Fuel 154 (2015) 140-151

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

Modelling of a fixed bed reactor for Fischer–Tropsch synthesis of simulated N₂-rich syngas over Co/SiO₂: Hydrocarbon production

Nima Moazami, Miroslaw L. Wyszynski^{*}, Hamid Mahmoudi, Athanasios Tsolakis, Zhi Zou, Pooria Panahifar, Kiyarash Rahbar

School of Mechanical Engineering, College of Engineering and Physical Sciences, The University of Birmingham, Edgbaston, Birmingham B15 2TT, UK

HIGHLIGHTS

• Pseudo-homogeneous mathematical modelling of fixed bed reactor for FT synthesis.

- Prediction of conversion rate and products' selectivity for the designed FT plant on cobalt-silica catalyst.
- Calculation of kinetic parameters for the proposed model using experimental data.
- Numerical investigation on effects of operating conditions on conversion and selectivity.

ARTICLE INFO

Article history: Received 16 May 2014 Received in revised form 9 February 2015 Accepted 18 March 2015 Available online 1 April 2015

Keywords:

Fischer–Tropsch synthesis Fixed bed reactor Mathematical modelling Interpreting kinetic data Ultra-clean fuel production Hydrocarbon selectivity

ABSTRACT

A numerical pseudo-homogeneous one-dimensional mathematical model of a mini-scale laboratory fixed bed reactor for Fischer–Tropsch (FT) synthesis was developed. FT synthesis was modelled for simulated N₂-rich syngas (17%Vol CO, 33%Vol H₂, and 50%Vol N₂) on a cobalt-silica (i.e. Co/SiO₂) catalyst/support. The performance of the reactor model for gas/liquid fuel production was studied at different operating conditions i.e. temperature of 503–543 K, pressure of 10–25 bar and gas hourly space velocity (GHSV) of 1800–3600 Nml g_{cat}^{-1} h⁻¹. An algorithm was written in order to calculate the conservation of species, pressure drop, reaction rate equations and physicochemical and thermodynamic properties' relationships along the axial dimension i.e. in the flow direction. The program code was executed in a MATLAB environment to describe the profiles of concentration of each individual component in the gas phase along the reactor. The model was capable of predicting the selectivity of different product species and conversion of CO and H₂ in the flow direction.

The power law rate expression was chosen for the rate of reaction and the dominating FT and Water Gas Shift (WGS) reaction equations were considered in accordance with the literature. After the mechanisms and rate equations were derived, the kinetic data (e.g. rate constant (k_j), for reaction 'j') for the proposed reaction equations were obtained as "integral reactor data" where the total conversion is measured as a function of: catalyst weight to flow rate ratio (i.e. W/F), inlet pressure, final conversion obtained by experiment, and inlet fluid temperature. The pre-exponential factors (A_j) were calculated by the classic Arrhenius equation using the predicted k_j and literature-derived activation energies (E_j). Finally, the partial order of reactions with regard to CO (m_j) and H₂ (n_j) were calculated for the power law rate equation using MATLAB Global Optimization Toolbox with additional in-house procedures according to the results acquired from experiments with the Co/SiO₂ catalyst.

The predicted results of the model were validated successfully against 16 experimental conditions with respect to conversion of CO and selectivity of products species such as CO_2 , CH_4 , C_2 , C_3 , C_4 , and C_{5+} . The error between the predicted and experimental results was negligible. Finally, the influence of the GHSV, temperature and inlet pressure of fluid mixture on components' selectivity and conversion, were also investigated and the conclusions were in agreement with the literature.

© 2015 The Authors. Published by Elsevier Ltd. This is an open access article under the CC BY-NC-ND licenses (http://creativecommons.org/licenses/by-nc-nd/4.0/).

* Corresponding author. Tel.: +44 121 414 4159, mobile: +44 7968 157 909. *E-mail address*: M.L.Wyszynski@bham.ac.uk (M.L. Wyszynski).







Nomenclature

Symbols		0£	density of the fluid (kg m ^{-3})
a_j	pre-exponential factor of rate constant in reaction 'j'	PJ Dp	density of the bulk ($kg_{cat} m^{-3}$)
-	$(\text{mol Pa}_{j}^{-(m+n)} g_{\text{cat}}^{-1} s^{-1})$	ГБ V;;	stoichiometric coefficient of component 'i' in reaction 'i
Ar	reactor surface area, (m ²)	υy	(-)
C_i	concentration of species 'i' (mol m^{-3})	ф	From factor $(-)$
d _i	inner reactor diameter (m)	Ψ	Liguin luctor ()
$\dot{d_0}$	outer rector diameter (m)	Subcominta	
d_n	average particle diameter. (m)		
E;	activation energy of reaction ' <i>i</i> ' (I mol ^{-1})	0	
F	inlet molar flow rate of the fluid (mol s^{-1})	Ĵ.	fluid phase
f	friction factor (-)	1	species 1
$h_{\rm P}$	reactor hed height (m)	j	jth reaction
k.	rate constants (mol Pa ^{-(m+n)} σ^{-1} s ⁻¹)	т	mixture
M	molecular weight of mixture $(\alpha \text{ mol}^{-1})$	Ζ	axial dimension
M.	molecular weight of species (i') (g mol ⁻¹)		
m	partial order of the reactant with respect to carbon	Abbreviations	
ш	monovide ()	BFD	Backward Finite Difference
*	nononide (-)	Со	Cobalt
וו ח	partial processing of aposics (i) (har)	EM	Euler Method
P _i	total pressure (bar)	Fe	Iron
P_T	total pressure (Dar) Valumatria flavu rata of the fluid ($m^3 a^{-1}$)	FT	Fischer-Tropsch
Q_v	volumetric now rate of the fluid ($m^2 S^{-1}$)	GHSV	Gas Hourly Space Velocity
K _j	rate of reaction $f(mol g_{cat} s^{-1})$	GC	Gas Chromatogram
Re	Reynolds number $(-)$	HC	Hydrocarbon
R_u	universal gas constant 8.314 (J mol ⁺ K ⁺)	LHHW	Langmuir Hinshelwood Hogan Watson
S _i	selectivity of species 'i' (mole%)	Mn	Manganese
T_f	fluid temperature (K)	MS	Manganese Mass Spectrometry
t_w	wall thickness (m)	Ni	Nickel
u_s	superficial fluid velocity (m s ⁻¹)	NR	Number of Reaction
W	catalyst weight (g)	NS	Number of Species
x	conversion (mole%)	ODE	Ordinary Differential Equation
Y_i	mole fraction of species ' i ' (–)		Dartial Differential Equation
			Process Dath Flow
Greek letters		PPF Der	Process Path Flow
β	volume fraction of active site of the solid particles (–)	KU CiC	Kullelliulli Silisen Carbida
ϵ	void fraction (–)	SIC	
μ_i	dynamic viscosity of species ' <i>i</i> ' (kg m ^{-1} s ^{-1})	51U ₂	Silica Water Can Shift
μ	dynamic viscosity of the mixture (kg m ⁻¹ s ⁻¹)	WG2	water Gas Shift
r-m			

1. Introduction

Fischer–Tropsch (FT) synthesis has great potential for the production of ultraclean transportation fuels like diesel and jet fuel from synthesized gas produced from more abundant resources such as coal, natural gas and biomass [1]. FT synthesis has also shows great promise for obtaining second generation biofuels i.e. the BTL process [2,3]; as well as for producing chemical feedstock or motor fuels without the production of the environmentally harmful compounds encountered in direct hydrogenation [4]. It has been found that several metals such as nickel (Ni), cobalt (Co), ruthenium (Ru) and iron (Fe) can be activated for FT reaction [5]. Fe and Co catalysts are the most common commercial FT synthesis catalysts. The Co catalysts are preferred due to their high FT synthesis activity, high selectivity to long chain hydrocarbons (HCs), better catalyst stability in hydrogen rich environments and lower selectivity to oxygenated compounds [6–8].

In general, modern FT synthesis is conducted through various types of reactors including: fixed bed, slurry bed, trickle bed, fluidized bed and a liquid phase slurry reactor [9,10]. The fixed bed reactor has an advantage of ease of scale-up from a single tube to a pilot plant and the absence of the requirement to separate the catalyst from the product [11]. Atwood and Bennett [12] proposed a one-dimensional (1D) heterogeneous plug flow model

with a tubular reactor over an Fe catalyst. Bub and Baerns [13] delivered a two-dimensional (2D), pseudo-homogeneous plug flow model with a fixed bed reactor over an Fe 16% and manganese (Mn) 84% catalyst, but only exclusively for converting N₂ rich syngas. Wang et al. [14] proposed a 1D heterogeneous model with fixed bed reactor to account for pore diffusion limitations. De Swart et al. [15] compared the performance of the slurry reactor with the simulated performance of the FT trickle bed reactor over a Co catalyst. Philippe et al. [16] studied the effect of operating conditions and thermal properties of a Co-based catalyst on the behaviour of a fixed bed reactor for FT synthesis using a 2D pseudo-homogeneous model. Guttel and Turek [17] compared different reactor types based on a 1D approach (fixed bed, slurry, monolithic reactor and micro-reactor); including all mass transfer resistances for Co used as a catalyst, showing the potential of new reactor concepts to decrease the mass transfer resistance. Jess and Kern [18] interpreted the use of fixed bed multitubular reactors meant for FT synthesis over Fe and Co catalysts by using 1D and 2D pseudo-homogeneous models. Jess et al. [19] established a pseudo-homogeneous 2D model for industrial multitubular FT reactors on an Fe catalyst, using nitrogen-rich syngas (50%). Quina et al. [20] studied a 2D heterogeneous fixed bed reactor over V_2O_5/TiO_2 (i.e. Vanadium oxide/Titanium dioxide) with large pore particles. It referred to the partial oxidation of o-Xylene (C_8H_{10}) Download English Version:

https://daneshyari.com/en/article/6635431

Download Persian Version:

https://daneshyari.com/article/6635431

Daneshyari.com