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DESIGN OF SLURRY REACTOR FOR INDIRECT LIQUEFACTION APPLICATIONS: QUARTERLY TECHNICAL STATUS REPORT, APRIL--JUNE 1991

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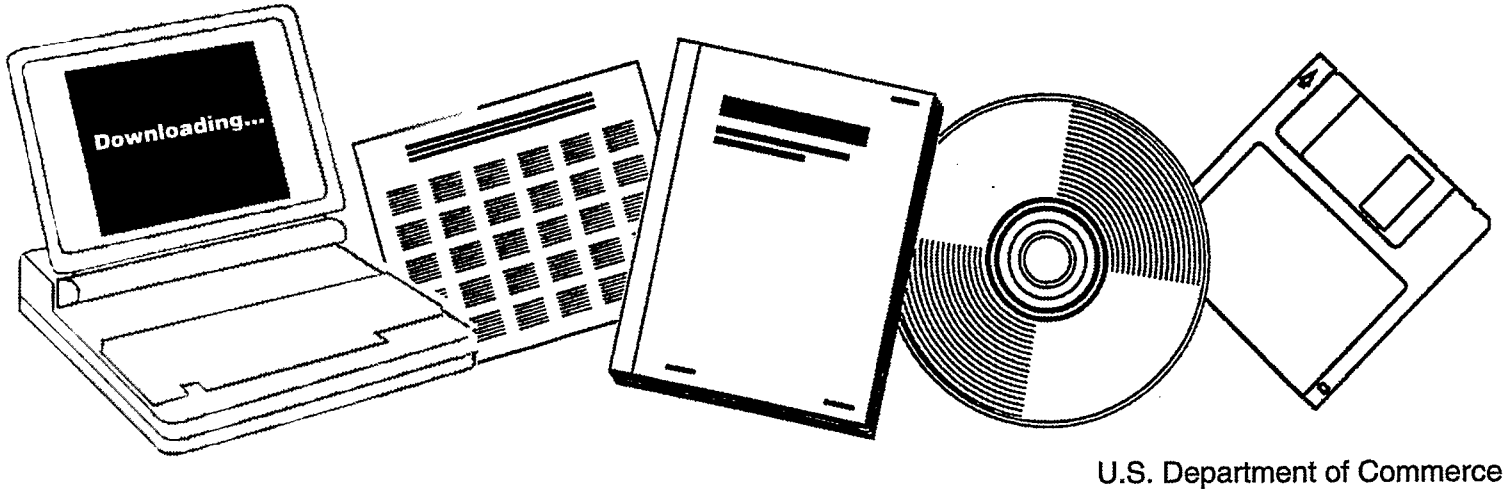

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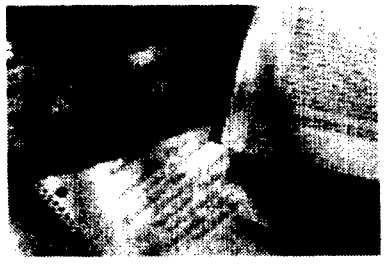

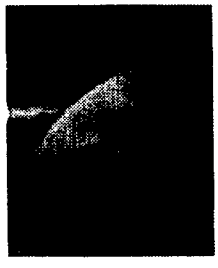

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Introduction

The objective of this project is to design a conceptual slurry reactor for two indirect liquefaction applications;production of methanol and production of hydrocarbon fuels via Fischer-Tropsch route. The work will be accomplished by the formulation of reactor models for both the processes and use computer simulation. Process data, kinetic and thermodynamic data, heat and mass transfer data and hydrodynamic data will be used in the mathematical models to describe the slurry reactor for each of the two processes. The cost of current vapor phase reactor systems will be compared with cost estimated for the slurry reactor systems. For the vapor phase systems, upstream and downstream processing equipments may have to be included during cost analysis for a meaningful cost comparison.

Finally, we will point out any inadequacies in the technical database currently available for a commercial design of the slurry reactor and identify research needs to improve upon the slurry reactor design. Assumptions used in the design will be documented.

Project Status

During this month, work was performed in the following areas

- Mathematical description and formulation of reactor model for FT synthesis reactor.
- Selection of correlations/models for model parameters estimation.
- Phase equilibria calculations for FT products.
- Development and testing of computer codes.

MASTER

Fischer-Tropsch Synthesis:

For FT synthesis reactor design, the problem has been divided into two parts.

1) Estimation of syn gas conversion in a given reactor volume.

2) Detailed calculation of compositions of vapor and liquid product streams based on phase equilibria.

Reactor Model

The development of a reactor model starts with writing the differential mass and energy balance equations. The resulting differential equations can then be solved using suitable boundary conditions. Given the large number of products formed during FT synthesis, it is not practical to make individual component balance. For design purposes, however, some products can be grouped together without significant loss of accuracy. The reactor design configuration and its operating conditions also allow for some simplifying assumptions to be made.

The following assumptions were made for the development of FT synthesis reactor model.

Assumptions for FT reactor model:

1) The synthesis products obey Schulz-Flory distribution. This assumption has been found to be valid over the entire range of products of an iron catalyst (Satterfield and Huff, 1982).

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$$m_n = \alpha m_{n-1} = \alpha^{n-1} m_1 \quad (1)$$

Here, m_n refers to the product distribution as formed on the catalyst. The probability of chain growth α is taken to be constant over the entire carbon distribution.

2) The products consist only of n-alkanes. These are in fact the main products of catalysts and little design error is introduced by lumping the methyl branched isomers and n-alkenes with the n-alkanes.

3) For gas flow calculation along the reactor, component balance is performed only for i) CO, ii) H_2, iii) CO_2, iv) H_2O and v) C_1 to C_3 hydrocarbons. The contribution of hydrocarbons heavier than C_3 is estimated to be less than 4% of the gas flow rate in the reactor.

4) The effectiveness factors for the catalyst particles are taken as unity. Due to the relatively small particle sizes (< 50 μm) used in the reactors, diffusional limitations should be negligible.

5) Again, as a consequence of the small particle size, mass and heat transfer resistances between the catalyst and liquid are assumed to be negligible.

6) The gas and slurry phases are modeled using the axial dispersion model, the most appropriate model for bubble column reactors (Deckwer et al., 1983).

7) The catalyst is not uniformly distributed in the reactor and the sedimentation-dispersion model (Cova, 1966; Kato et al., 1972, Smith et.al, 1985) is used for modeling the catalyst concentration.

8) The hydrodynamic parameters, namely gas holdup, interfacial area, heat and mass transfer coefficients and dispersion coefficients are assumed to be spatially independent.

9) The temperature dependence of the gas phase concentration $C_G = P/RT$ can be neglected since

$$d(1/T)dz = -1/T^2(dT/dz) \sim 0$$

10) Steady-state conditions prevail

Model Equations:

Based on the above assumptions, mass and energy balance were developed for the reactor model. Component balance were made for the following components. Definitions of the variables, coefficients and dimensionless groups are given in the Notation.

1) CO

2) H_2

3) CO_2

4) H_2O

5) C_1 to C_3

Gas Phase Mass Balance:

The gas phase mass balance with axial dispersion for component i can be written as:

$$\frac{1}{Pe_G}\frac{d^2y_i}{dz^2} - \frac{d(vy_i)}{dx} - (St_{G,i})(y_i - x_i) = 0 \qquad (2)$$

subject to the following boundary conditions:

$$vy_i - \frac{1}{Pe_G}\frac{dy_i}{dz} = y_{i,o} \qquad at\ z=0 \qquad (3)$$

$$\frac{dy_i}{dz} = 0 \qquad at\ z=1 \qquad (4)$$

The molar flow rate of gas will vary along the column due to reaction. The effect of change in molar flow rate on the superficial gas velocity can be determined by writing an overall mass balance. Thus

$$-\frac{dv}{dz} - \Sigma\, St_{G,i}(y_i - x_i) = 0 \qquad (5)$$

The above equation is subject to the boundary condition

$$v = 1 \qquad at\ z = 0 \qquad (6)$$

The volumetric flow rate of the gas will also vary along the column due to change in hydrostatic head. The local pressure along the column is given as

$$P(z) = P_T\,[1+\omega(1-z)] \qquad (7)$$

where

$$\omega = \rho_{SL} g(1-e_g) L/P_T \qquad (8)$$

Liquid Phase Mass Balance:

The liquid phase mass balance for component i can be written as:

$$\frac{1}{Pe_L}\frac{d^2x_i}{dz^2} - \frac{dx_i}{dz} + St_{L,i}(y_i - x_i) + \Sigma\theta_{i,k}(1-e_g)C_{cat,k}(H_i L/PU_L) = 0 \qquad (9)$$

subject to the following boundary conditions:

$$-\frac{1}{Pe_L}\frac{dx_i}{dz} + x_i = x_{i,o} \qquad at\ z=0 \qquad (10)$$

$$dx_i/dz = 0 \qquad at\ z = 1 \qquad (11)$$

Solid Phase Mass Balance:

The axial distribution of catalyst is governed by gravitational settling and axial dispersion due to agitation of the catalyst slurry by the gas flow. From assumption (vi) the volume fraction of the liquid is constant along the column length and hence the mass balance on catalyst can be written as:

$$\frac{1}{Pe_s}\frac{d^2w}{dz^2} + \frac{dw}{dz} = 0 \qquad (12)$$

with boundary conditions:

$$w - 1/Pe_s(dw/dz) = 021 \tag{13}$$

$$w - 1/Pe_s(dw/dz) = 0 \tag{14}$$

$$\int_0^1 w dz = 1 \tag{15}$$

An analytical solution to the above equation is possible and is given below:

$$w = \frac{Pe_s \exp(-Pe_s z)}{[1 - \exp(-Pe_s)]} \tag{16}$$

Model Parameters Estimation:

Gas Holdup

Recently Bukur et al. (1990) investigated hydrodynamics of three-phase slurry Fischer-Tropsch bubble column reactors. Experiments were conducted in both batch bubble column mode and continuous bubble column mode to investigate the effects of solids concentration (0 to 30 wt. %), solid particles type and size (iron oxide and silica particles; 0-5 μm and 22-44 μm). Two types of liquids, namely hydrotreated reactor wax (FT-300) and SASOL reactor wax were used. The operating conditions were generally selected to closely simulate slurry bubble column reactors for Fischer-Tropsch synthesis.

Bukur et al. (1990) tested various literature correlations using their experimental data. It was found that correlation of Zheng et al. (1988), Badjugar et al. (1986) and Hughmark (1967) could provide reasonable estimates of gas holdups in slug flow and churn turbulent regimes. It may be pointed out that we selected the correlation of Hughmark (1967) for methanol synthesis reactor simulation based on a test of various literature correlations using the experimental data of Air Products PDU operation. Based on the observation of Bukur et al. (1990), the correlation of Hughmark (1967) could also be used for a Fischer-Tropsch reactor model.

Bukur et al. (1990) also developed a general correlation for gas holdup by combining the data od two-phase studies (Bukur et al., 1987a,b) and three-phase studies. This correlation is recommended by the authors for estimation of gas holdups in Fischer-tropsch slurry bubble column reactors operating in slug flow and churn turbulent regime

$$e_G = 0.24 Fr_G^{0.28} Bo^{0.14} \qquad (17)$$

It may be pointed out that Bukur et al. (1990) conducted their experiments at atmospheric pressure, using one gas only, therefore the effect of operating pressure (or gas density) was not incorporated. Moreover, the correlation of Bukur et al. (1990) may not properly account for the effect of solid concentration higher than 30 wt. %. This correlation is being tested against the experimental data of Air Products PDU operation.

Effect of Operating Pressure on Gas Holdup

Recent studies show that gas holdup in bubble columns generally increases with increasing

operating pressure hence gas density (Idogawa et al., 1987; Clark, 1990: Kojima et al., 1991). The influence of pressure has been found to depend on pressure level, distributor type, gas velocity and solids concentration. These results show that a correlation for gas holdup should account for the effect of operating pressure (or gas density). Most of the literature correlations, however, are based on data obtained at atmospheric pressure and usually for one gas as a result these equations do not account for any influence of gas density. In solid-free bubble columns, a few gas holdup equations have been developed based on high pressure operation (Idogawa et al., 1985 and 1987) or experiments using various gases (Reilly et al., 1986; Hammer et al., 1984). There is, however, a lack of systematic research to investigate the influence of pressure on gas holdup in slurry bubble columns. The limited gas holdup values that have been reported in the literature for slurry bubble columns operating under high pressure are generally relatively high (Brown, 1984; Tarmy et al., 1984; Clark, 1990). Based on available data, it is expected that the influence of gas density in two and three-phase bubble columns will be similar when volume fraction of solids is not high. Available literature correlations are being tested to predict the influence of gas density for Air Products experimental data.

Volumetric Mass Transfer Coeff.

For the methanol synthesis reactor model, the correlation of Nguyen-tien et al. (1985) was selected for the estimation of volumetric mass transfer coefficient

$$k_{La}=0.39(1-\epsilon_{s,slurry}/0.58)U_g^{0.67} \qquad (18)$$

Nigam and Schumpe (1987), however, observed that for slurry bubble columns with batch

operation of the liquid phase, the mean solid fraction ($e_{s,sus}$) should be replaced by solid fraction at the reactor bottom ($e_{s,0}$).

Gas-liquid mass transfer in suspensions of fine particles (<10μm) was also measured by Schumpe et al. (1987). The suggested correlation by these authors accounts for the effects of solids in the pseudo-plastic suspensions by an effective viscosity term (μ_{eff}).

$$k_{la}=0.042U_g^{0.82}\mu_{eff}^{-0.39} \tag{19}$$

Here

$$\mu_{eff}=k\gamma_{eff}^{n-1} \tag{20}$$

The effective shear rate γ_{eff} can be calculated from a relation suggested by Nishikawa et al. (1977).

$$\gamma_{eff}=CU_g \tag{21}$$

Schumpe and Deckwer (1987) suggested the coefficient C=2800 m^{-1} based on k_la measurements in various pseudoplastic liquids (1>n>0.18).

Although the correlation of Schumpe et al. (1987) is based on a large set of data, it requires the knowledge of fluid consistency index (k) and flow behavior index (n) for the slurry. This information may be difficult to obtain at reactor conditions. This correlation can be useful if μ_{eff} can be calculated by a suitable correlation for the given system.

Development of Computer Codes:

The model equations for the Fischer-Tropsch synthesis reactor constitute a set of coupled second-order non-linear differential equations. These equations are not amenable to an analytical solution and therefore, a numerical method was selected for solution. Orthogonal collocation techniques are particularly suitable for the solution of boundary value problems and the software package, COLSYS, developed by Ascher et al. (1981) was selected for the numerical solution of the model equations. This method is based on spline collocation at Gaussian points using a B-spline basis. Approximate solutions are computed on a sequence of automatically selected meshes until a user-specified set of tolerances is satisfied.

Computer codes for the reactor model are being developed with a modular approach to computer programming, to ensure easy modifications by the user. Standard FORTRAN 77 is being used for writing the codes since this will ensure transfer to other compatible systems.

Vapor-Liquid Equilibrium Calculations in Fischer-Tropsch Synthesis:

The major constituents of the products from Fischer-Tropsch synthesis are the hydrocarbons ranging from methane to high melting paraffins with relatively small quantities of olefinic compounds. For iron catalyst, carbon dioxide is one of the major products formed with relatively small amounts of product water. In the case of cobalt catalyst, however, due to its poor activity for water gas shift reaction, water will be the major byproduct with relatively small amount of carbon dioxide. Small quantities of other byproducts such as alcohols, aldehydes, ketones etc.

are also formed. Straight-chain paraffins along with some 2-methylated branched paraffins predominate among the saturated hydrocarbons; major olefins are terminal olefins.

The products and the unreacted synthesis gas leaving the top of the slurry reactor will be assumed to be in equilibrium with the liquid phase in the reactor. A computer program has been developed to study the phase equilibria of the vapor and the liquid streams leaving the slurry reactor. Such information will be helpful in determining the relative flow rates and the composition of vapor and liquid streams which can be further used in the process design of the downstream units in the Fischer-Tropsch Plant. The conversion and the production yields from the slurry reactor model will be used to determine the overall composition for the phase equilibrium calculations. The problem presented here is identical with that of determining vapor and liquid compositions in a multi-component flash separation. Following assumptions will be made regarding the products formed during the reaction. The hydrocarbon products consists of only n-alkanes. These are, in fact, the main products for many of the FT catalyst and little design error will be introduced by lumping the methyl-branched isomers and n-alkenes with the n-alkanes. In the lower oxygenates, ketones and primary alcohols are formed in relatively small amounts as compared to water and hence these compounds will be lumped with water. The light hydrocarbons (C_5 to C_{11}) will be lumped together; heavy hydrocarbons (C_{12} to C_{15}) will be lumped together and hydrocarbons C_{16} and heavier will be considered as the slurry reactor wax with an average composition of C_{40} paraffin. The olefin to paraffin split of the hydrocarbon products can be obtained from the literature. For example, unreacted synthesis gas and reaction products from the Mobil's pilot plant for Fischer-Tropsch synthesis may be characterized into following fourteen components:

Component No.	Component(s)
1	Carbon Dioxide
2	Water + Ketones & Primary Alcohols (Acetone & 1-Propanol)
3	Hydrogen
4	Carbon Monoxide
5	Methane
6	Ethylene
7	Ethane
8	Propylene
9	n-Propane
10	Butylene
11	n-Butane
12	C_5 to C_{11} Light Hydrocarbons Lumped as n-Octane
13	C_{12} to C_{15} Heavy Hydrocarbons as n-Tridecane
14	C_{16} and Heavier as Slurry Reactor Wax (C_{40} Paraffin)

Phase Equilibrium Calculations for Multicomponent Vapor-Liquid Phase Equilibria:

A technique has been presented by Bendale, 1991, to predict multicomponent vapor-liquid equilibria from the optimized binary interaction parameters obtained from the Peng-Robinson equation of state, which is given as:

$$P = \frac{RT}{(V - b_{mix})} - \frac{a_{mix}}{V(V + b_{mix}) + b_{mix}(V - b_{mix})} \tag{22}$$

For a multicomponent mixture, the parameters a_{mix} and b_{mix} are given by the following expressions:

$$a_{mix} = \sum_i \sum_j x_i x_j \sqrt{a_i a_j} (1 - \delta_{ij}) \tag{23}$$

$$b_{mix} = \sum_i x_i b_i \tag{24}$$

In the above equation, δ_{ij} is defined as an interaction parameter that describes the deviation of parameter a_{mix} from the geometric mean of the pure component parameters a_i and a_j and is assumed to be constant. The pure component parameters a_i and b_i are given as:

$$a_i = a(T_c)\, \alpha(T_r, \omega) \tag{25}$$

$$a(T_c) = 0.45724\, (R^2 T_c^2 / P_c) \tag{26}$$

$$\alpha(T_r, \omega) = [1 + \kappa (1 - \sqrt{T_r})]^2 \tag{27}$$

$$\kappa = C_a (0.37464 + 1.54226\,\omega - 0.26992\,\omega^2) \tag{28}$$

If ω is greater than 0.5, then

$$\kappa = C_a (0.379642 + 1.48503\,\omega - 0.164423\,\omega^2 + 0.016666\,\omega^3) \tag{29}$$

$$b_i = C_b [0.0778\, (RT_c / P_c)] \tag{30}$$

The optimized values of correction factors C_a and C_b for pure components are evaluated which minimize the sum of absolute relative errors of calculated and experimental saturated vapor

pressure and saturated liquid density. The values of these correction factors approach unity for small molecules and non-polar gases which the Peng-Robinson equation of state is known to model accurately. If these values are not available, then the default values are assigned as unity. The expression for the fugacity coefficient obtained from the evaluation of the following equation,

$$RT\ln\Phi_i = \int_V^{\infty}[(\frac{\partial P}{\partial n_i}) - \frac{RT}{V}]\,dV - RT\ln Z \tag{31}$$

is given as:

$$\ln\Phi_i = \frac{b_i}{b_{mix}}(Z-1) - \ln(Z-B) + [\frac{\sum_k x_k(a_{ik}+a_{ki})}{a_{mix}} - \frac{b_i}{b_{mix}}] \times \frac{a_{mix}}{2.414bRT}\ln[\frac{Z-0.414B}{Z+2.414B}] \tag{32}$$

$$B = \frac{b_{mix}P}{RT} \tag{33}$$

Phase equilibrium calculations are performed at constant temperature and pressure and known overall composition to determine the flow rates and compositions of vapor and liquid streams. The governing equations include overall and component material balances, mole fraction constraints, and thermodynamic equilibrium criterion of equal fugacities of each component in each phase. For an N component system at constant temperature and pressure, there will be 2N independent expressions for these components equilibrated in two phases, with 2N unknowns, L, V, x_i's and y_i's, respectively.

On the basis of one mole of mixture F (unreacted reactants and products formed), an overall material balance and a component balance for each component can be represented as follows: with the following constraints:

$$L + V = F = 1 \tag{34}$$

$$\sum_i z_i = \sum_i x_i = \sum_i y_i = 1, \qquad i = 1 \text{ to } N \tag{36}$$

and thermodynamic criteria,

$$f_i^V = f_i^L \quad or \quad \phi_i^V y_i P = \phi_i^L x_i P \quad or \quad \phi_i^V y_i = \phi_i^L x_i, \quad i = 1 \text{ to } N \tag{37}$$

To perform Flash calculations, temperature T and pressure P are considered as the known variables, which are used to calculate the unknown mole fractions x_i's and y_i's of the iiquid and vapor phases, respectively. In addition to system temperature and pressure, the input data required consists of critical temperature, critical pressure and acentric factor of each component as well as the optimized binary interaction parameters, δ_{ij} as applied to the Peng-Robinson equation of state. The liquid and vapor phase fugacity coefficients for each component can be readily calculated from the expression 11. The set of equations 13, 14, 15 and 16 are solved simultaneously to determine the flow rates and mole fractions of liquid and vapor streams.

NOMENCLATURE

a	gas-liquid interfacial area, m^{-1}
a_{mix}	Peng-Robinson attractive parameter for mixture [atm cm^6 / $gmole^2$
a_i	Peng-Robinson attractive parameter for component i [atm cm^6 / $gmole^2$]
b_{mix}	Peng-Robinson repulsive parameter for mixture [cm^3 / gmole]
b_i	Peng-Robinson repulsive parameter for component i [cm^3 / gmole]
C	coefficient in Equation 21
C_a, C_b	Correction factors in the Peng-Robinson EOS
C_{cat}	catalyst concentration, gm/cc slurry
$C_{ct,avg}$	average catalyst concentration, kg/m^3 slurry
$C_{G,i}$	gas-phase concentration of component i, $kmol/m^3$
$C_{L,i}$	liquid-phase concentration of component i, $kmol/m^3$
C_G	total gas-phase concentration, $kmol/m^3$
C_P	heat capacity, kJ/kg.K
D_G	gas-phase dispersion coefficient, m^2/s
D_L	liquid-phase dispersion coefficient, m^2/s
D_S	solid-phase dispersion coefficient, m^2/s
F	Moles in feed in flash calculations
f_i^V	Fugacity of component i in vapor phase [atm]
f_i^L	Fugacity of component i in liquid phase [atm]
H_i	Henry's constant for component i, $atm.m^3/kmol$
k	fluid consistency index, $Pa.s^n$
$k_{L,i}$	liquid-side mass transfer coefficient for component i,

L	reactor length, m in reactor model or moles of liquid phase in flash calculations
m_i	solubility coefficient for component i, $(mol/m^3)_G/(mol/m^3)_L$
m_n	mole fraction of hydrocarbon products with carbon number n
n	flow behaviour index
P	Reaction Pressure [atm]
P_c	Critical pressure [atm]
P_{ri}	Reduced pressure of component i
P_T	pressure at reactor top, atm
R	universal gas constant, 0.082 m^3-atm/kmole/K
r_k	reaction rate for kth reaction, kmol/kg.s
T	Reaction temperature [K]
T_c	Critical temperature [K]
T_{ri}	Reduced temperature of component i
T_w	reactor wall temperature, K
U_G	gas superficial velocity, m/s
U_{Go}	inlet gas superficial velocity, m/s
U_L	liquid superficial velocity, m/s
U_S	settling velocity of catalyst particles in swarm, m/s
v	dimensionless gas-phase superficial velocity (U_G/U_{GO})
V	Moles of vapor in flash calculations
w	dimensionless catalyst concentration
x_i	dimensionless liquid-phase concentration of component i ($C_{L_i}H_i/P$) in slurry reactor model or mole fraction of component i in liquid phase in flash calculations
y_i	mole fraction of component i in the vapor (or gas) phase

z	dimensionless axial distance (x/L)
z_i	Overall Mole fraction of component i in feed in flash calculations
Z	Compressibility factor of the liquid or vapor phase

Dimensionless Numbers

Bo : Bond number ($D_c^2 \rho_{SL} g/\sigma_L$)

Fr_G : Froude number for gas (U_G^2/gD_c)

Pe_G : gas-phase Peclet number ($U_{Go}L/D_G e_G$)

Pe_L : liquid-phase Peclet number ($U_L L/D_L e_L$)

Pe_S : solid-phase Peclet number [$(U_S - U_L/e_L)(L/D_S)$]

St_G : gas-phase Stanton number ($K_{L,i}aL/U_{Go}$)

$St_{L,i}$: liquid-phase Stanton number for component i ($K_{L,i}aL/U_L$)

Greek Letters

δ_{ij}	Binary interaction parameter in Peng-Robinson EOS with one-parameter mixing rule
Φ_i^v	Fugacity coefficient of component i in vapor phase [atm]
ϕ_i^L	Fugacity coefficient of component i in liquid phase [atm]
ω	Accentric factor
θ_{ik}	stoichiometric coefficient of component i in reaction k
e_G	gas holdup
e_L	liquid holdup
$e_{s,o}$	volume fraction of solids at reactor bottom
$e_{s,sus}$	average volume fraction of solids in reactor

ρ_L	density of the liquid phase, kg/m^3
ρ_{SL}	density of slurry, kg/m^3
ω	ratio of hydrostatic pressure to the head pressure
α	probability of chain growth
μ_{eff}	effective viscosity of suspension, Pa.s
γ_{eff}	effective shear rate s^{-1}

Subscripts

L	liquid phase
G	gas phase
i	component i
k	kth reaction
o	inlet condition
S	solid phase

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