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Interfacial mass transfer limitations of the Fischer-Tropsch synthesis operated in a slurry bubble column reactor at industrial conditions

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HIGHLIGHTS

- Gas-liquid mass transfer for the Fischer-Tropsch synthesis was studied.
- Conversion varied in the range 45–90% depending on choice of mass transfer model.
- Conversion decreased linearly with increased inlet Sauter-mean diameter.
- Bubble size dependency of the mass transfer coefficient showed effect on conversion.

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ABSTRACT

At high catalyst volume fractions the Fischer-Tropsch synthesis (FTS) operated in a slurry bubble column (SBC) is driven into the mass transfer limited regime. This study utilized literature models for the gas-liquid mass transfer coefficients in a multifluid-population balance model in which the gas-phase composition was a function of bubble size. The results confirmed that mass transfer limitations occur and that the choice of mass transfer coefficient model is crucial, yielding final conversion results ranging from 45% to 92% depending on the choice of k_L models. At smaller k_L values the composition is highly dependent on bubble size, whilst for the largest k_L values the composition is not a function of bubble size at all. The population balance modeling (PBM) allowed for explicitly keeping track of the bubble size distribution. Varying the inlet Sauter-mean diameter (SMD) resulted in a linear decrease in conversion as the inlet SMD was increased from 5 mm to 20 mm. Illustrative models for the bubble size dependency of k_L were implemented, which provided additional information compared to traditional models which use (bubble size) averaged values for the liquid-phase mass transfer coefficient k_L and/or the gas-liquid interfacial area a and composition.

1. Introduction

Bubble column and slurry bubble column (SBC) reactors are widely used in the chemical, biochemical, petroleum and metallurgical industries (Leonard et al., 2015). Bubble column reactors and the mathematical models to describe them are presented in e.g. Deckwer (1992) and Jakobsen (2014). Bubble column applications include different types of chemical reactions such as oxidation, chlorination, alkylation, polymerization, esterification and hydrogenation (Leonard et al., 2015). Bubble columns can also be used for fermentation, biological wastewater treatment and the production of liquid fuels from synthesis gas through the Fischer-Tropsch synthesis (FTS) (Leonard et al., 2015), an example of gas-to-liquid processes. A review of gas-to-liquid processes in slurry reactors is given in Wang et al. (2007). This study considers the FTS in an SBC, illustrated in Fig. 1.

1.1. The FTS

The FTS is of interest when seeking renewable sources for liquid fuels. Lignocellulosic material such as forestry residue is a potential raw material for advanced biofuels. Torrefied and gasified biomasses are converted to hydrocarbons via synthesis gas. The FTS produces hydrocarbons of various lengths from synthesis gas over a catalyst through the reaction:

$$nCO + (2n + 1)H_2 \rightarrow C_nH_{2n+2} + nH_2O \quad (1)$$

The catalyst type applied in this study is cobalt. Most biomass-to-liquid concepts have utilized cobalt, as it can be operated at higher

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Nomenclature

Latin letters

A	bubble surface area [m^2]
A	amplitude of $f_{d,\text{in}}$ in Eq. (9), $A = \sum_{\xi} \frac{\alpha_{G,in}(\xi)\rho_{G,in}(\xi)\sigma\sqrt{(2\pi)}}{exp[-(\xi-\bar{\xi})^2/(2\sigma^2)]W_{\xi}(\xi)}$ [$kg\ m^{-1}\ m^{-3}$]
a	kinetic parameter [$kmol\ s^{-1}(kg\ cat)^{-1}\ Pa^{-2}$]
a_L	gas-liquid interfacial area [$m^2\ m^{-3}$]
b	kinetic parameter [Pa^{-1}]
C_p	heat capacity [$J\ K^{-1}\ kg^{-1}$]
D	diffusion coefficient [$m^2\ s^{-1}$]
D_C	reactor inner diameter [m]
$D_{G,z,\text{eff}}$	effective axial dispersion coefficient [$m^2\ s^{-1}$]
D_H	reactor hydraulic diameter [m]
D_t	distance between cooling tubes [m]
d_s	Sauter-mean diameter [m]
d_S	solids average particle diameter [m]
f_d	mass density function [$kg\ m^{-1}\ m^{-3}$]
$F_{G,z}$	cross-sectionally averaged force term [$kg\ m\ s^{-2}$]
g	standard acceleration due to gravity [$m\ s^{-1}$]
h	mass averaged enthalpy [$J\ kg^{-1}$]
H	reactor height [m]
n	number of moles [mol]
k	turbulent kinetic energy [$m^2\ s^{-2}$]
K_s	weight based vapor-liquid equilibrium constant [–]
k_L	liquid-phase mass transfer coefficient [$m\ s^{-1}$]
p	pressure [Pa]
$q_{G,z}$	cross-sectionally averaged heat transfer term [$J\ kg^{-1}\ s^{-1}$]
Q	total flowrate [$m^3\ s^{-1}$]
r_{CO}	reaction rate of CO [$kmole\ s^{-1}(kg\ cat)^{-1}$]
S_m	source term due to coalescence and breakage in the equation of change for mass [$kg\ m^{-1}\ m^{-3}\ s^{-1}$]
$S_m\omega_s$	source term due to coalescence and breakage in the equation of change for species mass [$kg\ m^{-1}\ m^{-3}\ s^{-1}$]
$S_m v_z$	source term due to coalescence and breakage in the equation of change for momentum [$kg\ m^{-3}\ s^{-2}$]
$S_m h$	source term due to coalescence and breakage in the equation of change for momentum [$J\ m^{-3}\ m^{-1}$]
t	time [s]
T	temperature [K]
u_{rel}	relative velocity [$m\ s^{-1}$]
V	volume of bubble [m^3]
v_L	cross-sectionally averaged liquid velocity [$m\ s^{-1}$]
v_z	cross-sectionally averaged gas velocity [$m\ s^{-1}$]
v_ξ	growth velocity [$m\ s^{-1}$]
v_t	terminal velocity [$m\ s^{-1}$]
w	wetted perimeter [m]
x_s	mole fraction of s in the liquid phase [–]
z	axial direction [m]

Greek letters

α	volume fraction [–]
α	product distribution parameter [–]
γ	size-dependent mass transfer term [s^{-1}]
γ_s	size-dependent mass transfer term for species s [s^{-1}]
Γ_s	mass transfer term for species s [$kg\ m^{-3}\ s^{-1}$]
ϵ	turbulent dissipation rate [$m^2\ s^{-3}$]
η	Kolmogorov scale [–]
$\lambda_{G,z,\text{eff}}$	effective turbulent conductivity in spatial space [$W\ m^{-1}\ K^{-1}$]
μ	viscosity [Pa s]
$\mu_{G,z,\text{eff}}$	cross-sectionally averaged effective (and turbulent) viscosity for the gas phase [$kg\ m^{-1}\ s^{-1}$]
ν	kinematic viscosity [$m^2\ s$]
ξ	bubble diameter [m]
σ	standard deviation for the inlet distribution of $f_{d,\text{in}}$. $\sigma = 10 \times 10^{-4}$ [–]
σ_{G-L}	gas-liquid surface tension [$N\ m^{-1}$]
ϕ_S	weight fraction solids in gas-free slurry [–]
ψ_S	volume fraction solids in gas-free slurry [–]
ρ	density [$kg\ m^{-3}$]
$\omega_{G,s}$	mass fraction of species s in the gas phase [–]
$\omega_{L,s}$	mass fraction of species s in the liquid phase [–]

Subscripts

b	bubble
c	continuous
d	dispersed
eff	effective
G	gas phase
$G-L$	gas-liquid
in	inlet
L	liquid phase
L	integral scale
max	maximum
min	minimum
s	species s
S	solid phase
SL	slurry phase
t	terminal
z	axial (z) direction
λ	Taylor scale

Superscripts

$*$	at the interface
0	at the inlet
s	superficial

Abbreviations

BC	bubble column
FTS	Fischer-Tropsch synthesis
ID	inner diameter
PBE	population balance equation
PBM	population balance model
SBC	slurry bubble column
SMD	Sauter-mean diameter

conversion rates (Imhof and van der Waal, 2013). In this work a conventional 25 wt%Co/Al_2O_3 catalyst is applied. The kinetic model by Yates and Satterfield (1991) was applied in this study, given as:

$$-r_{CO} = \frac{a p_{CO} p_{H_2}}{(1 + b p_{CO})} \tag{2}$$

where p_{CO} and p_{H_2} are the partial pressures of CO and H_2 and a and b are temperature-dependent kinetic parameters. Eq. (2) was re-written into liquid concentrations by reformulating the partial pressures in terms of liquid concentrations by use of a Henry's law constant (as in e.g. Sehabiague et al. (2008) and Troshko and Zdravistch (2009)) to obtain for Eq. (2):

$$-r_{CO} = \frac{a K_{H_2} x_{H_2} K_{CO} x_{CO} p^2}{(1 + b K_{H_2} x_{H_2} p)} \tag{3}$$

where p is pressure, K_s is the constant for species s and x_s is the liquid mole fraction of species s. Values for K_s were calculated by means of Aspen HYSYS.