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OPTIMIZATION OF VARIOUS COAL-CONVERSION SYSTEMS

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Abstract

It is well known that the identification of flow regimes is important in scale-ups and designs of multiphase reactors. Therefore, it is natural that the selections of parameter prediction methods for the reactor models should be based on flow regimes. Very few correlations, theories and models are capable of covering the whole spectrum of flow regimes. Often, accuracy is sacrificed for generality. By concentrating on each individual flow regime and its characteristics, the correlations and models selected can be expected to give better results.

In this period, the evaluation of correlations for phase holdups and liquid dispersion coefficient have been evaluated for both the slurry reactors and the three-phase fluidized bed reactors.

Statement of Work

As the models for process units are the most lacking elements in the proposed project, a substantial portion of the two years' research effort will be devoted to the establishment of unit models. Special attention will be paid to the liquefier as it is the least understood part of the liquefaction process.

Task I

a. Review literature on the hydrodynamics of two-phase flow, and incorporate relevant material to the development of a liquefier unit model.

b. Analyze the effect of coal minerals and other catalysts on the kinetics and mechanism of coal dissolution and hydrogenation.

c. Develop a kinetic and hydrodynamic model of coal dissolution and hydrogenation, and compare the model's predictions with experimental data.

d. Study the effect of the various operating parameters such as temperature, pressure, reactor size and degree of mixing on the performance of the liquefier.

e. Study the transient behavior of the liquefier due to operational changes.

Task II

a. Integrate unit models developed in Task I into process models for the simulation of selected liquefaction processes such as SRC-II and H-Coal.

Slurry Bubble Column Reactor

Physical Properties

Recently, Thurgood, et al. (1982) studied the rheological characteristics of coal liquefaction preheater slurries at high temperature and pressure. They showed that in the range of 400 to 700°K, the coal-solvent slurry (35 wt% coal) was pseudoplastic and can be modeled by a power-law equation. Javdani, et al. (1977) had found that coal slurry behaved like a homogeneous Newtonian liquid up to 27.1 wt% concentration at low temperatures (approx. 20-30°C). Since the experimental data presented by Thurgood et al. more closely resembled the coal liquefaction conditions, non-Newtonian behaviors must be considered and direct applications of the results obtained for gas-liquid two-phase flow may not be possible.

Flow Regime Map

The flow regime map developed by Taitel et al. (1980) and later modified by Knickle and Kirpekar (1982) was used in analyzing the experimental data for gas-liquid flow. Two problems were encountered. First, the demarcation lines sometimes overlapped and judgment had to be used to select which line was correct. Second, the distributor effects were not accounted for in the flow regime map. Literature (Otake, et al. (1981), Deckwer, et al. (1980), Ohki and Inoue (1970)) had shown that at certain orifice diameter, the uniform bubbling regime may be nonexistent or indistinguishable. Therefore, for orifice diameter greater than 0.2 cm, the nonexistence of the uniform bubbling regime was assumed in our analysis.

Evaluation of Parameters

The correlations for gas holdup and liquid axial dispersion coefficients are evaluated based upon the approach presented by Mandhane, et al. (1975). The most appropriate correlations in a given flow regime are selected from the results of the evaluation. Table 1 summarizes the findings.

Reactor Modeling

The model developed by Hatate, et al. (1981) will be used to test the results of the parameter selection. However, dispersion in the gas phase will also be included.

Table 1. Results of the Evaluation for Holdup and Dispersion Coefficients.

	Correlations Recommended	
Flow Regime	Dispersion Coefficient	Gas Holdup
Bubbling	Shah and Deckwer (1982)	Kawagow et al. (1976)
Bubble-Slug Transition	Deckwer et al. (1980)	Mersmann (1978)
Slug	Kato and Nishiwaki (1972)	Kumar (1976)
Churn	Cova (1974)	Hikita et al. (1980

Alvarez-Cuenca, et al. (1980) proposed that there are two regions of mass transfer in the bubble column and Deckwer, et al. (1973) observed zones of different mixing in the bubble column. Therefore, a "two-zone" model is being considered.

Future Work Planned

Numerical solution to the dispersion model will be continued and modifications added as needed. Non-Newtonian behavior will be studied and applicability of gas-liquid studies to the coal slurry systems will be continued.

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B. Three-Phase Fluidization

In the past months, the phase holdups, bubble behavior, dispersion coefficients, mass transfer, heat transfer, and flow regime map have been reviewed. Data and correlations were collected to examine the applicability of correlations. In this period, the pressure drops, expansion and contraction, and flow regimes are reviewed. Phase holdups and dispersion coefficient of liquid phase have been evaluated. Also, the data for mass transfer and heat transfer have been collected.

Pressure Drops

The pressure drop in a three-phase fluidized bed is approximately proportional to the height of the bed.

$$\frac{-dP}{dZ} = (\varepsilon_g \rho_g + \varepsilon_\ell \rho_\ell + \varepsilon_s \rho_s) g$$

Or, in an integrated form

$$\Delta P = L(\varepsilon_g \rho_g + \varepsilon_\ell \rho_\ell + \varepsilon_s \rho_s) g$$

Usually, $\varepsilon_g \rho_g$ can be neglected from the above equations. Dhanuka and Stepanek (1978) compared the measured values of pressure drop and the values evaluated based on the above equation and found the maximum deviation was $\pm$ 4 percent.

Bed Expansion and Contraction

Bed contraction is a unique feature of three-phase fluidization. Many studies have revealed that bed contraction does not occur in beds of relatively large particles, e.g., glass spheres of d_p > 3 mm

(Michelsen and Østergaard, 1970; Dakshinamurty et al., 1971; Kim et al., 1972; Mukherjee et al., 1974). The most up-to-date work on this subject is by Epstein and Nickes (1976). They used the generalized wake model to predict the initial bed expansion or contraction:

$$\left.\frac{d\varepsilon}{dU_g}\right|_{U_g \to 0} > 0 \quad \text{bed expansion}$$

$$\left.\frac{d\varepsilon}{dU_g}\right|_{U_g \to 0} < 0 \quad \text{bed contraction}$$

where

$$\left.\frac{d\varepsilon}{dU_g}\right|_{U_g \to 0} = \frac{[n/(n-1) + k]\,\frac{U_\ell}{\varepsilon_\ell} - [(1+k)U_\ell + k\,\frac{U_{g\ell}}{n-1}]}{[n(n-1)](\frac{U_\ell}{\varepsilon_\ell})(U_\ell/\varepsilon_\ell + U_{g\ell})}$$

Usually, bed contraction is accompanied by bubble coalescence while bed expansion is accompanied by uniform bubbling; when the gas velocity is increased more, the bed reaches the bubble coalescence regime.

Flow Regimes

For the purpose of reactor design, it is necessary to express the state of fluidization in terms of its flow regimes. Although a few research studies are available, flow regimes in three-phase fluidized beds have not been completely investigated (Javdane et al., 1977; Mukherjee et al., 1974; and Muroyama et al., 1978).

Several research studies have found the same flow regions exist as in those of gas-liquid systems. These are: uniform bubbling, bubble coalescence, slug and annular flow regions. For practical operation, the behaviors of the bed in uniform bubbling and bubble coalescence regions are important. In the former case, the gaseous phase forms a uniform dispersion of small bubbles and disintegration of bubbles can occur. On the other hand, bubble coalescence and larger bubble sizes are the characteristics of the latter case.

Darton and Harrison (1975) analyzed these two flow regimes by means of drift flux. Vasalos et al. (1979) observed that transition from uniform bubbling to bubble coalescence flow occurred at higher velocity as the liquid velocity increased. Østergaard (1981) also stated that bubble coalescence dominated at all gas velocities when liquid velocity was below 7 cm/s at 3 mm particle size. In general, higher gas velocities accelerate the bubble coalescence and further increase gives rise to slug formation. At sufficiently high gas flow rate, film or annular flow is obtained.

As observed in liquid-solid fluidization, particles are entrained from the bed when flow rate exceeds the terminal velocity of particles. Increase of gas flow rate may lower this critical liquid flow rate.

Begovich and Watson (1978) analyzed the minimum fluidization velocity of liquid ($U_{\ell mf}$) in three-phase systems. They showed a generalized equation that predicted a decrease in $U_{\ell mf}$ with an increase in gas flow rate. The minimum fluidization velocity of gas at the condition of stagnant liquid was studied by Narayaman et al. (1969).

Based on these results, a rough flow map of three-phase systems is drawn in Figure 1. The scales of both gas and liquid superficial velocities are arbitrary. Point A is obtained from the terminal

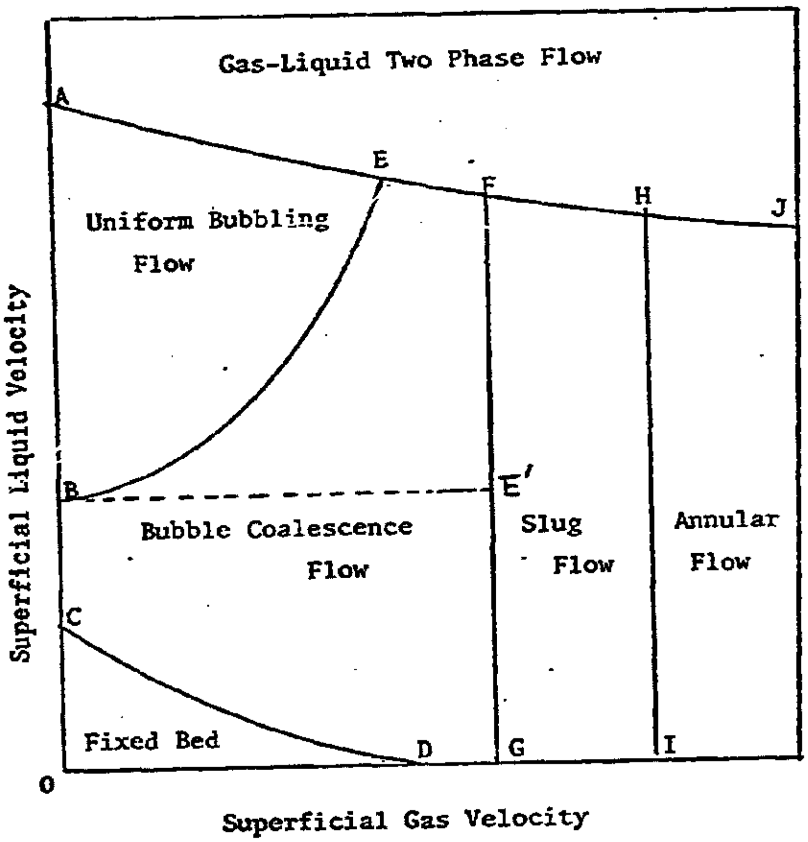

Fig.1 Flow Regime Map in Three Phase Fluidized Bed

velocity of the particle, and point C is calculated using the correlation of Wen and Yu (1966). Point D is given by Narayaman et al. (1969) as stated above. Also, line CD is calculated by the correlation of Begovich and Watson (1978). Lines FG and HI may be nearly straight, like in gas-liquid flow (Taitel et al., 1980). In 6- and 10-cm columns, 10 cm/s is reported for point G by Muroyama et al. (1978). The most difficult to describe is line BE that separates uniform bubbling and the bubble coalescence flow. This is because the particle size affects the bubble flow. Michesen and Østergaard (1970) discovered that small particles tend to promote bubble coalescence while large particles tend to reduce it.

It appears that the line BE may be different for each particle size, but the exact nature of this line is not clear and experimental data concerning flow region transfer are needed. The line BE in Figure 1 represents a general boundary between two regions. Although Muroyama et al. (1978) showed that this boundary is a horizontal line like BE', it is more likely to go upward with an increase in gas flow rate according to the finding by Darton et al. (1975) and Vasalos et al. (1978). For the lines AEJHJ and CD, it is apparent that these lines move upward with increase in particle diameters.

Evaluation of Correlations of Holdups and Phase Mixing

No complete flow regime map has yet been devised. Muroyama et al. (1978) studied three-phase fluidization with glass beads of six different sizes (0.215 - 6.9 mm), alumina beads (2.0 mm), and Raschig rings (5.2 mm) in columns of 6 cm and 10 cm in diameter. Flow patterns were classified into three regions: coalescence bubble flow ($U_\ell <$ 8 cm/sec, $U_g <$ 10 cm/sec); dispersed bubble flow ($U_\ell >$ 8 cm/sec, $U_g <$ 10 cm/sec, $d_p \leq$ 2 mm); and slug flow ($U_g >$ 10 cm/sec). In different flow regimes, phase holdups, phase mixings, mass transfer, and heat transfer will be different.

Three hundred and thirty points (Mischelsen and Østergaard, 1970; Dakshinamurty et al., 1971; Dhanuka and Stepanek, 1978; Darton and Harrison, 1974; Østergaard, 1965; Bruce and Revel-Chion, 1974; and Efremov and Vakhrushev, 1970) for holdups were used to evaluate the holdup correlations. In uniform bubbling regime, Dakshinamurty et al.'s (1971) correlation is the "best" one for predicting overall bed voidage ($\varepsilon_\ell + \varepsilon_g$). It is not surprising, because most of the data used in deriving this correlation were in uniform bubbling conditions. For gas holdup prediction, Begovich et al.'s (1978) correlation is the best one. In bubble coalescence and slugging regimes, correlations proposed by Begovich et al. (1978) are the best for both overall bed voidage and gas holdup.

One hundred and thirty-four data points (Vail et al., 1968; Michelsen and Østergaard, 1970; and El-Temtamy et al., 1979) were used to evaluate the liquid phase dispersion. In the uniform bubbling regime, El-Temtamy et al.'s (1979) correlation is the best one among the tested correlations. The reason is that many data obtained by El-Temtamy et al. (1979) were used in data base. In bubble coalescence and slugging regimes, the correlation by Kato et al. (1972) is the best one for liquid dispersion prediction. This coincides with Shah's (1979) conclusion, i.e., small particles in small column correspond to bubble coalescence and slugging. A more detailed presentation of the evaluation for holdup and dispersion will be given in the annual report.

The phenomena in three-phase fluidization are similar to those in bubble columns. In the uniform bubbling regime, the gas phase can be described as plug flow. The degree of mixing is low in the liquid phase; therefore, the dispersion model can be applied to the liquid phase. In the bubble coalescence regime, mixing in the gas phase becomes important. Both liquid and gas phases can be described by the dispersion model. In the slugging regime, the existence of particles becomes less important, and phase mixings are analogous to the conditions in bubble columns.

Future Plans

1. Continue to evaluate the parameters for characterizing three-phase fluidization.

2. Analyze the effect of coal minerals and catalysts on the kinetics and mechanism of coal dissolution and hydrogenation.

3. Develop a kinetic and hydrodynamic model of coal dissolution and hydrogenation, and compare the model's predictions with experimental data.

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