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ON

HYDRODYNAMIC MODELS FOR SLURRY

BUBBLE COLUMN REACTORS

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HYDRODYNAMIC MODELS FOR SLURRY BUBBLE COLUMN REACTORS

ABSTRACT

The objective of this investigation is to convert our "learning gas-solid-liquid" fluidization model into a predictive design model. The IIT hydrodynamic model computes the phase velocities and the volume fractions of gas, liquid and particulate phase. Model verification involves a comparison of these computed velocities and volume fractions to experimental values.

This report presents the Ph.D. thesis of Mr. Y. Wu. All but a small fraction of his thesis dealt with the work of this project. A summary of his results are as follows.

A hydrodynamic model for multiphase flows, based on the principles of mass conservation, momentum balance and energy conservation for each phase, was developed and applied to model gas-liquid, gas-liquid-solid fluidization and gas-solid-solid separation. To simulate the industrial slurry bubble column reactors, a computer program based on the hydrodynamic model was written with modules for chemical reactions (e.g. the synthesis of methanol), phase changes and heat exchangers. Also the kinetic theory was programmed to compute the viscosity of the solid phase.

In the simulations of gas-liquid two phases flow system, the gas hold-ups, computed with a variety of operating conditions such as temperature, pressure, gas and liquid velocities, agree well with the measurements obtained at Air Products' pilot plant. The hydrodynamic model has more flexible features than the previous empirical correlations in predicting the gas hold-up of gas-liquid two-phase flow systems.

In the simulations of gas-liquid-solid bubble column reactors with and without slurry circulation, the code computes volume fractions, temperatures and velocity distributions for the gas, the liquid and the solid phases, as well as concentration distributions for the species (CO, H_2, CH_3OH, ...), after startup from a certain initial state. A kinetic theory approach is used to compute a solid viscosity due to particle collisions. Solid motion and gas-liquid-solid mixing are observed on a color PCSHOW movie made from computed time series data. The steady state and time average catalyst concentration profiles, the slurry height and the rates of methanol production agree well with the measurements obtained at an Air Products' pilot plant. The temperature movie shows heat transfer behavior of the internal heat exchangers. The simulations may be useful as a guide for industrial reactor design such as for determining reactor size, distributor design, positions of heat exchangers, mixing type, and erosion of heat exchanger tubes.

SIMULATION OF METHANOL SYNTHESIS

IN SLURRY BUBBLE COLUMN REACTORS

BY

YUANXIANG WU

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requirements for the degree of
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Approved _____
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Y. W.

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LIST OF SYMBOLS

Symbol	Definition
A	coefficient matrix
a	interfacial area per unit volume (cm^2/cm^3)
B	coefficient matrix
C_D	drag coefficient
C_j^{ℓ}	concentration of j in bulk liquid phase
$C_j^{g-\ell}$	concentration of j in g-l interface
C_k	fluctuating velocity of particle
C_{pg}	specific heat of gas
C_{pk}	specific heat of phase k
d_k	diameter of solid particle or liquid droplet
e_k	restitution coefficient of phase k
F_g	forces acting on gas phase
F_k	forces acting on phase k
E	strength of electric field
f_j	fugacity of j
H_j	Henry's constant of j
H_g	enthalpy of gas
H_k	enthalpy of phase k
h_{vk}	gas-phase k heat transfer coefficient
G( )	solid compressive stress modules
g	gravity acceleration
g_{0k}	radial distribution of phase k
[I]	unit tensor
K_{eq}	reaction equilibrium constant
K_r	reaction kinetic coefficient
$K_{j\ell}$	mass transfer coefficient of j in liquid phase
k_g	thermal conductivity of gas

Symbol	Definition
k_k	thermal conductivity of phase k
k_g^0	mean thermal conductivity of gas
k_k^0	mean thermal conductivity of phase k
k_k^*	effective thermal conductivity of phase k
M^j	molecular weight of j
$\overline{M}_g$	average gas molecular weight
M_k	number of reactions in phase k
$\dot{m}_k$	rate of generation of phase k
N	total number species
Nu_k	Nusselt number
P_g	gas pressure
P_k	pressure of phase k
Pr	Prandtl number
q_k	surface charge of phase k
r_{ik}	rate of ith reaction in phase k
R	gas constant
R_k^j	rate of mass transfer, j specie in phase k
Re_k	Reynolds number
T	temperature
T_g	gas temperature
T_k	temperature of phase k
T_g^0	reference gas temperature
T_k^0	reference temperature of phase k
u	velocity in x direction
v	velocity in y direction
y_k^j	weight fraction of i in phase k
z	compressible factor

Greek letters:

α_{ik}^j	stoichiometric coefficient of ith reaction in k phaseξ_k

Symbol	Definition
$\beta_{k\ell}$	frictional coefficient between phase k and l
γ_k	collisional energy dissipation
ΔH_{ik}	reaction heat of ith reaction in phase k
ε_k	volume fraction of phase k
Θ	granular temperature
κ_k	conductivity of fluctuating energy
μ_k	viscosity of phase k
ξ_k	bulk viscosity
ρ_k	density of phase k
τ_{ck}	cohesive force
τ_k	shear stress of phase k
Φ_k	energy dissipation
ψ_k	sphericity of particle or droplet

Subscripts:

g, ℓ, s	gas, liquid, solid respectively
i	ith reaction
k	solid or liquid phase

Superscripts

j	species

ABSTRACT

In this study, a hydrodynamic model for multiphase flows, based on the principles of mass conservation, momentum balance and energy conservation for each phase, was developed and applied to model gas-liquid, gas-liquid-solid fluidization and gas-solid-solid separation. To simulate the industrial slurry bubble column reactors, a computer program based on the hydrodynamic model was written with modules for chemical reactions (e.g. the synthesis of methanol), phase changes and heat exchangers. Also the kinetic theory was programmed to compute the viscosity of the solid phase.

The slurry bubble column reactor, a typical multiphase flow system, is used to produce methanol from syn-gas (CO, H_2, ...). The hydrodynamic model was used to simulate the reactor's time-depended dynamic behavior. The code computes volume fractions, temperatures and velocity distributions for the gas, the liquid and the solid phases, as well as concentration distributions for the species (CO, H_2, CH_3OH, ...), after startup from a certain initial state. In this simulation, the gas is treated as a continuous phase while the solid (catalyst) and the liquid (wax) as a dispersed phase. A kinetic theory approach is used to compute a solid viscosity due to particle collisions. Solid motion and gas-liquid-solid mixing are observed on a color PCSHOW movie made from computed time series data. The steady state and time average catalyst concentration profiles and the rate of methanol production agree well with the measurements obtained at an Air Products' pilot plant. The temperature movie shows heat transfer behavior of the internal heat exchangers. The simulations may be useful as a guide for industrial reactor design

such as for determining reactor size, distributor design, positions of heat exchangers, mixing type, and erosion of heat exchanger tubes.

The model was also applied to understand the hydrodynamics of electrostatic separation of pyrites from coal. The model was modified to include an external electric force. The kinetic theory has been applied to predict the viscosities for both solid phases, coal and pyrites. The study showed that pyrites can be removed from coal in an inclined electro-fluidized bed. A series of pictures from simulations show the hydrodynamic behavior, such as solid flow patterns and pyrites concentrations, in the electrostatic separator. This study indicates that dilute feeding results a high coal recovery and leads to an improved design of electrostatic separators.