

Mathematical simulations of the performance of trickle bed and slurry reactors for methanol synthesis

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Abstract

Three- and two-phase reactor models were developed to simulate the performance of trickle bed and slurry reactors for methanol synthesis. The combination of orthogonal collocation and quasi-linearization was used to solve the trickle bed reactor model incorporating resistance to interparticle and intraparticle diffusion and resistance to mass transfer between gas and liquid phases. Model parameters were estimated independently from either published correlations or literature data. The model predicts significant resistance to intraparticle diffusion on the performance of trickle bed reactors. However, comparisons between pilot size trickle bed and slurry reactors illustrate the superior performance of trickle bed reactors over the slurry reactors for methanol synthesis even with diffusion limitations.

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1. Introduction

Methanol has been widely used as a basic feed-stock in many chemical processes. It is used as a fuel additive and it is the starting chemical for producing formaldehyde and other solvents. Moreover, it is a key reactant for synthesis of methyl tertiary butyl ether (MTBE), which was a favored gasoline additive for reducing air pollution, but problems developed with its use because of water pollution. With the increasing concern over the environment, the demand for methanol will increase significantly in the near future as a result of increasing pressure to convert methane to liquid fuels and to produce olefins from methanol. Methanol may also be converted to a synthetic fuel by the methanol-to-gasoline (MTG) process employing a ZSM-5 catalyst (Satterfield, 1991). In addition, it might be used potentially as a cleaner and more reliable

fuel than the petroleum-based fuel for the future (Boutacoff, 1989; Gray & Alson, 1989).

Since the 1960s, most methanol has been produced in low-pressure processes, typically 240–260 °C and 5–10 MPa, from natural-gas-based synthesis gas consisting of hydrogen and carbon monoxide using gas-phase fixed-bed reactors (GPFBR) (Satterfield, 1991). However, because of the highly exothermic nature of the synthesis reactions, heat dissipation has been a bottle-neck in the reactor design, and the reactor configuration has tended to be complicated. Furthermore, GPFBRs are unsuitable for direct use of coal-derived synthesis gas that has a low hydrogen to carbon ratio because of the deposition of coke (Stiles et al., 1991).

To overcome the problems associated with GPFBRs, many reactor designs have been proposed (Kuczynski, Oyevaar, Pieters, & Westerterp, 1987; Satterfield, 1991; Westerterp, Bodewes, Vrijland, & Kuczynski, 1988; Westerterp, Kuczynski, & Kamphuis, 1989). In 1980s, people introduced slurry reactors for methanol synthesis (Frank, 1980; Frank & Mednick, 1982; Graaf, 1988; Weimer, Terry, & Stepanoff, 1987). Recently, Pass, Holzhauser, Akgerman, and Anthony (1990) and Tjandra, Anthony, and Akgerman (1993) investi-

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✱ The late Professor Akgerman made significant contributions to this work.

Nomenclature

a_v	packing external surface area (m^{-1})
c_{pg}	gas average heat capacity ($\text{J}/(\text{mol K})$)
c_{pl}	liquid average heat capacity ($\text{J}/(\text{mol K})$)
$C_{g,i}$	concentration of component i in gas phase (mol/m^3)
C_l	total liquid concentration (mol/m^3)
$C_{l,i}$	concentration of component i in liquid phase (mol/m^3)
$C_{s,i}$	concentration of component i in solid phase (mol/m^3)
d_h	Krischer and Kast hydraulic diameter, $d_p(16\varepsilon_b^3/(9\pi(1-\varepsilon_b)^2))^{1/3}$ (m)
d_p	particle diameter (m)
d_r	reactor diameter (m)
$D_{e,i}$	effective diffusion coefficient of component i in liquid phase (m^2/s)
D_i	molecular diffusion coefficient of component i in liquid phase (m^2/s)
D_l	axial dispersion coefficient of liquid phase (m^2/s)
f	surface wetting coefficient
F	total mole flow rate in feed (mol/s)
F_g	total gas mole flux ($\text{mol}/(\text{m}^2 \text{ s})$)
$F_{g,i}$	mole flux of component i in gas phase ($\text{mol}/(\text{s m}^2)$)
Fr_l	liquid Froude number, $a_v G_l^2/(\rho_l^2 g)$
Fr'_l	modified liquid Froude number, $u_l^2/(h_l^2 d_p g)$
g	gravity acceleration (m/s^2)
G_g	gas mass velocity ($\text{kg}/(\text{m}^2 \text{ s})$)
G_l	liquid mass velocity ($\text{kg}/(\text{m}^2 \text{ s})$)
h_l	liquid hold-up
h_w	overall wall heat transfer coefficient ($\text{J}/(\text{m}^2 \text{ s K})$)
H_i	dimensionless Henry's constant of component i
H'_i	Henry's constant of component i (MPa l/mol)
$(-\Delta H)_I$	heat of reaction for the CO hydrogenation to CH_3OH reaction (J/mol)
$(-\Delta H)_{II}$	heat of reaction for the water gas shift reaction (J/mol)
$k_{gs,i}$	gas–solid mass transfer coefficient of component i (m/s^{-1})
$k_{ls,i}$	liquid–solid mass transfer coefficient of component i (m/s^{-1})
$(ka)_{gl,i}$	gas–liquid volumetric mass transfer coefficient of component i (s^{-1})
$(ka)_{gs,i}$	gas–solid volumetric mass transfer coefficient of component i (s^{-1})
$(ka)_{ls,i}$	liquid–solid volumetric mass transfer coefficient of component i (s^{-1})
K_{II}	equilibrium constant for the water gas shift reaction

K_i	phase equilibrium constant of component i
L	total length of reactor (m)
M	total number of interior collocation nodes for catalyst particle
M_w	average molecular weight (kg/mol)
N	total number of interior collocation nodes for reactor
p_i	partial pressure of component i (MPa or atm)
P	pressure (Pa)
Pe_l	liquid Peclet number based on reactor length, $u_l L/D_l$
Pe'_l	modified liquid Peclet number based on particle diameter, $u_l d_p/h_l D_l$
Pr'''_l	modified liquid Prandtl number, $c_{pl} \mu_l/\lambda_l$
r	radius of catalyst particle (m)
r_I	reaction rate of the CO hydrogenation to CH_3OH reaction ($\text{mol}/(\text{kg h})$)
r_{II}	reaction rate of the water gas shift reaction ($\text{mol}/(\text{kg h})$)
$r_{g,i}$	radius of gyration of component i (\AA)
R	gas constant ($\text{J}/(\text{mol K})$)
Re_l	liquid Reynolds number based on particle diameter, $G_l d_p/\mu_l$
Re'''_l	modified liquid Reynolds number based on particle diameter, $u_l \rho_l d_p/(\varepsilon_b \beta)$
R_p	total radius of catalyst particle (m)
$Sc_{l,i}$	liquid Schmidt number, $\mu_l/(\rho_l D_i)$
$Sh^*_{l,i}$	modified liquid Sherwood number of component i , $(ka)_{gl,i} d_h^2/D_i$
SV	gas phase space velocity (at standard condition) (h^{-1})
T	temperature (K)
T_{ref}	reference temperature (K)
T_w	wall temperature (K)
u_g	gas superficial velocity (m/s)
u_l	liquid superficial velocity (m/s)
V	vapor mole flow rate in effluent (mol/h)
w_{cat}	catalyst loading (kg)
We_l	liquid Weber number, $G_l^2 d_p/(\rho_l \sigma_1 a_v)$
We'''_l	modified liquid Weber number, $G_l^2/(\rho_l \sigma_1)$
x_i	liquid mole fraction of component i
X_g	modified liquid Lockhart–Martinelli parameter, $G_g/G_l(\rho_l/\rho_g)^{0.5}$
z	reactor length (m)

Greek symbols

β	liquid saturation of bed voidage
ε_b	void fraction of reactor
ε_p	particle porosity
λ_l	liquid thermal conductivity ($\text{J}/(\text{m s K})$)
μ_g	gas viscosity (Pa s)
μ_l	liquid viscosity (Pa s)
$\nu_{j,i}$	stoichiometric coefficient of component i for reaction j

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