



Comprehensive Fischer–Tropsch reactor model with non-ideal plug flow and detailed reaction kinetics

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ABSTRACT

This paper presents a detailed first principle Fischer–Tropsch reactor model including detailed heat transfer calculations and detailed reaction kinetics. The model is based on a large number of components and chemical reactions. The model is tuned to a fixed bed nearplug flow reactor but can also be applied to slurry and micro-channel reactors.

The presented model is based on a cascade of ideally stirred reactors. This modelling approach is novel for Fischer–Tropsch reactors and has the advantage of being able to represent none-ideal reactors. Using a large number of components and reactions makes it possible to better represent the product slate than with conventional modelling based on distribution models.

The results of the simulations emphasise that temperature control is important. Global conversion and product yields are dependent on operating conditions especially the temperature. The model is used to calculate the dimensions of an industrial reactor from a laboratory scale reactor.

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1. Introduction

Biomass to liquids (BtL), gas to liquids (GtL) and coal to liquids (CtL) processes transform a carbon based feedstock into a synthesis gas by gasification that is in turn transformed into a liquid fuel. A wide variety of fuels can be synthesised from synthesis gas, including methanol, ethanol, gasoline, kerosene and diesel. The production of methane (methanation) also falls in this category of processes even though it is a gas. Long and shorter chain alkanes are the main products of the Fischer–Tropsch process. After fractionation the liquids are naphtha, kerosene, diesel and waxes. Wax can be cracked to produce lighter products (upgrading). Produced kerosene and diesel are fossil fuel substitutes with slightly different characteristics (Collins et al., 2006). The Fischer–Tropsch process combines hydrogen with carbon monoxide to produce alkanes, alkenes, oxygenates and water. Fischer–Tropsch reactions can be modelled and simulated in different ways, depending on the use of the model.

Fischer–Tropsch production is often represented by an Anderson Flory Schultz (ASF) product distribution. While this globally represents the product slate, it is incapable to precisely describe the products (Masuku et al., 2012b; Qian et al., 2013). Often two or more ASF distributions need to be superimposed to correctly describe the product slate (Fox and Tam, 1995; Masuku et al., 2012a). Fischer–Tropsch reactor models in process simulators and techno-economic studies are often based on a global conversion of carbon monoxide. The product slate is assumed or calculated from a simple model often based on the Anderson Flory Schultz (ASF) distribution (Haarlemmer et al., 2012; Kim et al., 2009; Tock et al., 2010; van Vliet et al., 2009). These models are simple to configure and fast to execute, but lack precise responses to solicitations by varying operating conditions.

More detailed models are based on a kinetic model for the conversion of syngas. The product slate is then calculated from a simplified kinetic model to describe the overall advancement of the reaction followed by a distribution equations to calculate different products (Almeida et al., 2013; Ellepola et al., 2012; Maretto and Krishna, 1999; Visconti and Mascellaro, 2012). Computational fluid dynamics studies of Fischer–Tropsch reactors are often limited to the CO conversion (Shin et al., 2013). This allows the estimation of the heat production and the modification of the composition, without taking into account the full reaction scheme.

Some detailed reaction (micro-) kinetics have been presented (de Deugd, 2004; Mazzone and Fernandes, 2006; Qian et al., 2013;

Abbreviations: ASF, Anderson Flory Schultz; BtL, biomass to liquids; CSTR, continuously stirred tank reactor; CtL, coal to liquids; GtL, gas to liquids; SRK, Soave Redlich Kwong.

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Nomenclature

Variable

A	heat transfer area (m^2)
Ant (1–6)	coefficients Antoine's equation
Bo	Bodenstein number (–)
CD	amount of catalyst per reactor volume (kg m^{-3})
C_p	heat capacity ($\text{J mol}^{-1} \text{K}^{-1}$)
c_t	molar density (mol m^{-3})
d	channel width (m)
D	diffusion coefficient ($\text{m}^2 \text{s}^{-1}$)
D^*	dispersion coefficient ($\text{m}^2 \text{s}^{-1}$)
e	wall thickness (m)
E	energy (J mol^{-1})
F	mol flow rate (mol s^{-1})
g	gravitational acceleration (m s^{-2})
h	film (heat transfer) coefficient ($\text{W m}^{-2} \text{K}^{-1}$)
H	enthalpy flow (J s^{-1})
H_r	heat of reaction (J mol^{-1})
k	kinetic constant (s^{-1} or $\text{bar}^{-1} \text{s}^{-1}$)
L	length (m)
m	mass (kg)
M_w	mol weight (kg mol^{-1})
n	number of reactors
nc	number of components
N	number of moles (mol)
Nu	Nusselt number (–)
NL	moles in liquid phase (mol)
NT	concentration total active sites (mol m^{-3})
NV	moles in gas phase (mol)
p_i	partial pressure (Pa)
P	total pressure (Pa)
Pe	Péclet number (–)
Pr	Prandtl number (–)
Q	heat transferred (J s^{-1})
r	rate of reaction ($\text{mol m}^{-3} \text{s}^{-1}$)
R	universal gas constant ($\text{J mol}^{-1} \text{K}^{-1}$)
Re	Reynolds number (–)
s	reaction channel dimension
t	time (s)
T	temperature, total (K)
u	velocity (m s^{-1})
U	heat transfer coefficient ($\text{W m}^{-2} \text{K}^{-1}$)
V	reactor volume (m^3)
w	width flow channel (m)
x	mole fraction (–)

Greek symbols

*	active site
Δ	difference
θ	fraction active sites (–)
λ	conductivity ($\text{W m}^{-1} \text{K}^{-1}$)
μ	dynamic viscosity (Pa s)
ν	stoichiometric coefficient
σ	variance
ρ	density (kg m^{-3})

Sub- and super scripts

a	activation
cata	catalyst
f	fluid side, internal reactor
FT	Fischer–Tropsch
g	gas
h	hydraulic

i	index used for components
In	inlet
j	reaction number
l	liquid
Out	outlet
ref	reference
tot	total
r	residence
s	saturated
tot	total
Wall	reactor wall
Water	water side

Storsaeter et al., 2006; van Dijk, 2001) sometimes with models based on these kinetics. These models are capable to represent more accurately the observed products. Research papers generally focus on the calculation of the reactor products; fully integrated models (including detailed kinetics and heat transfer) are rarely presented.

To estimate the cost of synthetic fuels, simple yield models are usually sufficiently accurate, given the precision that can be obtained in techno-economic studies, generally in the 50% accuracy range (Haarlemmer et al., 2012). When more detailed evaluations are performed to evaluate process choices on the economic result of the process plant, it is interesting to be able to use a model that produces precise responses to changing compositions and operating conditions. This is especially important when looking at the amount of inert components; recycle rates, operating pressures and temperatures. Interesting optimisations have been performed with very detailed models outside process simulators (Rafiee and Hillestad, 2012).

Fischer–Tropsch reactors are often simulated as idealised reactors. Chemical reactors rarely operate as a single ideally mixed reactor or perfect plug reactor. Hooshyar et al. (2012) showed that both slurry and fixed bed reactors show non-ideal behaviour.

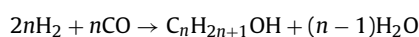
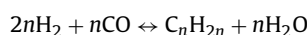
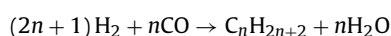
This paper presents a model that is detailed in reactor kinetics and heat transfer. It takes into account operating conditions and the reactor geometry. This allows the evaluation of specific choices in the process engineering of synthetic fuel plants.

2. Modelling the Fischer–Tropsch reactor

The model of the Fischer–Tropsch reactor includes, apart from balance equations, reaction kinetics and heat transfer calculations. The approach taken in this study is to simulate the reactor by a limited number of ideal reactors the choice of the number of ideal reactors is explained in this section.

2.1. Fischer–Tropsch reaction mechanism

The reaction mechanism of the Fischer–Tropsch mechanism has received a great deal of attention. The global reactions of Fischer–Tropsch synthesis are the following:



These reactions occur at any pressure (generally between 5 and 40 bar) and at temperatures between 170 and 350 °C in the presence of a catalyst which can be a transition metal such as iron,

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