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Ted Knowlton*

S. B. Reddy Karri†

J. S. Smith‡

*PSRI, Chicago, IL., USA, tmkpsri@ix.netcom.com

†PSRI, Chicago, IL. USA

‡Smith Engineering Services, Texas City, Texas, USA

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HYDRODYNAMIC SCALE-UP OF CIRCULATING FLUIDIZED BEDS

T.M. Knowlton and S.B. Reddy Karri
Particulate Solid Research, Inc.
4201 W. 36th St, Suite 200
Chicago, IL 60632, USA

J.S. Smith
Smith Engineering Services
9207 Stingray Court
Texas City, TX 77591

ABSTRACT

A general procedure that can be used to scale up circulating fluidized beds is presented. It consists of developing a mathematical model in conjunction with measuring 1) the radial dispersion coefficient (D_r) using gas tracers, 2) the radial solids velocity profile using a Pitot tube and 3) the radial distribution of solids density ($1 - \epsilon$) using an optical probe. If the resulting information is obtained in a riser 200 mm or greater in diameter, it can be used in conjunction with the mathematical model for scale-up.

INTRODUCTION

"Scale-up is still not an exact science, but is rather a mix of physics, mathematics, witchcraft, history and common sense which we call engineering" – J. Matsen (1)

Scale-up is an issue that weighs large on the minds of every process designer. It is well known that, in general, the hydrodynamics of small-scale fluidized beds can differ significantly from the hydrodynamics of large fluidized beds, and that often this difference leads to negative results. If this hydrodynamic difference is not taken into account in design, the yields from the large process may be inferior to that experienced on the small scale. Therefore, engineers charged with overseeing process design and scale-up are extremely concerned about how to translate the results from small scale to commercial size.

Several authors have written about the effects of scale on hydrodynamics in fluidized systems (Matsen (1), Glicksman (2), Werther (3)). Because it is difficult and expensive to obtain hydrodynamic data on large-scale systems are limited.

Circulating fluidized beds (CFBs) are attractive reactors for conducting moderate to fast heterogeneous catalytic reactions and combustion reactions. Examples of

processes employing CFBs are fluid catalytic cracking, maleic anhydride from the partial oxidation of n-butane, methanol-to-olefins, methanol-to-gasoline and combustion of coal. Key features of these processes are (1) a large circulation of solids to help with heat transfer, (2) the means to continuously regenerate the catalyst in catalytic reactions, and (3) the use of smaller equipment due to the inherently large solids and fluid fluxes employed.

Development of mathematical models that adequately describe the transport mechanisms at work in CFBs is valuable for predicting reactor conversion and selectivity. The more complex computational fluid dynamics (CFD) models are tools that can be used to extrapolate or predict scale up parameters from a limited amount of experimental data. However, using CFD codes to exclusively model and scale-up a CFB is extremely risky at this stage of CFD development. Simpler models comprising material balances superimposed on the CFB solids flow structure are easier to build, and require very little computer time to optimize. For example, given the typical CFB core-annular structure, the information required from a hydrodynamic perspective is the solids volume fraction, how the gas flows (upward or downward) through the solids and how it undergoes axial and radial dispersion. This approach assumes axisymmetric flow, and that gas diffusion and particle diffusion are either negligible or lumped into the chemical kinetics. This approach is limited to the upper accelerated section of the CFB. A separate model is needed for the acceleration region; and the two can then be combined for a complete model of the CFB.

SCALE-UP APPROACH

The overall approach described to scale-up CFB reactors is to: 1) develop a hydrodynamic model for the CFB, and 2) determine the solids holdup, solids velocity profile and the radial gas dispersion coefficient in a cold model of the riser.

1. Develop or select a hydrodynamic model for the CFB hydrodynamics.

The development of a hydrodynamic mathematical model or the selection of an existing hydrodynamic model is the basis of the CFB scale-up procedure. The hydrodynamic model can be developed in-house or selected from the literature. The model is generally a 2D model that assumes circumferential symmetry, although a 3D model can be used. However, it is generally not necessary to use a 3D model because the gas and solids velocity profiles in a riser are normally axisymmetric. This significantly reduces the complexity of the modeling. After the model is developed/selected, it can be combined with the kinetics of the process to determine process yields and selectivities.

The most important hydrodynamic parameters to estimate for CFB scale-up are:

- a) Solids holdup or the volume fraction of the solids suspended in the gas-solids suspension ($1 - \epsilon$).
- b) The gas velocity (or solid velocity) profiles in the riser
- c) The radial gas dispersion coefficient

2. Determine the solids holdup, solids velocity profiles and the radial gas dispersion coefficient in a cold flow model of the riser.

The solids holdup, gas velocity profile and gas dispersion coefficient can be determined in a cold flow model of the riser operating over the range of solids mass fluxes and gas velocities to be used in the commercial riser. The cold flow model of the riser should be at least 200 mm in diameter. In general, wall effects in small diameter units can have a major effect on experimental parameters, and the parameters can vary significantly with size. However, after a certain diameter, the effect of size often reaches an asymptote as indicated in Figure 1. In risers, this asymptote is thought to be reached at a size of approximately 200 mm. Evidence for this is shown in Figure 2, which shows how the pressure drop per unit length, $\Delta P/Lg$, varies with the superficial gas velocity in the riser for three different riser diameters – 100, 200 and 300 mm. The figure shows that the $\Delta P/Lg$ vs. velocity curve for the riser zone above the acceleration region is lowest for the 100 mm diameter riser. However, the $\Delta P/Lg$ vs. velocity curves for the 200 and 300 mm diameter risers are essentially the same. This indicates that the values of $\Delta P/Lg$ in are essentially the same for risers larger than approximately 200 mm, and cold and hot model measurements should be conducted in risers of this diameter or larger.

Solids Holdup ($1-\epsilon$)

Solids holdup in the riser is the most important hydrodynamic parameter to consider for the scale-up of processes. If the solids holdup is not estimated accurately, reaction yields and selectivities will not be predicted correctly. A common method of determining solids holdup in the riser cold model is to traverse an optical probe radially across the riser at several axial locations for the range of solids mass fluxes and gas velocities to be used in the commercial riser.

To calculate the holdup in the commercial riser, a technique using the slip factor is generally used. The definition of the slip factor, ψ , is:

$$\psi = \frac{U_g}{\epsilon U_p} = \frac{U_g \rho_p (1-\epsilon)}{\epsilon G_s} \quad (1)$$

The slip factor can be estimated using the Patience *et al.* (4) correlation:

$$\psi = 1 + \frac{5.6}{Fr} + 0.47 Fr_t^{0.41} \quad (2)$$

The Patience correlation predicts that the slip velocity will change with riser diameter and gas velocity.

The radial distribution of the solids in the riser can be predicted by a power law. A simple expression that can be shown to fit the experimental radial solids distribution is:

$$\frac{1-\epsilon}{1-\epsilon_{avg}} = \frac{q+2}{q+2f} \left[1 + (f-1) \left(\frac{r}{R} \right)^q \right] \quad (3)$$

where f is the ratio of the solids volume fraction at the wall divided by that in the center, and q is the power law exponent. Equation (3) has been derived such that the mass balance of the solids distribution has been preserved. The factor f is often

approximately 6, and q approximately 4. $(1 - \epsilon_{avg})$ is determined from the slip factor relationship in Equation (1).

Differential pressure measurements per unit length in the riser at several axial locations in conjunction with particle concentration measurements at different radial positions using an optical probe can be used to determine the slip factor and correlation parameters, q and f .

A plot showing the density variation in a riser operating at high fluxes and velocities in an FCC riser is shown in Figure 3.

Velocity Profiles

The gas and solids velocity profiles are important in CFB scale up. Researchers have almost universally reported that the solids velocity (or equivalently the gas velocity) profiles in a riser are parabolic (Bader et al (5), Van Breugel et al (6)). However, the gas profile may be nearly turbulent (uniform across the diameter) in the case of low solids mass fluxes, parabolic for moderate solids fluxes and approach a triangular shape for high solids fluxes. The shape of the gas velocity profile affects the contact between gas and particles, and may limit product conversion and/or selectivity in some applications.

Although the average slip factor in a CFB may range from 1.2 to 2.5, the local slip factor at any radial position is nearly 1. This is important because the shape of the gas velocity profile is then approximately the same as the particle velocity profile. The reason why the local slip factor is near 1 while the average is much greater than 1 is because the average slip factor takes into account the radial distribution of particle volume fraction, $(1-\epsilon)$, as shown in Equation (4) in dimensionless form.

$$\psi = \frac{\int_0^1 u_{avg} (1-\phi) \xi d \xi}{\int_0^1 (1-\phi) \xi d \xi} \quad \frac{\int_0^1 u_{particle} \phi \xi d \xi}{\int_0^1 \phi \xi d \xi} \quad (4)$$

Thus, a measurement of the solids velocity profile expressed as $u/u_{avg}(r/R)$ is nearly identical to the gas velocity profile. This is why a Pitot tube (discussed below and which measures the solids velocity profile) may be used to infer the gas velocity profile from the solids velocity profile.

The actual parabolic shape of the velocity profile for the solids used and the solids flux and gas velocity ranges anticipated in the commercial riser can be determined in a riser cold model. This is done by radially traversing a Pitot tube or an optical probe across the riser.

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When using the Pitot tube, it is assumed that the gas contribution to the momentum measured by the Pitot tube is negligible. If the gas momentum is negligible, then the following equation applies to the Pitot tube:

$$\Delta P = \frac{K_p G_s U_p}{g_c} \quad (5)$$

where K_p is the Pitot tube coefficient that is determined by calibration. The particle velocity is calculated by rearranging the equation to give:

$$U_p = \frac{\Delta P g_c}{G_s K_p} \quad (6)$$

Axial and Radial Dispersion Coefficients

Axial Dispersion Coefficient

Namkung and Kim (7), and Li and Wu (8) have reported axial dispersion coefficients (D_x) for CFBs on the order of 0.3 to 1.0 m²/s. Liu *et. al.*, (9) reported axial Péclet numbers of the order of 9, which corresponds to axial dispersion coefficients on the order of 3.7 m²/s – probably because of a relatively short riser. Assuming these coefficients are representative of the CFB regime, an estimate of commercial riser axial Péclet numbers using the relation:

$$Pe_x = \frac{UL}{D_x} \quad (7)$$

can be made. For a gas velocity of 9 m/s, an axial dispersion coefficient of 0.3 m²/s, and a reactor height of 30 m, the axial Péclet number is 900. If a coefficient of 3.7 m²/s is selected, the Péclet number is 65. With such relatively large Péclet numbers, axial dispersion is extremely low in CFBs. Martin, *et. al.* (10) and Werther, *et. al.* (11) reported that axial mixing of the gas in CFBs is negligible, and that radial dispersion is the primary mechanism limiting plug flow of the gas. Thus, axial dispersion kinetics are insignificant compared to the convection kinetics. Axial Péclet numbers can easily be on the order of several hundreds in CFBs, particularly for tall CFB riser reactors.

Radial Dispersion Coefficient

Several investigators have reported radial dispersion coefficients in risers. Table 1 summarizes some of the values reported. Operating conditions and geometries vary widely for the data shown. The radial dispersion coefficient in Table 1 measured in the largest riser is that reported by Derouin *et. al.* (12). Their reported radial dispersion coefficient was approximately 0.03 m²/s for a riser diameter of approximately 1 m and a riser height of approximately 30 m. For an industrial-sized

reactor with this radial dispersion coefficient, operating at a velocity of 8 m/s and with a radius of 1 m, the radial Peclet number is:

$$Pe_r = \frac{UR}{D_r} = \frac{8(1)}{0.03} = 270 \quad (8)$$

Table 1. Typical Values of the Radial Dispersion Coefficient in CFB's

Radial Dispersion Coefficient (m ² /s) (averaged)	Authors
0.0006	Wei, <i>et. al.</i> , 2001* (13)
0.0035	Sternéus, <i>et. al.</i> , 2000 (14)
0.0012	Namkung & Kim, 2000 (15)
0.0018	Mastellone & Arena, 1999 (16)
0.0300	Derouin, <i>et. al.</i> , 1997 (12)
0.0024	Amos, <i>et. al.</i> , 1993 (17)
0.0019	Werther, <i>et.al.</i> , 1992 (11)
0.0024	Martin, <i>et. al.</i> , 1992 (10)
0.0037	Li & Wu, 1990 (8)

* Very low gas velocity, 2 - 3.5 m/s

Radial and axial dispersion coefficients in CFB risers are commonly determined by injecting a continuous tracer gas (helium, CO₂, etc.) into the center of the column. The gas should be injected at a velocity slightly lower than or equal to the gas velocity in the center of the riser. Gas sampling probes are then traversed radially at several axial locations, and the tracer concentration is measured as a function of radial position. Knowing the shape of the velocity profile (determined as described above), the dispersion coefficients can be obtained from the experimental data.

A gas tracer can also be injected circumferentially at the wall of the CFB. This allows the determination of the amount of gas backmixing in a CFB if the annular solids flow downward along the wall. Tracer gas sampling probes are then traversed radially both above and below the injection gas injection point. Gas injected at the wall is usually injected slowly and through sintered disks to ensure that the gas remains near the wall and does not jet into the center of the bed.

Most investigators have calculated the radial dispersion coefficient in risers using the analytic solution from Klinkenberg *et. al.*, (18):

$$\frac{c}{c_{avg}} = 1 + \sum_{n=1}^{\infty} \frac{J_0(\alpha_n r/R) e^{-(\alpha_n^2 z/(RPe_r))}}{J_0^2(\alpha_n)} \quad (9)$$

Where:

$$J_1(\alpha_n) = 0$$

and

$$Pe_r = \frac{U(2R)}{D_r}$$

This analytic solution for the trace concentration profile employs an average riser gas velocity.

If the gas velocity profile is not flat, then the two approaches are available. In the first approach, a parabolic velocity profile is assumed in the riser. In the second approach, a general Ostwald-de Waele velocity profile is assumed.

In the first approach the starting point is the general non-steady-state diffusion equation in cylindrical coordinates with a parabolic profile assumed:

$$\frac{\partial c}{\partial t} = \frac{D_r}{r} \frac{\partial}{\partial r} \left(r \frac{\partial c}{\partial r} \right) - 2u_{avg} \left(1 - \left(\frac{r}{R} \right)^2 \right) \frac{\partial c}{\partial z} \quad (10)$$

After converting the equation to a dimensionless form, it can be solved to obtain the Taylor Dispersion Model (Taylor (19)):

$$\frac{\partial \bar{c}}{\partial \tau} = \frac{Pe_r}{48} \frac{\partial^2 \bar{c}}{\partial \xi^2} \quad (11)$$

where

$$Pe_r = \frac{u_{avg} R}{D_r} \quad (12)$$

Equation (10) describes a decaying tracer impulse that is injected into a flowing fluid. The solution is:

$$\bar{c} = \frac{m/A}{\sqrt{4\pi \frac{(u_{avg} R)^2}{48 D_r} t}} \exp \left[-\frac{(z - tu_{avg})^2}{4 \frac{(u_{avg} R)^2}{48 D_r} t} \right] \quad (13)$$

where the mass injected per area is m/A .

If the tracer pulse is applied to a riser with a parabolic profile, the axial dispersion coefficient can be calculated as:

$$D_x = \frac{(U_{avg} R)^2}{48 D_r} \quad (14)$$

with

$$Pe_x = \frac{U_{avg} L}{D_x}, \text{ and } Pe_r = \frac{U_{avg} R}{D_r}, \text{ then}$$

$D_x = \frac{U_{avg} R}{Pe_x}$, and $D_r = \frac{U_{avg} R}{Pe_r}$, and by substitution:

$$\frac{U_{avg} L}{Pe_x} = \frac{(U_{avg} R)^2}{48} \frac{Pe_r}{U_{avg} R} \text{ and}$$

$$Pe_x = \frac{48 L}{Pe_r R} \quad (15)$$

In terms of diameter instead of radius,

$$Pe_x = \frac{2(48) 2L}{Pe_{r,D} D} = \frac{192 L}{Pe_{r,D} D} \quad (16)$$

Arena (20) also explains that the axial Péclet number is related to the radial Peclet number through the general form of Equation (16), i.e

$$Pe_x = \frac{1}{\beta Pe_{r,D}} \frac{L}{D} \quad (17)$$

He states that β (a dimensionless constant that describes the uniformity of the gas profile in the riser) for a parabolic velocity profile has a value of 1/192, which is the same as the value obtained from the Taylor Dispersion model shown in Equation (16). The value of β changes with the shape of the gas velocity profile. Derouin et. al. (12) found a near parabolic velocity profile in their large 1-m-diameter riser. Therefore, the equivalent axial Péclet for their 1-m-diameter riser 30 m tall and using the Pe_r value (270) from Equation (8) is:

$$Pe_x = \frac{192 L}{Pe_{r,D} D} = \frac{192 30}{270 1} = 21 \quad (18)$$

It can be seen that a low radial Péclet number is desirable if plug flow is preferred in a riser because it increases the value of Pe_x . Plug flow is generally preferred for catalytic processes. Plug flow is not generally preferred for combustion processes. Increasing D_r (which decreases the value of Pe_r) is desirable if plug flow is required.

Werther et al (21), reported a value of Pe_r of 465 from tests with 130 micron quartz sand in a 0.4-m-diameter riser. Jiang et al (22) reported that Pe_r values ranged from 100 to 1000 for Group A material. It seems that a good range for Pe_r for Group A and small Group B materials is approximately 200 to 500. Most CFBs operate with particles of this size range. An average value for this size range would be for a Pe_r of approximately 350.

Namkung and Kim (15) reported in a log-log plot in their paper that the radial dispersion coefficient increased essentially linearly with reactor diameter (Figure 4). This result suggests that the radial Péclet number is relatively constant within the CFB flow regime, and that radial dispersion can “keep up” with the increase in riser diameter. However, log-log plots can often mask the true variability in a parameter,

and although D_r increases with column diameter, it is recommended that D_r be determined for the actual solids used, and for the gas velocity and solids mass flux ranges to be used in the CFB. As stated above, a range of Pe_r from 200 to 500 is likely for most CFBs operating with Group A material.

The second approach to determine the radial dispersion coefficient is to use the Ostwald-de Waele general velocity profile. This was the approach used by Derouin *et al.* (12).

The Ostwald-de Waele velocity profile is:

$$\frac{u}{u_{avg}} = \frac{3n+1}{n+1} \left[1 - \left(\frac{r}{R} \right)^{\frac{n+1}{n}} \right] \quad (19)$$

In this approach, the velocity profile in Equation (10) is replaced by the Ostwald-de Waele velocity, Equation (19). After substitution and manipulation and converting the equation into dimensionless form, the following Taylor Dispersion-Ostwald-de Waele equation is obtained:

$$\frac{\partial \bar{c}}{\partial \tau} = \left[\frac{n^2}{2(5n+1)(3n+1)} \right] Pe_r \frac{\partial^2 \bar{c}}{\partial \xi^2} \quad (20)$$

If $n = 1$, Equation (20) reduces to the Taylor Dispersion Equation with a parabolic velocity profile, Equation (11). It can also be used to obtain radial dispersion and velocity data in a cold flow riser and calculate the equivalent axial Peclet number for use in a 1-D hydrodynamic model. Other possibilities are shown for different values of n in Table 2. An n value of 0.1 would give a value of β equal to 1560. This value of β is close to the turbulent velocity profile value of 2000, as reported by Arena (20).

Table 2. Ostwald-de Waele-Taylor Dispersion Equivalency Chart for CFB Reactors

Ostwald-de Waele Index	Gas Phase Hydrodynamic Equivalency
$n = 0.1$	$Pe_x = \frac{1560 L}{Pe_{r,D} D}$
$n = 0.5$	$Pe_x = \frac{280 L}{Pe_{r,D} D}$
$n = 1.0$	$Pe_x = \frac{192 L}{Pe_{r,D} D}$
$n = 4.0$	$Pe_x = \frac{136 L}{Pe_{r,D} D}$

Equation (19) cannot be applied with the gas velocity profile is negative (as in the case when the solids flow downward near the wall). In general, the velocity profile can be fitted by Equation (20).

$$u = (u_{avg} - k) \frac{3n+1}{n+1} \left[1 - \left(\frac{r}{R} \right)^{\frac{n+1}{n}} \right] + k \quad (20)$$

Equation (20) is a modification of the Ostwald de Waele velocity profile that allows for a negative component to the velocity profile for $k < 0$. The equation is derived such that, upon integration, the k value drops out and the average velocity, u_{avg} , is obtained. When $k = 0$, the conventional form of the Ostwald de Waele equation results.

Overall Model

A general combined hydrodynamic and kinetic model that can be used for this scale up strategy is given below:

$$\frac{\partial c_i}{\partial t} = \frac{1}{Pe_r} \frac{1}{\xi} \frac{\partial}{\partial \xi} \left[\xi \frac{\partial c_i}{\partial \xi} \right] - \frac{u}{u_{avg}} (\xi) \frac{\partial c_i}{\partial \eta} + R_i(T, P, \varepsilon(\xi)) \quad (21)$$

Where

$$\tau = \frac{U_{avg} t}{R}, \quad \xi = \frac{r}{R}, \quad \text{and} \quad \eta = \frac{z}{R}$$

For each species, i , the model includes: the radial Peclet number (Pe_r), the velocity profile ($U(r)$), and the solids radial distribution ($1 - \varepsilon(r)$). How to determine these three parameters has been described above. In this general case, the solids distributed radially may be either a reactant or a catalyst. The R_i terms represent the net molar production rate of species “ i ”. Although kinetics are outside the scope of this paper, a good kinetics model, derived from appropriate laboratory and pilot plant reactors, is essential for scale-up of the process.

A non steady-state system of equations is necessary for a riser because the solids velocity profile may exhibit local values of zero or values less than zero (i.e., if the solids in the annulus flow downward along the wall). This can be seen in Figure 5 for the case of high mass fluxes and low gas velocity for FCC catalyst (Karri and Knowlton (23)). The zero and/or negative values prevent a direct integration of the steady-state form of the equation. The general solution strategy is to convert the system to a set of Ordinary Differential Equations and relax the system in time to a steady-state using a technique called the Method of Lines. The three parameters and/or empirical expressions are typically functions of gas velocity, solids mass flux, and the diameter of the column. The relative order of importance of the variables in affecting the system is: the gas velocity (U), the solids mass flux (G_s) and the column diameter (D_t). Therefore,

$$\begin{aligned} Pe_r &= f_1(U, G, D_t) \\ \varepsilon(r/R) &= f_2(U, G_s, D_t) \\ v(r/R) &= f_3(U, G_s, D_t) \end{aligned}$$

Although the scale up methods and modeling strategies presented here are general, the functions f , g , and h must be developed for a particular reactor scale-up application.

NOTATION

D, D_t	=	Column diameter, m
D_r	=	Radial Dispersion Coefficient, m^2/s or cm^2/s
D_x	=	Axial Dispersion Coefficient, m^2/s
f	=	Ratio of solids volume fraction at the wall to that at the center, (-)
Fr	=	Froude Number, $U_g/(gD)^{0.5}$, (-)
Fr_t	=	Froude Number based on terminal velocity, $U_t/(gD)^{0.5}$, (-)
G	=	Gravitational constant, m/s^2
G_s	=	Solids Mass Flux, $kg/(s \cdot m^2)$
L	=	Riser length, m
Pe_r	=	Radial Peclet Number, (-)
Pe_x	=	Axial Peclet Number, (-)
q	=	Power law exponent, (-)
r	=	Radius variable, m
R	=	Radius, m
R_i	=	Net molar production rate of species i , moles/s
U, U_g	=	Superficial gas velocity in riser, m/s
U_p	=	Particle velocity, m/s
z	=	Height variable, m
β	=	Dimensionless constant characterizing the uniformity of the riser gas velocity profile, (-)
ΔP	=	Pressure drop, kPa
ε	=	Voidage, (-)
ε_{avg}	=	Average voidage, (-)
ρ_p	=	Particle density, kg/m^3
ψ	=	Slip factor, (-)

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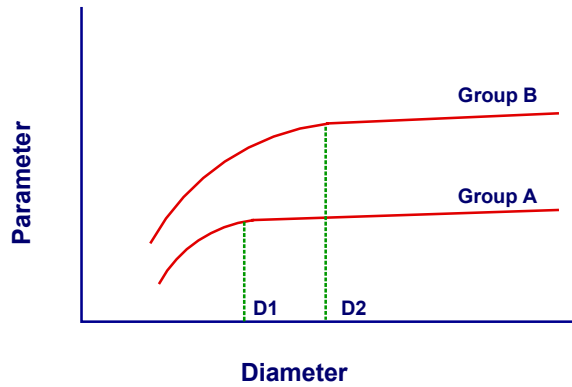


Figure 1. Effect of Diameter on Hydrodynamic Parameters

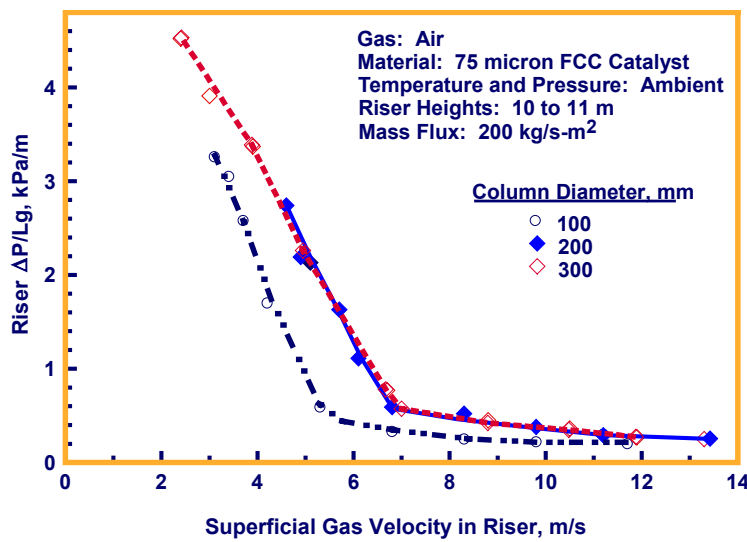


Figure 2. Riser $\Delta P/L$ vs. Gas Velocity for Different Riser Diameters

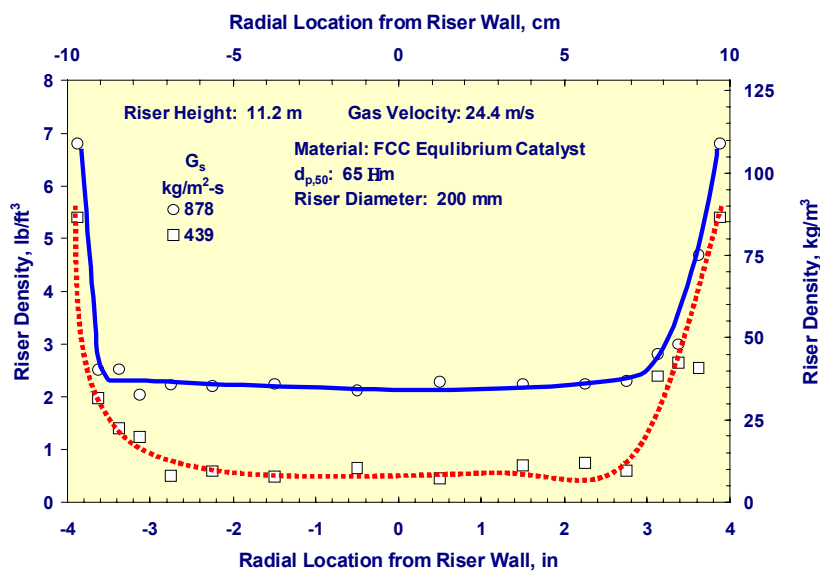


Figure 3. Riser Density as Function of Radial Position

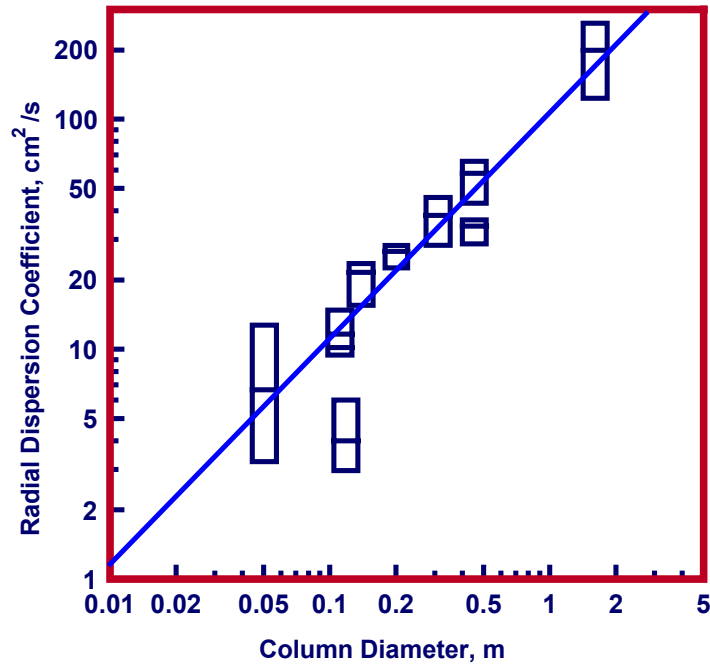


Figure 4. The Effect of Riser Diameter on the Radial Dispersion Coefficient

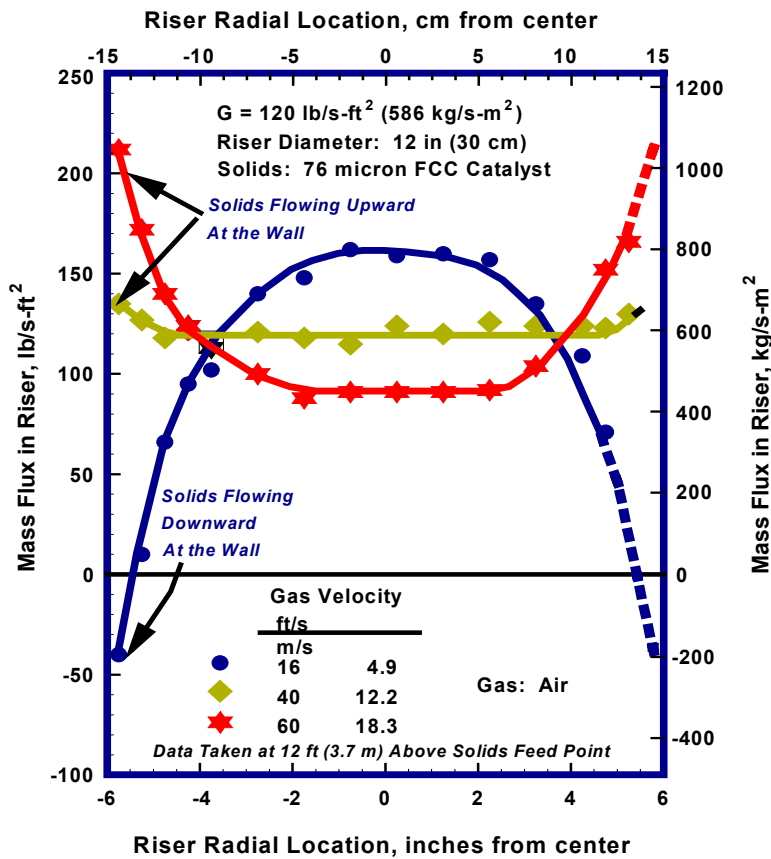


Figure 5. The Effect of Gas Velocity on the Radial Distribution of Solids Mass Flux