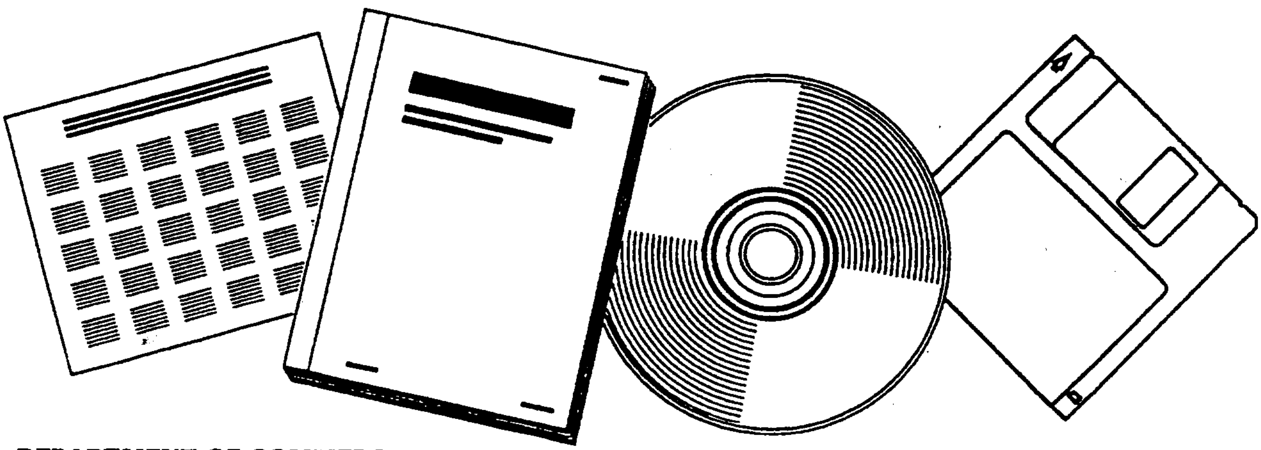
DE85013465

COPY

MODIFIED SEDIMENTATION-DISPERSION MODEL FOR SOLIDS BEHAVIOR IN COAL LIQUEFACTION REACTORS

DEPARTMENT OF ENERGY, PITTSBURGH, PA.
PITTSBURGH ENERGY TECHNOLOGY CENTER

1984



U.S. DEPARTMENT OF COMMERCE
National Technical Information Service

CONF-841121--19

DE85 013465

A MODIFIED SEDIMENTATION-DISPERSION MODEL FOR SOLIDS BEHAVIOR IN COAL LIQUEFACTION REACTORS

by

Dennis N. Smith,* John A. Ruether, and Gary J. Stiegel
Pittsburgh Energy Technology Center
U.S. Department of Energy
P.O. Box 10940
Pittsburgh, Pennsylvania 15236

and

Yatish T. Shah
University of Pittsburgh
Chemical and Petroleum Engineering Department
Pittsburgh, Pennsylvania 15261

ABSTRACT

A modified sedimentation-dispersion model for solid phase behavior in a three-phase slurry reactor is presented. The model incorporates a mass balance of solids that is described by solids dispersion, hindered settling and convection transport. The modified sedimentation-dispersion model incorporates boundary conditions that provide for a closed form solution of the axial solids distribution as a function of hindered settling and solids dispersion and can account for the spatial distribution of particle size and concentration in polydispersed systems. The application of the model to indirect coal liquefaction processes is briefly discussed.

*Speaker

To be presented at the Annual AIChE Meeting, San Francisco, California, November 20-25, 1984 (Modeling of Coal Conversion Processes Session).

INTRODUCTION

In the design of slurry bubble column reactors such as the ones used in coal liquefaction processes, the hydrodynamic behavior of dispersed solids must be considered especially if the solid phase is catalytic. Several investigations have been reported in the literature concerning the axial solids concentration distribution for monodispersed particles [Cova 1966, Kato et al. 1972, Smith and Ruether 1984]. The solids distribution in a slurry bubble column has been successfully described with a one-dimensional sedimentation-dispersion model. This model has two parameters, hindered settling velocity and axial solids dispersion coefficient, which are generally related to column geometry, flow rates, and particle and liquid thermophysical properties through empirical correlations.

Up to now, the sedimentation-dispersion model has only been applied to monodispersed narrow-sized fractions of solids. It is the purpose of this communication to develop the theory necessary to apply the sedimentation-dispersion model to polydispersed solid systems consisting of particle size or particle density distributions. The modified sedimentation-dispersion model also incorporates boundary conditions that allow for a closed form solution for the prediction of solids concentration as a function of axial position. Experimental results obtained from a 10.8-cm diameter slurry bubble column will be compared to the modified sedimentation-dispersion model for monodispersed as well as polydispersed solids systems. The effect of gas and slurry velocities, particle size and density, and distributor-type on the hindered settling velocity and solids dispersion coefficient will be discussed.

EXPERIMENTAL

The description of the slurry bubble column apparatus has been reported elsewhere [Smith and Ruether 1984, and Smith et al. 1984). A schematic of the slurry bubble column apparatus is shown in Figure 1. Two types of distributor plates have been used in this study, a single bubble cap and a multiple orifice plate. The gas, liquid, and solid phases employed in this study were nitrogen, water and glass beads. The temperature and pressure were constant for each experimental condition at approximately 303 K and 1.07 atmospheres, respectively. Four narrow-sized particles were used having mean particle diameters of 48.5-, 81.0-, 96.5-, and 193.5 x 10^{-6}m. Three solids densities of the glass beads were used: 2420-, 2990-, and 3990-Kg/m^3. The gas and slurry velocities were varied from 0.03- to 0.20-m/s and 0.007- to 0.02-m/s, respectively.

Slurry was sampled at six axial positions in equal intervals of 0.35-m beginning at 0.05-m from the distributor plate. The solids concentrations in the slurry was obtained from the slurry sample weight, dried solids weight, and known liquid and solids densities. In addition to slurry samples taken in the slurry bubble column, slurry samples were taken in the slurry feed line and the solids concentration in the slurry feed was obtained in the same way as in the column. The average solids concentration in the slurry bubble column was obtained from the volume of slurry in the column (obtained after sudden interruption of the gas and slurry flows), the slurry feed concentration, and the known amount of solids and liquid initially charged to the slurry bubble column apparatus. The gas holdup was calculated from level differences of the gas-liquid-solid dispersion and static slurry height. All slurry samples were taken at steady-state conditions where the solids concentration did not change with time (experimentally verified to be less than one hour for the entire range of experimental conditions).

For the polydispersed solids systems studied, in addition to the above-mentioned sampling procedure, the particle size distribution of each sample of dried solids was determined from sonic screening and subsequent weighing of the weight distribution on each screen.

MODEL DEVELOPMENT

The solids concentration distribution in a cocurrent upward flow slurry bubble column can be described by a one-dimensional sedimentation-dispersion model for monodispersed particle systems [Kato et al. 1972, and Smith and Ruether 1984]. A differential mass balance for the solid phase considering solids dispersion, hindered settling and convection as the mechanisms of solid motion may be written for steady-state conditions and monodispersed particles as follows:

$$\frac{-E_s}{L}\frac{dC_s}{dx} + \left[\frac{\bar{U}_{sL}}{(1-\varepsilon_g)} - \bar{\Psi}_L U_P\right] C_s = U_{sL} C_s^f \qquad (1)$$

Up to now, the boundary condition for integration of Equation (1) has not been identified on a theoretical basis. Cova [1966] suggests the solids concentration at the top of the column is the same as the slurry effluent or feed concentration. Kato et al. [1972] and Smith and Ruether [1984] provide empirical correlations for the solids concentration at the top of the column.

The boundary conditions chosen in the present model development is located at the top of the column. The concentration gradient, dC_s/dx, is given as follows:

$$\frac{dc_s{}^1}{dx} = C_s{}^f - C_s{}^1 \; ; \; x = 1 \tag{2}$$

The flux of solids entering the bubble column by hindered settling at $x = 1$ is given as the product, $\Psi_L U_p C_s{}^f$. With these criteria established, Equation (1) and Equation (2) may be combined to represent the boundary condition at $x = 1$.

$$\frac{-E_s}{L} (C_s{}^f - C_s{}^1) + \frac{\bar{U}_{sL}}{(1-\varepsilon_g)} C_s{}^1 - \bar{\Psi}_L U_p C_s{}^f = U_{sL} C_s{}^f \tag{3}$$

Upon rearrangement of Equation (3), the solids concentration at the top of the column may be expressed in terms of the slurry feed or effluent solids concentration.

$$C_s{}^1 = [1 - \frac{\Psi \, U_p}{(E_{s/L}) + U_{sL}}] \, C_s{}^f \tag{4}$$

Integration of Equation (1) with the boundary condition given in Equation (4) gives the following expression:

$$C_s = \{(\frac{E_s+\bar{\Psi}_L U_p L}{E_s+U_{sL}L})(\frac{\bar{\Psi}_L U_p}{\bar{\Psi}_L U_p - U_{sL}}) \, C_s{}^f \exp [\frac{-(\bar{\Psi}_L U_p - U_{sL})L(x-1)}{E_s}]\}$$
$$-(\frac{U_{sL} C_s{}^f}{\bar{\Psi}_L U_p - U_{sL}}) \tag{5}$$

For polydispersed particle systems, the solids concentration of the i^{th} particle size fraction is related to the total solids concentration by the following expression:

$$C_s = \sum_i C_{si} \tag{6}$$

where C_{si} may be expressed as:

$$C_{si} = \left[\left(\frac{E_{si}+\bar{\Psi}_L U_{pi} L}{E_{si}+U_{sL} L}\right)\left(\frac{\bar{\Psi}_L U_{pi}}{\bar{\Psi}_L U_{pi}-U_{sL}}\right) C_{si}^{f} \exp\left[\frac{-(\bar{\Psi}_L U_{pi}-U_{sL})L(x-1)}{E_{si}}\right]\right] - \left(\frac{U_{sL} C_{si}^{f}}{\bar{\Psi}_L U_{pi}-U_{sL}}\right) \tag{7}$$

For the theoretical prediction of axial solids concentration distribution, two parameters, U_p and E_s, are needed. In the present investigation, U_p and E_s are obtained from a nonlinear regression analysis of Equation (5) or Equation (7) with the best fit of measured solids concentration being optimized with the parameters U_p and E_s. The best fit is defined as the minimum residual sum of squares between the observed and calculated solids concentration. A search method described by Ahrendts and Baehr [1981] was used to obtain the best fit of the observed solids concentration.

RESULTS AND DISCUSSION

Empirical correlations have been developed for the hindered settling velocity and solids dispersion coefficient obtained from the nonlinear least squares optimization of observed solids concentration distribution and that predicted from Equation (5) or Equation (7). The effects of gas and slurry velocity, particle size, density and concentration, and distributor type were considered in developing the correlations for hindered settling velocity and the solids dispersion coefficient.

The hindered settling velocity is dependent on the particle terminal velocity, gas velocity, and liquid fraction in the slurry. The following empirical correlation was obtained:

$$U_p = 1.44\, U_t^{0.78}\, \bar{U}_g^{0.23}\, \bar{\Psi}_L^{3.5} \tag{8}$$

where: 0.002 m/s $< U_t < 0.025$ m/s, 0.03 m/s $< \bar{U}_g < 0.20$ m/s, and $0.90 < \Psi_L < 0.98$.

No effect of slurry velocity or distributor type was observed on the hindered settling velocity. The absolute relative deviation of Equation (8) from the observed hindered settling velocity is 9.6 percent for 128 experimental conditions.

For the solids dispersion coefficient, all of the operating variables mentioned above had a significant effect. The following dimensionless empirical correlation was obtained for the perforated plate distributor.

$$Pe_p = 6.7\, (Fr_g^{6}/Re_g)^{0.106}\, (1 + 0.06\, Ar^{\frac{1}{2}}) \tag{9}$$

where: $0.3 < Pe_p < 1.2$, $0.03 < Fr_g < 0.20$, $2100 < Re_g < 29000$, $0.007 < Fr_L < 0.02$, and $5 < Ar < 360$.

The solids Peclet number, Pe_p, has been used to correlate the observed solids dispersion coefficient in a similar manner as given by Riquarts [1981] for the liquid dispersion coefficient in a bubble column. The effect of column diameter was not examined in this study and caution should be used in employing Equation (9) for other column diameters. The average absolute relative deviation of Equation (9) from the observed solids Peclet number is 18.3 percent for 62 experimental conditions.

The solids dispersion coefficient for a bubble cap distributor has been reported elsewhere [Smith and Ruether 1984].

$$Pe_p = 9.6\ (Fr_g^{\ 6}/Re_g)^{0.114} + 0.019\ Re_p^{\ 1.1} \tag{10}$$

The absolute relative deviation of Equation (10) from the observed solids Peclet number was 15.7 percent for 66 experimental conditions. In comparing the solids dispersion coefficient obtained from the bubble cap and perforated plate distributor, the solids dispersion coefficient for the bubble cap distributor has less dependency on gas velocity than that for the perforated plate distributor. The solids mixing is slightly greater for the perforated plate as compared to the bubble cap distributor for small particles at low slurry velocities. At high slurry velocities, the solids mixing is slightly less for the perforated plate as compared to the bubble cap distributor.

A comparison of the observed and predicted axial solids concentration distribution as a function of operating variables is shown in Figures 2 through 5. Figure 2 illustrates the effect of particle density on the axial solids concentration distribution for a perforated plate distributor. Increasing particle density increases the variance of the solids distribution. Figure 3 illustrates that increasing particle diameter increases the variance of the axial solids concentration distribution. Figure 4 shows a relatively small effect of superficial gas velocity on the axial solids concentration profile. Increasing the gas velocity slightly decreases the variance of the axial solids concentration distribution. Figure 5 illustrates that the modified sedimentation dispersion model can accurately predict the particle size and solids concentrations distribution in polydispersed solids systems.

The model presented here should be useful in the design of Fischer-Tropsch slurry reactor. The models for F-T slurry reactor presented so far do not consider the effect of axial variations in particle distribution on the conversions of CO and H_2 and in particular, selectivity of the product distribution. The solid distribution model presented in this paper will allow better simulation of F-T slurry bubble column reactors.

NOMENCLATURE

Ar = Archimedes number, $(g\, d_p^3\ \rho_s\ (\rho_s \rho_L)/\mu_L^2)$

C_s = solids concentration if slurry, kg/m^3

C_s^f = solids concentration is slurry feed, kg/m^3

C_s^1 = solids concentration at top of column, kg/m^3

D = column diameter, m

d_p = particle diameter, m

E_s = solids dispersion coefficient, m^2/s

Fr_g = Froude number of gas phase, $(\bar{U}_g/(gD)^{\frac{1}{2}})$

g = gravitational acceleration, m/s^2

L = column length, m

Pe_p = solids Peclet number, $(\bar{U}_g D/E_s)$

Re_g = Reynolds number of gas phase, $(\bar{U}_g\ D\ \rho_L/\mu_L)$

Re_p = Reynolds number of particle, $(U_t\ d_p\ \rho_L/\mu_L)$

U = actual linear velocity, m/s

$\bar{U}$ = superficial velocity, m/s

U_p = hindered settling velocity, m/s

U_t = terminal particle velocity, m/s

X = dimensionless axial position from bottom of column, (z/L)

Z = axial position from bottom of column, m

Greek Symbols

ε_g = gas holdup

ρ_L = liquid density, kg/m^3

ρ_s = solids density, kg/m^3

Ψ_L = average fraction of liquid in slurry

μ_L = liquid viscosity, kg/m-s

Superscripts

i = i^{th} particle size or density fraction

g = gas phase

sL = slurry phase

LITERATURE CITED

1. Ahrendts, J., and Baehr, H., Int. Chem. Eng., 21, 572 (1981).

2. Cova, D.R., Ind. Eng. Chem., Process Des. Dev., 5, 20 (1966).

3. Kato, Y., Nishiwaki, A., Fukuda, T., and Tanaka, S., J. Chem. Eng. Japan, 5, 14 (1972).

4. Riquarts, H.-P., Ger. Chem. Eng., 4, 18 (1981).

5. Smith, D.N., and Ruether, J.A., "Dispersed Solid Dynamics in a Slurry Bubble Column," accepted by Chem. Eng. Sci. (1984).

6. Smith, D.N., Ruether, J.A., and Stiegel, G.J., "Polydispersed Solids Behavior in a Bubble Column," to be presented at Annual AIChE Meeting, San Francisco, Calif. (Nov. 25-30, 1984).

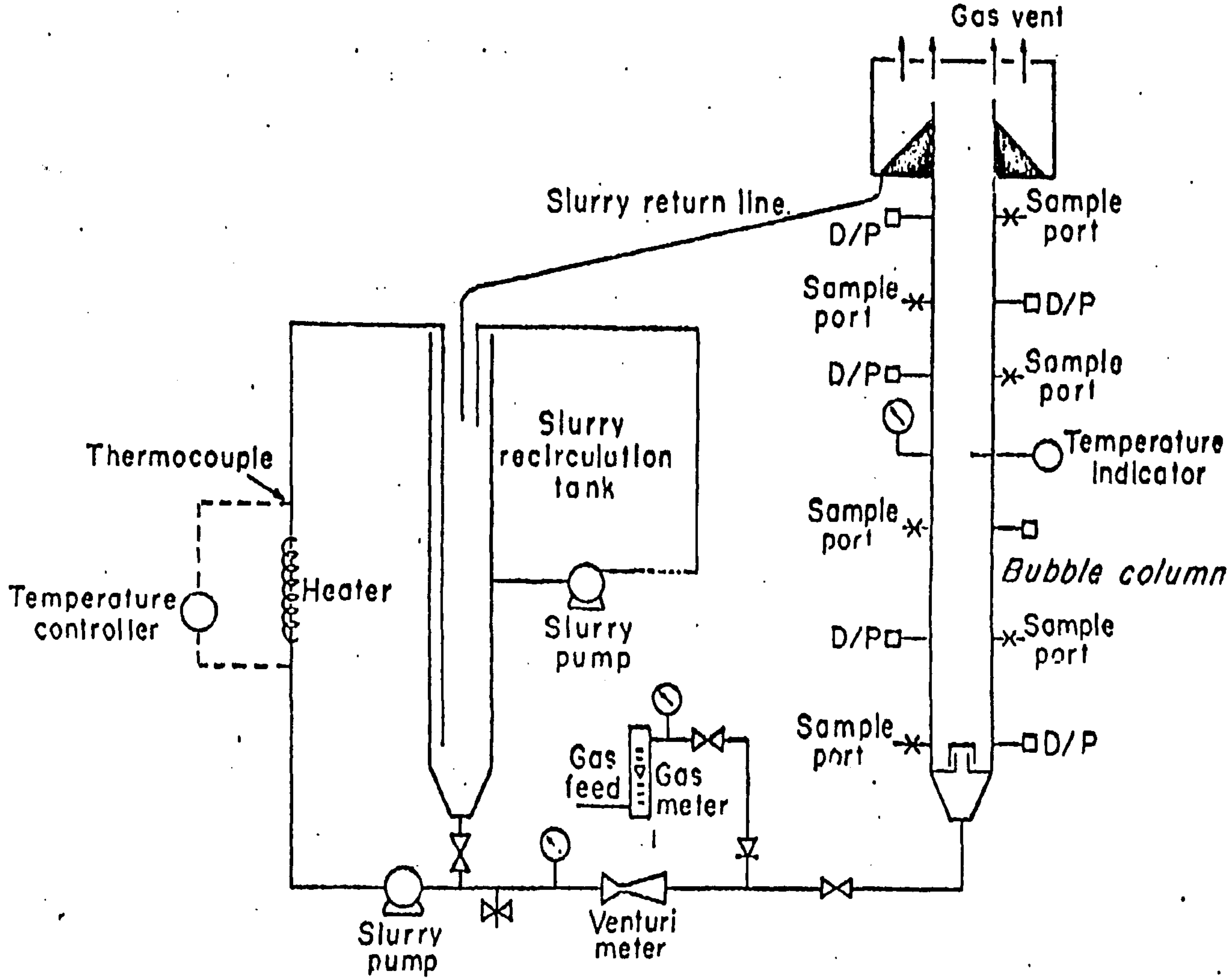


Figure 1. Schematic of slurry bubble column apparatus.

1-13-81 L-18107

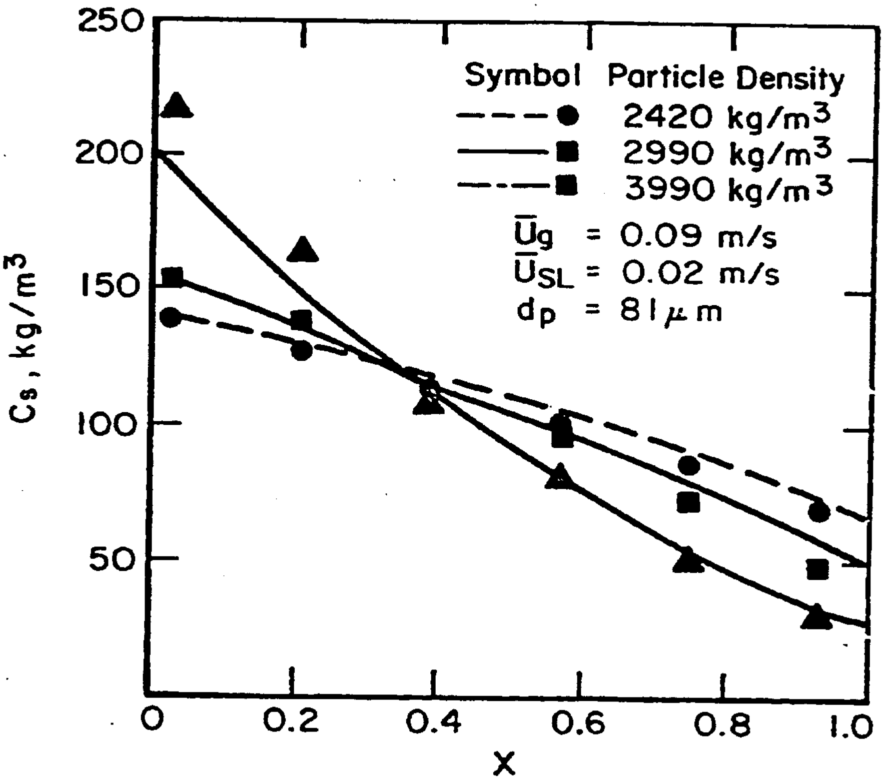


Figure 2 - Effect of particle density on axial solids concentration distribution.

BSI/6237

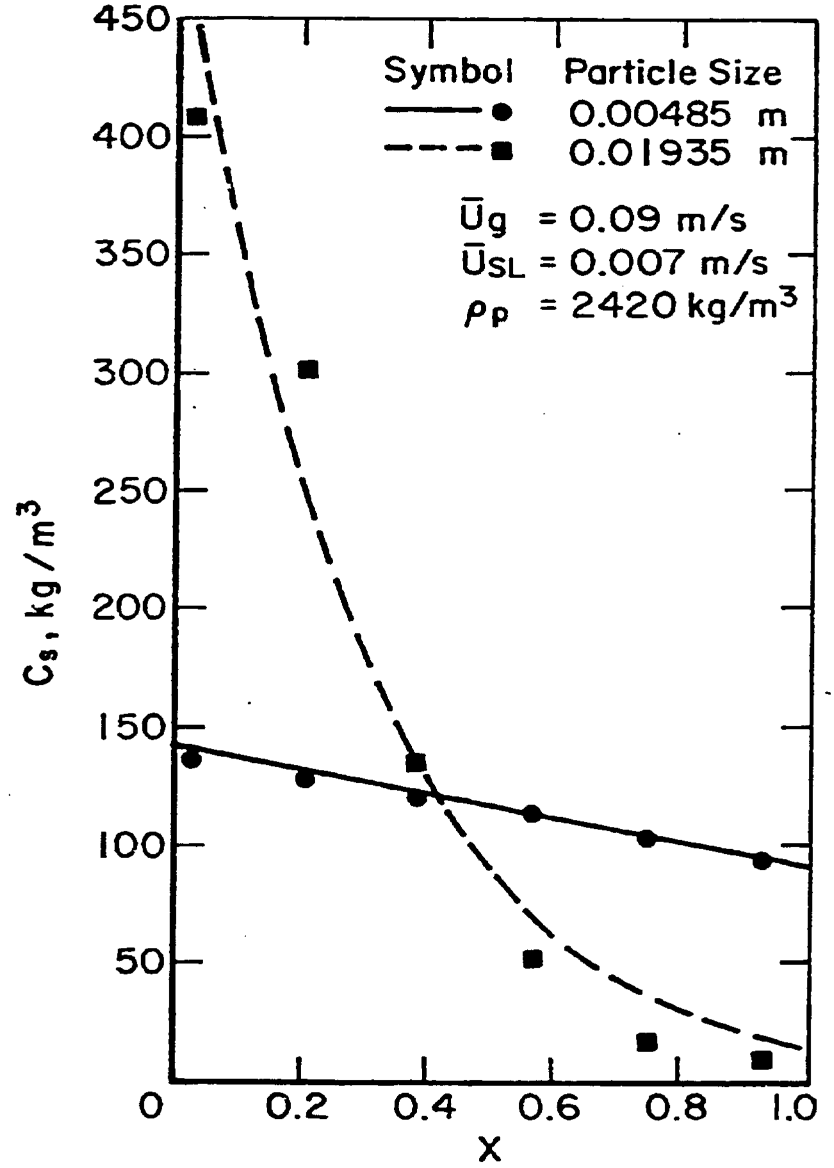


Figure 3 - Effect of particle diameter on axial solids concentration distribution.

BSI/6238

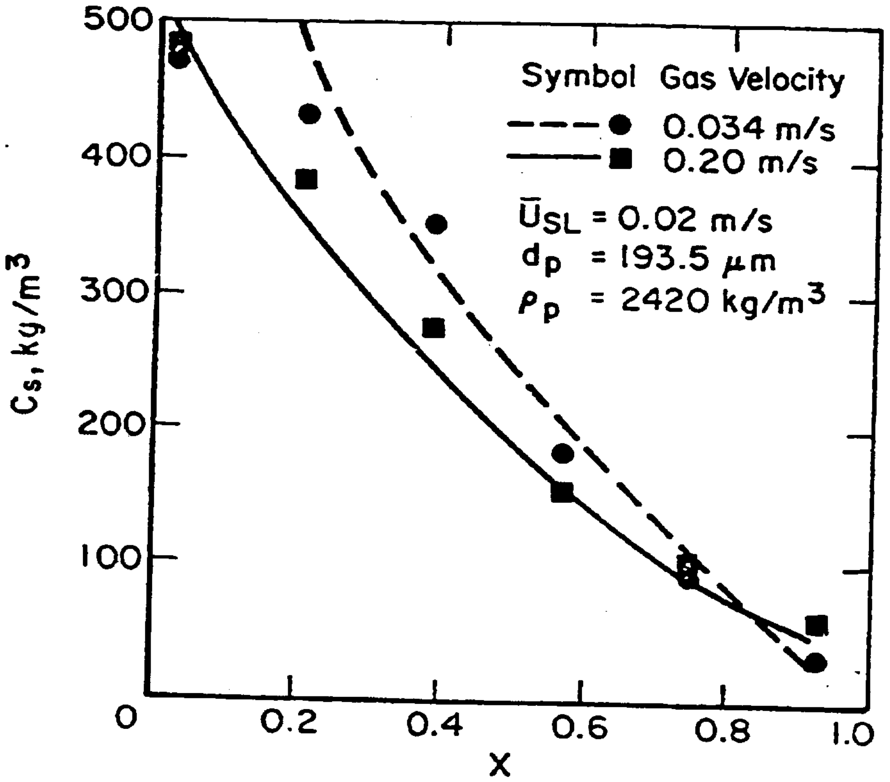


Figure 4 - Effect of gas velocity on axial solids concentration distribution.

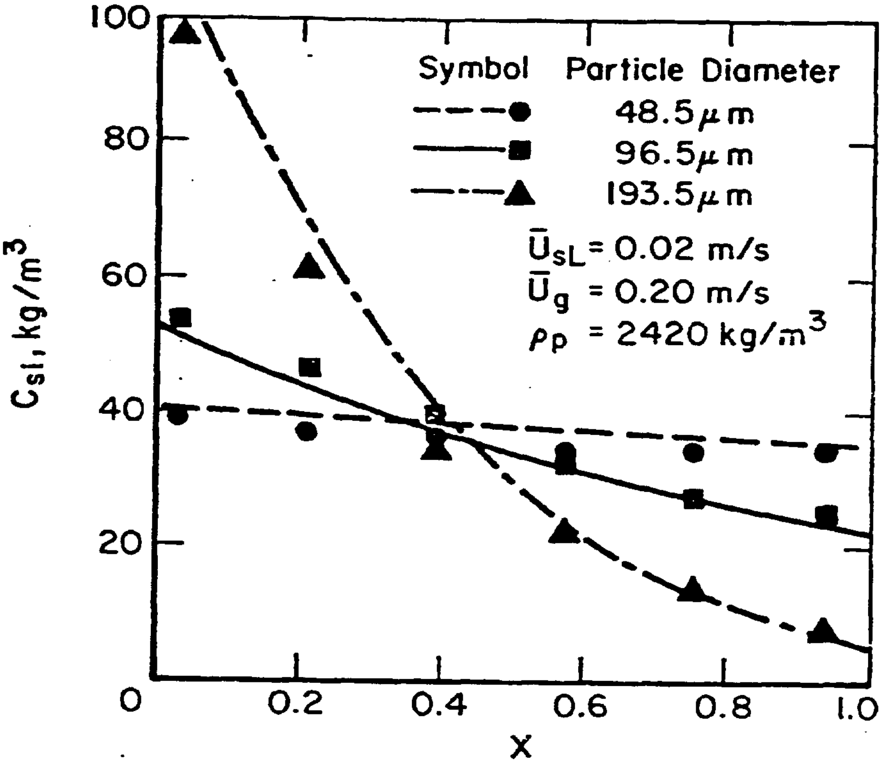


Figure 5-Axial solids concentration distribution for polydispersed solids system.