iron based catalyst. The reactor bed is modeled with cylindrical pellets and the model equations were solved employing finite volume method. The model is applied to predict the amount of conversion of reactants to products. In addition the amount of heat released by reactions is used to calculate the coolant data.

Keywords - Fischer-Tropsch Synthesis, GTL Technology, Fixed Bed Reactors, Computational Fluid Dynamics, Heat Transfer Analysis.

1. INTRODUCTION

Fischer-Tropsch Synthesis is a part of GTL technology which can be briefly defined as the means used to convert synthesis gas containing hydrogen and carbon monoxide to hydrocarbon products. The name comes from the founders of this technology 'Franz Fischer' and 'Hans Tropsch' who first developed it at Kaiser Wilhelm Institute for coal research in Mulheim (Ruhr), Germany, in 1920.

The present fossil-fuels used are non-renewable. Because of the growth in population and technology and faster depletion of fossil fuels, the need for fuels has also grown parallel. These non-renewable resources are bound to get over one day. So, it becomes important to look for alternate fuels where FTS is one of the best options.

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 which can be transported economically.

Most part of the world energy source is based on liquid hydrocarbons such as gasoline, kerosene, and diesel, so the conversion of abundant fossil fuels such as natural gas and coal into liquid hydrocarbons is very much necessary.

The qualities of Fischer-Tropsch products are excellent and their environmental properties are being recognized as very valuable in the ongoing drive towards cleaner fuels and engines in terms of absence of sulphur, nitrogen or heavy metal contaminants, and the low aromatic content. The kerosene/jet fuel produced has good combustion properties and high smoke points. The diesel and petrol fuels have higher cetane and octane numbers respectively.

Potential co-products may also utilize material and energy that is not directly associated with the FT hydrocarbons. For example, waste heat may be converted to electrical power for sale and nitrogen produced in the air separation unit may be used to make ammonia which may be further reacted with waste Carbon Dioxide to make Urea.

Currently there are two FT operating modes. The high-temperature (300-350⁰C) process with iron-based catalysts is used for the production of gasoline and linear low molecular mass olefins. The low-

temperature (200-240°C) process with either iron or cobalt catalysts is used for the production of high molecular mass linear waxes [3].

There are four types of catalysts used in FTS, Iron based, Cobalt based, Nickel based and Ruthenium based. Iron and Cobalt based catalysts are widely used.

There are four types of Fischer-Tropsch (FT) reactor in commercial use at present, circulating fluidized bed reactor; fluidized bed reactor; fixed bed reactor and slurry phase reactor.

The basic Fischer-Tropsch reaction can be described as formation of paraffinic or olefinic chains Eqs. (1) & (2) and a water-gas shift reaction Eq (3):



The main reaction, Eq. (1), is highly exothermic. The increase in temperature is undesirable because it, 1) favors increased methane formation, 2) favors catalyst deactivation mechanism (carbon deposition, sintering and fouling) and 3) Reduces the average chain length of the product molecules. Because of these undesirable effects it becomes very important to keep the reactor bed at an optimum temperature by cooling it by providing a cooling jacket around it and the coolant being the water.

2. GOVERNING EQUATIONS

2.1 Mass Conservation Equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (4)$$

2.2 Mass Conservation Equation

$$\frac{\partial(\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla \cdot p + S_i \quad (5)$$

Where, p is the static pressure(Pa), ρ is the density(kg/m³), \vec{v} is the velocity vector(m/s) and S_i is the source term for porous media.

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 Eq (5), and an inertial loss term the second term on the right-hand side of Eq (6)).

$$S_i = - \left(\sum_{j=1}^3 D_{ij} \mu v_j + \sum_{j=1}^3 C_{ij} \frac{1}{2} \rho |v| v_j \right) \quad (6)$$

Where, S_i 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_{ij} and C_{ij} 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 in the cell.

The prescribed matrices D_{ij} and C_{ij} are given by the famous Ergun equation for packed beds

$$D_{ij} = \frac{150(1 - \varepsilon)^2}{\varphi^2 d_p^2 \varepsilon^3} \quad (7)$$

$$C_{ij} = \frac{3.5(1 - \varepsilon)}{\varphi d_p \varepsilon^3} \quad (8)$$

Where, ε is the particle porosity, d_p is the particle diameter(m) and φ is the sphericity of the cylindrical particles or pellets".

The variation of density with pressure and temperature is dealt through the ideal gas equation.

$$p = \rho RT \quad (9)$$

Where, p is pressure (pa), ρ is the density(kg/m^3), R is the specific gas constant(J/kgK) and T is temperature(K).

2.3 Species Conservation Equation

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

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot J_i + R_i \quad (10)$$

Where, R_i is the net rate of production of species i by chemical reaction, Y_i is the local mass fraction of each species and J_i is the diffusion flux of species i .

2.4 Energy Conservation Equation

Eq (10) 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:

$$\frac{\partial(\varepsilon \rho_f E_f + (1 - \varepsilon) \rho_s E_s)}{\partial t} + \nabla \cdot (\vec{v} (\rho_f E_f + p)) = \nabla \cdot \left(k_{eff} \nabla T - \left(\sum_i h_i J_i \right) \right) + S_f^h \quad (11)$$

Where, E_f is the total fluid energy, E_s is the total solid medium energy, S_f^h is the fluid enthalpy source term and k_{eff} is the effective thermal conductivity of the medium given by

$$k_{eff} = \varepsilon k_f + (1 - \varepsilon) k_s \quad (12)$$

Where, k_f is the fluid phase thermal conductivity and k_s is the solid medium thermal conductivity.

3. GEOMETRIC MODEL AND GRID

The domain contains three regions. Top and the bottom fluid regions are the extrusions to allow the flow to develop. The middle reactor bed is filled with randomly arranged cylindrical pellets (catalysts) and with voids being fluid region. The pellets are modeled as porous region. The wall-pellets contact and pellets-pellets contacts are fused with an approximation for quality meshing. The geometry and the mesh are shown in Fig 1.

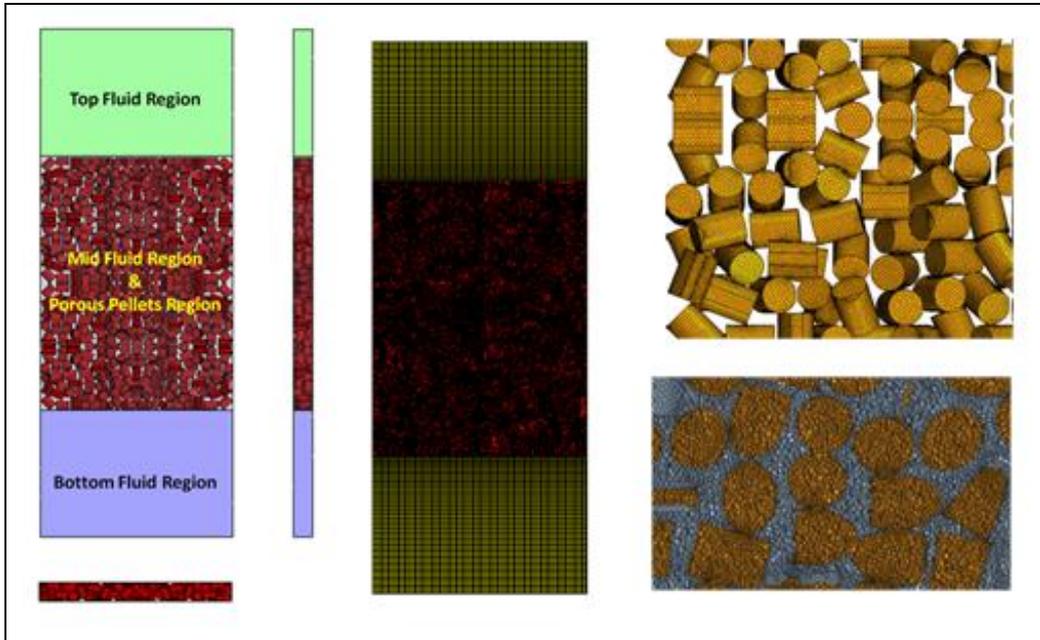


Fig 1: Geometry and Mesh

The reactor bed has been meshed with polyhedral cells. The upstream and downstream fluid regions are extruded to produce polyhedral prism layers. The total number of volume cells is around 2.01 million

4. BOUNDARY CONDITIONS

The inlet (top) is modeled as mass flow inlet and the outlet (bottom) is modeled as pressure outlet. The reactor bed walls are maintained at a constant temperature of 493 K and the domain operating pressure is 25bar. The porous resistance coefficients are calculated using the Eq (7) & (8). The pellets porosity is 0.7. The flow is steady and laminar. The PISO scheme is used for pressure-velocity coupling and upwind second order is used as discretization scheme.

5. SIMULATION AND DISCUSSION

5.1 Reaction Network

The FTS reactions happen inside the pellets. The FTS reactions include the species, H₂ (Hydrogen), CO (Carbon Monoxide), CH₄ (Methane), C₂H₄ (Ethylene), C₂H₆ (Ethane), C₃H₈ (Propane), n-C₄H₁₀ (n-Butane), i-C₄H₁₀ (iso-Butane), C₈H₁₈ (Octane Vapor), CO₂ (Carbon-Dioxide) and H₂O (Water Vapor). There are 11 species and 8 reactions which are listed in Table 6 as leading Fischer–Tropsch reactions.

Sl No.	Equation	Equation No
1	$CO + 3H_2 \xrightarrow{R_1} CH_4 + H_2O$	13
2	$2CO + 4H_2 \xrightarrow{R_2} C_2H_4 + 2H_2O$	14
3	$2CO + 5H_2 \xrightarrow{R_3} C_2H_6 + 2H_2O$	15
4	$3CO + 7H_2 \xrightarrow{R_4} C_3H_8 + 3H_2O$	16
5	$4CO + 9H_2 \xrightarrow{R_5} n-C_4H_{10} + 4H_2O$	17
6	$4CO + 9H_2 \xrightarrow{R_6} i-C_4H_{10} + 4H_2O$	18
7	$8CO + 17H_2 \xrightarrow{R_7} C_8H_{18} + 8H_2O$	19
8	$CO + H_2O \xrightarrow{R_8} CO_2 + H_2$	20

Table 1– FTS Reactions [2]

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	0.585	0.5982	0.02316	23564.3
8	0.5742	0.71	410.667	58826.3

Table 2: Kinetic Parameters Data [2]

The reaction rate equation is as follows [2],

$$R_i(\text{mol/hr.gr}_{\text{cat}}) = k_i \exp\left(-\frac{E_i}{R_g T}\right) P_{CO}^m \cdot P_{H_2}^n \quad (21)$$

Where, R_i is reaction rate, k_i is pre-exponential factor, E_i is activation energy, R_g is gas constant, P_{CO} and P_{H_2} are partial pressures of CO and H₂ respectively and m & n are power raised to partial pressures of CO and H₂ respectively. The units and values are changed according to the solver compatibility by using the bed density.

5.2 Concentration Contours

Concentration contours of some species along the length of reactor are shown in Fig 2. This figure indicates that as the reactions progress the concentrations of CO and H₂ decrease along the length of the reactor and the concentrations of the products such as: CH₄, C₂H₄, C₂H₆, C₃H₈, C₄H₁₀, and C₈H₁₈ increase.

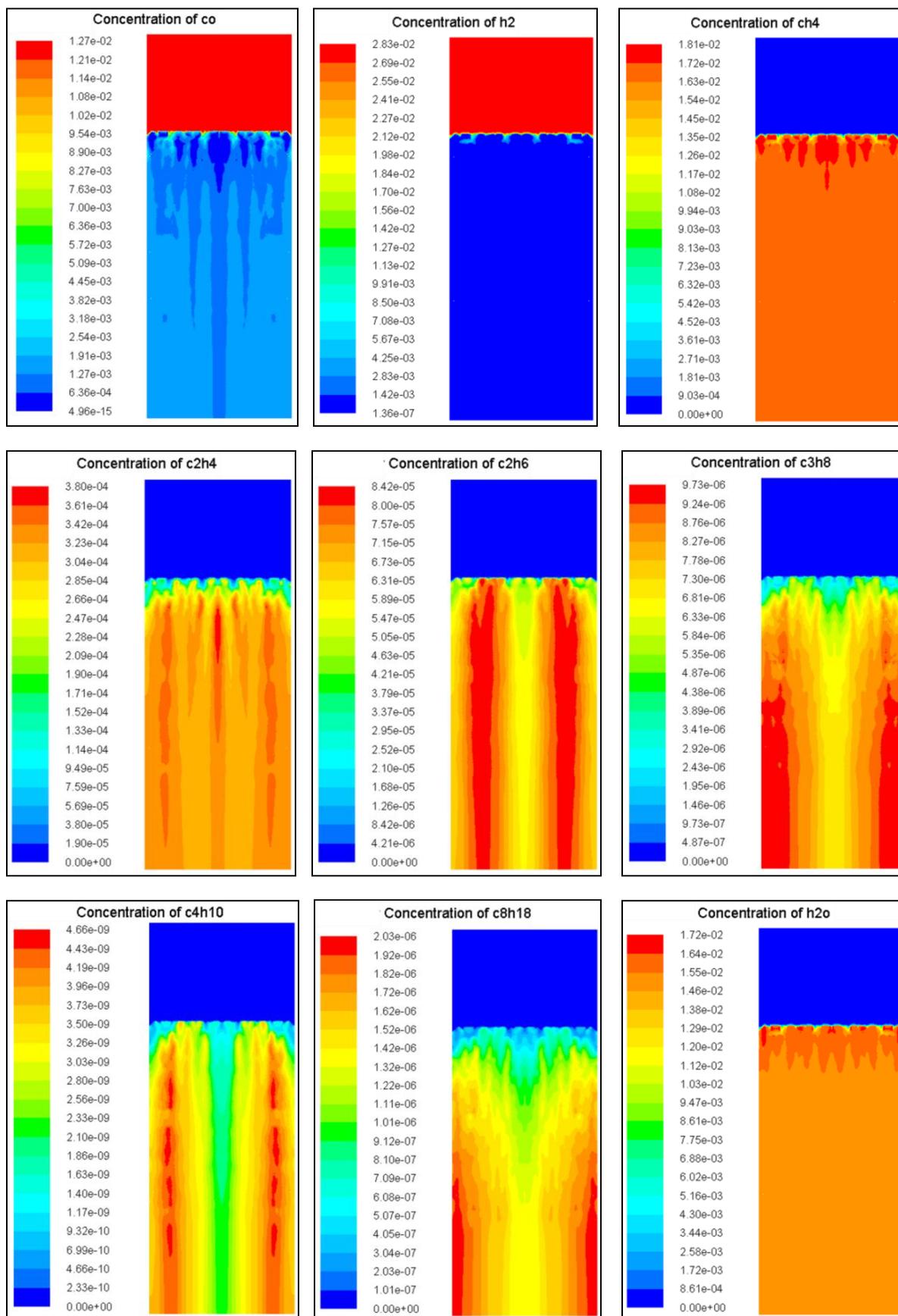


Fig 2: Molar Concentration Contours (kmol/m³) of Reactants and Products

5.3 Model Validation

The results of this study are compared with Reference [2]. As the geometry and boundary conditions considered are different in both the cases, it is not possible to have the direct comparison; instead the trend of the results has been compared.

Parameter	Present Study	Reference [2]
% Conversion of CO	93.61	70.11
% Conversion of H ₂	99.94	59.06
% Conversion of (CO+H ₂)	96.775	64.585

Table 3: Comparison of Percentage Conversion

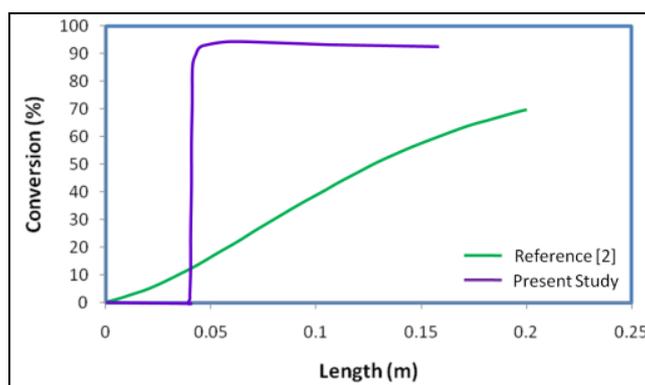


Fig 3: Comparison of Percentage Conversion of CO through the Domain

6. CONCLUSION

Simulation results indicate that the Carbon Monoxide and Hydrogen concentrations have decreased due to the reactions occurring along the length of the reactor and the concentrations of the product species (Methane, Ethylene, Ethane, Propane, n-Butane, iso-Butane, Octane, Carbon Dioxide and Water) have increased.

There is around 94.5% conversion of Synthetic gas. Methane, Carbon Dioxide and Water are the major products.

Both the temperature and the conversion of reactants to products are high because of the constant temperature condition on the reactor walls. Physically the rise in temperature leads to catalyst deactivation. So, the reactor has to be cooled to an optimum temperature. Once the cooling or the convection on the reactor walls is considered, the temperature will be reduced along with the reduction in the amount of conversion of reactants to products.

Around 8×10^3 KJ/kg of heat is being produced from the FTS reactions for the given boundary conditions. By considering a coolant jacket of 5 mm annulus, the mass flow rate of the coolant (water) is calculated to be 2.2×10^{-4} kg/s. The outlet temperature of water is calculated to be 364.1K.

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