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Design Methodology for the Fischer-Tropsch Reactor for the Production of Green Diesel from Coal Syngas

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ABSTRACT

The world is facing declining liquid fuel reserves at a time when energy demand is exploding. Alternative fuel is currently an important issue all over the world due to efforts on reducing the global warming which is contributed by the combustion of petroleum or petrol diesel. In order to achieve a secure and stable energy supply that does not cause environmental damage, renewable energy sources must be explored and promising technologies must be developed. In this study one of the renewable energy technology known and Fischer-Tropsch Synthesis is considered and a design methodology for the Fischer-Tropsch Reactor for the production of Green Diesel from Coal Syngas is presented.

Key words: Biodiesel, Renewable Energy, Global Warming, Fischer-Tropsch Synthesis

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INTRODUCTION

Biodiesel has become an important source of renewable energy because of its availability, no bad impacts on the environment and it can be produced by a variety of sources like from Coal Gas, vegetable oil and algae [1]. Coal is a best candidate for replacing the oil as an energy supply. It is source of energy rich and easily can be converted into liquids fuels by converting into syngas and then into biodiesel [2]. Although biodiesel is a fast emerging as the oil of future Biodiesel is able to decrease such gas emission which can cause the global warming because of its several factors like production methods, types of feed stocks etc. Another environmental effect of the biodiesel is that biodegradation rate of biodiesel is 5 times faster than petroleum diesel over a period of 28 days.

Biodiesel is a widely used as a diesel component worldwide as well as in Thailand. Even a lot of research papers are studied about Biodiesel. The aim of this study is to provide a design methodology for the Fischer-Tropsch Reactor for the production of Green Diesel from Coal Syngas [3].

Fischer-Tropsch Synthesis is a set of chemical reactions that can be used to produce the green diesel and a variety of chemicals from synthesis gas (a mixture of carbon monoxide and hydrogen). Synthesis gas can be obtained from the coal or natural gas usually. This process can be used to produce approximately carbon free and environment friendly fuels [4].

Reaction Kinetics

The major overall reactions involved in the Fischer-Tropsch Synthesis are as follows.

1. Paraffin $(2n+1)H2 + nCO\rightarrow/ CnH2n+02 + nH2O$
2. Olefins $2nH2 + nCO\rightarrow/ CnH2n + nH2O$
3. Water Gas Shift Reaction $CO + H2O\rightarrow/1\ CO2 + H2$

Side reaction involves in this process are

1. Alcohols $2nH2 + nCO\rightarrow CnH2n0+2O + (2n-1)4H2O$
2. Boudouard Reaction $2CO\rightarrow C + CO2$

Catalyst Modification will takes place in following reactions

1. Catalyst Oxidation/Reduction $MxOy + yH2\leftrightarrow/1\ yH2O + xM$
   $MxOy + yCO\leftrightarrow/1\ yCO2 + xM$
1. Bulk Carbide Formation $yC + xM\leftrightarrow MxCy$

Previous kinetics study on the Fischer-Tropsch Synthesis based on iron catalyst is shown in Table-1. In general for iron catalysts the FT reaction rate increases with H2 partial pressure and decreases with partial pressure of water. [5] Previous research show a reversible decrease of the catalyst activity by addition of 12 and 27 mol% water to the feed gas. However, after addition of 42 mol% water the catalyst did not regain its initial activity. Previous study shows a number of rate expressions for Iron based catalyst as follows [5-8]. Selectivity control in Fischer-Tropsch synthesis by process conditions and Catalyst modifications is shown in Table-2 [9].

Table-1

Sr. No.	**Rate Expressions**
1	KP_{H_2}
2	$KP_{H_2}P_{CO}$
3	$\frac{kP_{H_2}P_{CO}}{P_{CO} + aP_{H_2O}}$
4	$\frac{kP^2{}_{H_2}P_{CO}}{P_{CO}\,P_{H_2} + aP_{H_2O}}$
5	$\frac{kP^2{}_{H_2}\,P_{CO}}{1 + aP_{CO}P^2{}_{H_2}}$
6	$\frac{kP_{H_2}P_{CO}}{P_{CO} + aP_{CO_2}}$
7	$\frac{kP_{H_2}P_{CO}}{P_{CO} + aP_{H_2O} + bP_{CO_2}}$
8	$\frac{kP^{½}{}_{CO}P^{½}{}_{H_2}}{(1 + aP^{½}{}_{CO} + bP^{½}{}_{H^2})^2}$
9	$\frac{kP_{CO}P^{½}{}_{H_2}}{(1 + aP_{CO} + bP^{½}{}_{H_2})^2}$
10	$\frac{kP_{CO}P_{H_2}}{(1 + bP_{CO})^2}$

Table-2

Parameter	**1**	**2**	**3**	**4**	**5**	**6**
Temperature	↓	↑	*	↓	↑	↑
Pressure	↑	↓	*	↑	*	↓
H_2/CO	↓	↑	↓	↓	↓	↑
Conversion	*	*	↓	↓	↑	↑
Space Velocity	*	*	↑	↑	*	↓
Alkali Content in Iron Catalyst	↑	↓	↑	↑	↑	↓

Where
↑ Increasing ↓ Decreasing * Complex Relation

1. Chain Length
2. Chain Branching
3. Olefin Selection
4. Alcohol Selection
5. Carbon Deposition
6. Methane Selection

Design Calculations

Fischer-Tropsch Reactor is multi-tubular fixed bed reactor. It is used to convert synthesis gas to hydrocarbons at specified conditions.
Temperature = 250°C= 523K, Pressure = 25bar = 2.5MPa, Overall Conversion = 60%

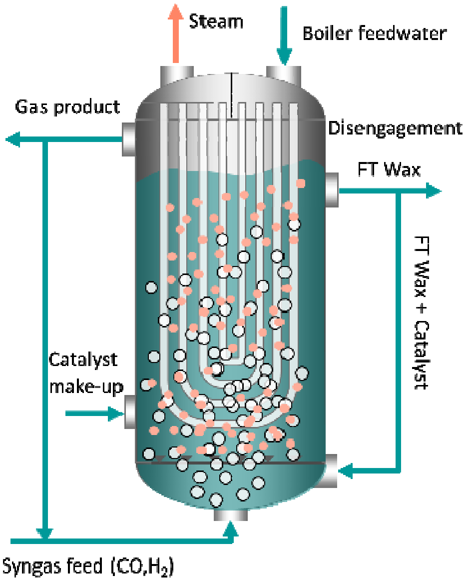

Fig. 1

Volume of Catalyst

We know that [10]

$$\frac{V}{F_{A_0}} = \int \frac{dx}{-r_A} \tag{1}$$

Where V= Volume of Catalyst, F_{A0}= Molar Feed Rate and $-r_A$= Rate of Reaction

For Fisher Tropsch reaction, at our desired operating conditions and catalyst rate of reaction can be calculated from this relation [8].

$$-r_A = \frac{kP_{H_2}^2 P_{co}}{1+aP_{co}P_{H_2}^2} \tag{2}$$

Where [11],

K= Rate Constant = 0.0339mol/kg.s.MPa, P_{H2}= Partial Pressure of Hydrogen

P_{CO}= Partial Pressure of Carbon Mono Oxide, a= Adsorption Parameter = 1.185MPa^{-1}

Rate constant k and a can be calculated at any temperature by using following empirical relation [8].

$$K = 8.27 \times 10^8 exp^{\left(-\frac{E}{RT}\right)} \tag{3}$$

At 250^{0}C the activation energy for Fischer-Tropsch Reaction is 104KJ/mol.

As we know that [12]

$$a = a_\infty exp^{\left(-\frac{\Delta H}{RT}\right)} \tag{4}$$

For partial pressure

$$P_i = X_i \times P_T \tag{5}$$

Where

P_T= Total Pressure, X_i=Mole Fraction, P_i= Partial Pressure

From material balance partial pressure of respected components can be calculated as follows,

X_{CO}= Mole Fraction of CO = 0.271, X_{H2}= Mole Fraction of H_2 = 0.581, P_T= Total Pressure = 25bar = 2.5MPa

So, by Dalton Law,

P_{CO} = 0.271×2.5 = 0.6775MPa and P_{H2} = 0.581×2.5 = 1.452MPa

by putting all the calculated values in the above expression (2) we have,

$$-r_A = \frac{0.0339 \times (1.45)^2 \times (0.6775)}{1 + (1.185) \times (0.6775) \times (1.45)^2} = 1.75 \times 10^{-5} \frac{Kmole}{Kg.sec.}$$

For the conversion of units, density of catalyst (Iron) will be multiplied with rate of reaction.

Density of Iron catalyst [13] = 7840kg/m^3

by multiplying density of feed with Rate, we have

$$-r_A = 1.75 \times 10^{-5} \times 7840 = 0.136 \frac{Kmole}{sec.m^3}$$

For 60% conversion now put the values in relation (1) we get

$$V = \frac{(1.38) \times (0.60 - 0)}{(0.136)} = 6.06m^3$$

Volume of Reactor

As we know that [10]

$$Volume\ of\ Vessel - Volume\ of\ Catalyst = Porosity\ of\ Catalyst\ Bed \times Volume\ of\ Vessel$$

Average Porosity of Catalyst Bed [14] = 0.64

Or

$$Volume\ of\ Reactor = \frac{Volume\ of\ Catalyst}{1 - Porosity\ of\ Catalyst\ Bed} = \frac{6.06}{1 - 0.64} = 16.84m^3$$

Dimension of Tubes [15]

D_i= Inner Diameter of Tube = 34.8mm, D_o= Outer Diameter of Tube = 38mm and L= Length of Tube = 4.88m

Number of Tubes

$$Inner\ Cross\ Sectioal\ Area\ of\ One\ Tube = \frac{\pi d^2{}_i}{4} = \frac{3.14 \times (34.8 \times 10^{-3})^2}{4} = 9.5 \times 10^{-4} m^2$$

$$Inner\ Volume\ of\ One\ Tube = Area\ of\ One\ Tube \times Length\ of\ Tube = 9.5 \times 10^{-4} \times 4.88 = 4.63 \times 10^{-3} m^3$$

$$N_T = \frac{Volume\ of\ Reactor}{Volum\ of\ One\ Tube} = \frac{16.84}{4.63 \times 10^{-3}} = 3637$$

Surface Area Available for One Tube

Surface area available for one tube can be calculated as follows

$$A = \pi d_o L = (3.14 \times (38 \times 10^{-3}) \times 4.88) = 0.4822m^2$$

Length of Shell

Let 10% additional length is given at top and 10% at bottom.

$$Total\ Additional\ Length = 0.2 \times Length\ of\ Tube = 0.2 \times 0.4822 = 0.976m$$

And

$$Lenth\ of\ Shell = Length\ of\ Tube + Additional\ Length = 4.88 + 0.976 = 5.856m$$

Diameter and Area of Shell [15]

Bundle diameter of tubes can be calculated as

$$D_b = d_o \left(\frac{N_T}{K_t}\right)^{\left(\frac{1}{n}\right)} \tag{6}$$

Where

Outer Diameter of Tube = d_o = 38mm, Number of Tubes = N_T = 3637,

Constant = n = 2.207 and Constant = K_t = 0.215

Put the values in above equation we get

$$D_b = d_o \left(\frac{N_T}{K_t}\right)^{\left(\frac{1}{n}\right)} = 38 \times 10^{-3} \left(\frac{3637}{0.215}\right)^{\left(\frac{1}{2.207}\right)} = 3.12m$$

For Fixed Tube

$$Shell\ Diameter + Bundle\ Diameter = Clearence = 0.097m$$
$$Shell\ Diameter + 3.12 = 0.097m$$
$$Shell\ Inner\ Diameter = 3.21m$$

As we know that

$$Area\ of\ Shell = \pi \frac{d^2{}_s}{4} = 3.14 \times \left(\frac{(3.21)^2}{4}\right) = 8.21m^2$$

$$Outer\ Area\ of\ Tubes = \pi \frac{N_T D_t{}^2}{4} = 3.14 \times 3637 \times \frac{38 \times 10^{-3}}{4} = 4.12m^2$$

Since, area of shell is greater than area of tubes (A_s>A_T) so design is satisfactory.

Pressure Drop [10, 16]

Pressure drop can be determined by the Ergun equation as follows.

$$\frac{\Delta P}{L} = \frac{fCG^2}{\rho D} \times 10^{-10} \tag{7}$$

$$C = \frac{1.75 \times 10^{10}}{144g} \times \frac{1-\varphi}{\varphi^3} \tag{8}$$

$$f = 1 + \frac{150}{1.75} \times \frac{DG}{\mu}^{-1} \times 1 - \varphi \tag{9}$$

Where

ΔP = Pressure Drop, L = Length = 4.88m, G = Mass Flow Rate = 19.5 Kg/sec, φ = Porosity of Catalyst Bed = 0.64, D_p = Diameter of Catalyst Particles = 0.66mm, μ = Viscosity of Feed Gas = 0.000018 Kg/m.sec.

$$G_{tube} = \frac{G}{A_t} = \frac{19.5}{4.12} = 4.73\ \frac{Kg}{m.sec.}$$

Put the values in (9) we get

$$f = 1 + \frac{150}{1.75}\left((\frac{1.92 \times 10^{-3} \times 3658.3}{4.45 \times 10^{-3}})^{-1} \right)(1 - 0.62) = 1.02$$

Put this value in (8) we get

$$C = \frac{1.75 \times 10^{11}}{144 \times (4.17 \times 10^8)} \left(\frac{1 - 0.64}{0.64^3}\right) = 0.45$$

Now put all of these values in (7) we get.

$$\frac{\Delta P}{L} = \frac{1.02 \times 0.45 \times 3658.3^2}{0.44 \times 1.92 \times 10^{-3}} \times 10^{-10} = 0.72$$
$$\Delta P = 0.72 \times L = 0.72 \times 15.616 = 11.35\ psi$$
$$\Delta P = 0.78\ bar$$

Pressure drop is less than 3 bar so it is reasonable hence design is satisfactory.

RESULTS

In this research we present a basic design methodology for the Fischer-Tropsch Reactor as follows.

Fischer-Tropsch Reactor			
Type	Multi-Tubular Fixed Bed Reactor	**Volume of Catalyst**	$6.06m^3$
Feed	Syngas	**Number of Tubes**	3637
Flow Rate	5000kgmole/hr.	**Outer Diameter of Tube**	38mm
Temperature	250-270°C	**Inner Diameter of Tube**	34.8mm
Pressure	25bar	**Length of Tubes**	4.88m
Catalyst	Iron	**Diameter of Shell**	3.21m
Composition of Catalyst (wt. basis)	100Fe 5Cu $5K_2O$ $5SiO_2$	**Length of Shell**	5.85m
Volume of Reactor	$16.84m^3$	**Pressure Drop**	0.78 bar

CONCLUSIONS

In this research we design a reactor for 60% conversion of Synthesis Gas in to the Green Diesel with the optimized reactor size of $16.84m^3$ in the presence of Iron based catalyst (100Fe, 5Cu, $5K_2O$, $5SiO_2$) supported catalyst in a Fischer-Tropsch Reactor (Multi-Tubular Fixed Bed Reactor). Our reactor design is satisfactory because of its pressure drop is less than 3bar which is 0.78bar.

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