

Refereed Proceedings The 12th International Conference on Fluidization - New Horizons in Fluidization

Engineering

Engineering Conferences International

Year~2007

PRESENTATION SLIDES: Hydrodynamic Scale-Up of Circulating Fluidized Beds

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HYDRODYNAMIC SCALEUP OF CIRCULATING FLUIDIZED BEDS

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Scale-Up

"Scale-Up is Not an Exact Science, but is Rather That Mix of Physics, Mathematics, Witchcraft, History and Common Sense That We Call Engineering"

--- John Matsen





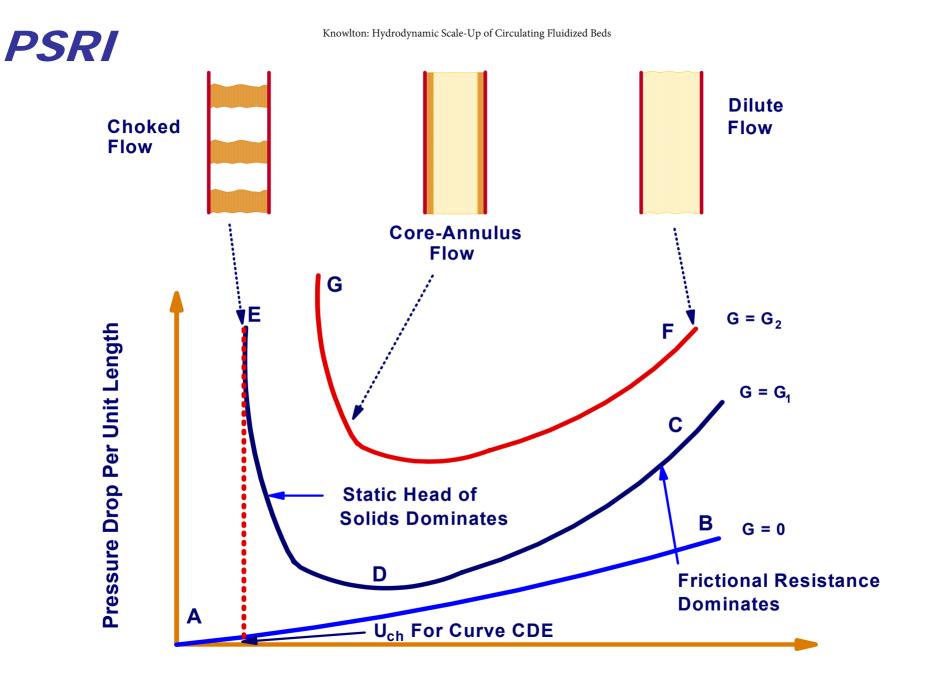
 It is Well Known That the Hydrodynamics of Small-Scale Fluidized Beds Can Differ Significantly From Those of Larger Beds

 If This Difference is Not Taken Into Account in Scale-Up, the Yields From the Large Commercial Process May be Inferior to That Experienced on a Smaller Scale





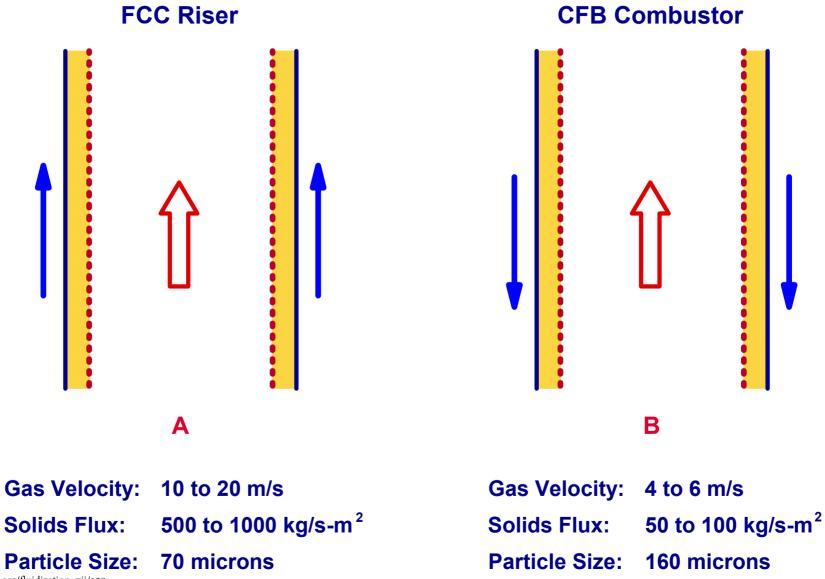
- Circulating Fluidized Beds (CFBs) Are Attractive Reactors for Conducting Moderate to Fast Heterogeneous Catalytic and Combustion Reactions
 - 1) Catalytic Cracking
 - 2) Combustion of Coal
 - 3) Methanol-to-Olefins
 - 4) Maleic Anhydride Production, etc.

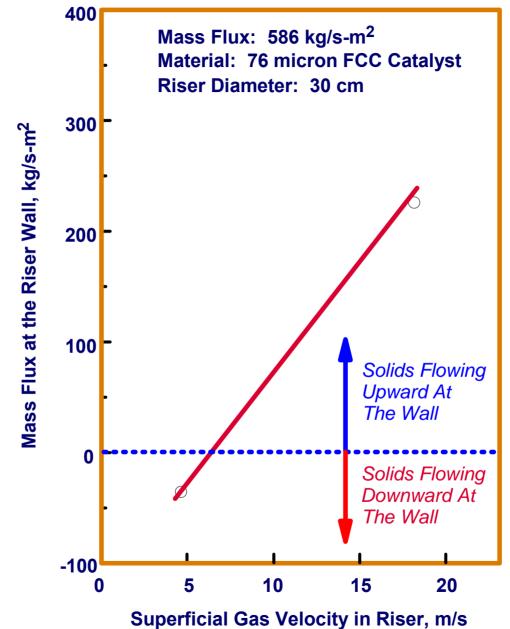


Superficial Gas Velocity, U



Annulus Flow Direction









- Mathematical Models That Adequately Describe the Hydrodynamic Mechanisms in CFBs are Valuable for Predicting Reactor Conversion and Selectivity
- The Complex Computation Fluid Dynamics (CFD) Codes are Tools That Can be Used to Extrapolate or Predict Scale-Up Parameters





 However, Using CFD Codes to Exclusively Model and Scale-Up a CFB is Extremely Risky at This Stage of CFD Development

 Although CFD is Not Ready to be Used Solely for Scale-Up, it is Now at a Point That it Can be a Useful Tool to Assist in Scale-Up if the CFD Code is Validated from Experimental Data



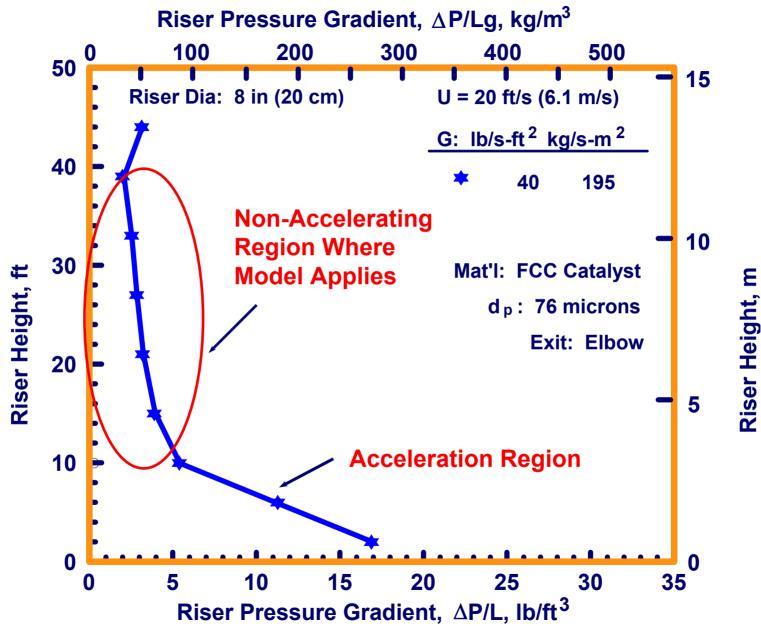


- At This Point, Simple Models Comprising Material Balances That are Superimposed on the on the CFB Solids Flow Structure are Easier to Build Than CFD Models, and Require (Relatively) Little Computer Time to Optimize
- Given a Core-Annular CFB Structure, the Information Required for Modeling/Scale-Up of a CFB is:
 - 1) the Solids Volume Fraction, (1 ε)
 - 2) How the Gas Flows Through the Solids
 - 3) Radial and Axial Gas Dispersion



Scale-Up

- This Approach Described Assumes Axisymmetric Flow, and That Gas Diffusion is Negligible or Lumped Into the Chemical Kinetics
- The Approach is Limited to the Non-Accelerating, Stead-State Section of the CFB







• Overall Approach:

1) Develop or Select a Hydrodynamic Model

2) Determine the Solids Holdup, Solids Velocity Profiles, and the Radial Gas Dispersion Coefficient in a Cold Flow Model



Hydrodynamic Model

- Development of The Hydrodynamic Model is the Basis for the Scale-Up Procedure
- The Model Can be Developed In-House or Selected From the Literature
- The Hydrodynamic Model is Generally a 2D Model That Assumes Circumferential Symmetry



Hydrodynamic Model

- It is Usually Not Necessary to Use a 3D Model Because Gas and Solids Velocity Profiles in a Riser are Generally Axisymmetric
- This Significantly Reduces the Complexity of the Modeling
- After the Model Has Been Developed/Selected, it Can be Combined With the Process Kinetics to Determine Yields and Selectivities, etc.





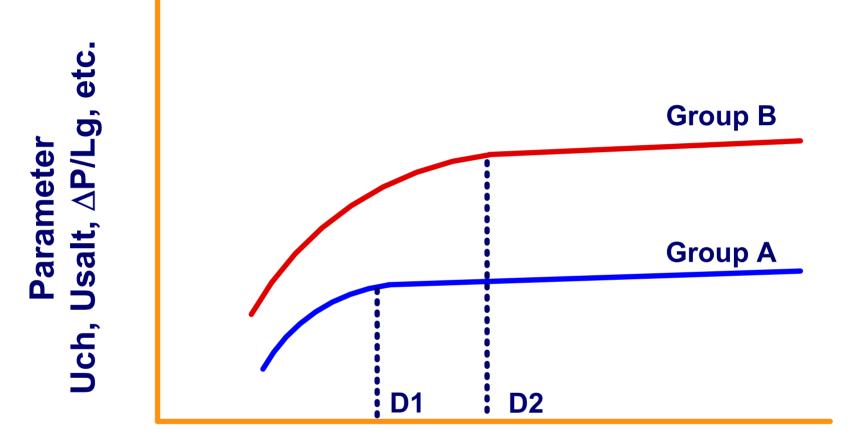
- The Most Important Hydrodynamic Parameters to Estimate for CFB Scale-Up are:
 - **1)** Solids Holdup Volume Fraction of Solids in the Suspension, (1ε)
 - 2) The Solid Velocity (or Gas Velocity) Profile in the Riser
 - 3) The Radial Gas Solids Dispersion Coefficient





- Determine Solids Holdup (1 ε), the Solids Velocity Profile, and the Radial Gas Dispersion Coefficient in a Cold Flow Model
 - 1) These Parameters can be Determined in a Cold Flow Model Operating Over the Mass Flux and Gas Velocity Ranges in the Commercial Riser
 - 2) Parameters Can Vary Significantly with Diameter for Small Diameter Risers, but Often This Effect Reaches an Asymptote After a Certain Diameter (the asymptote is often a function of particle size)





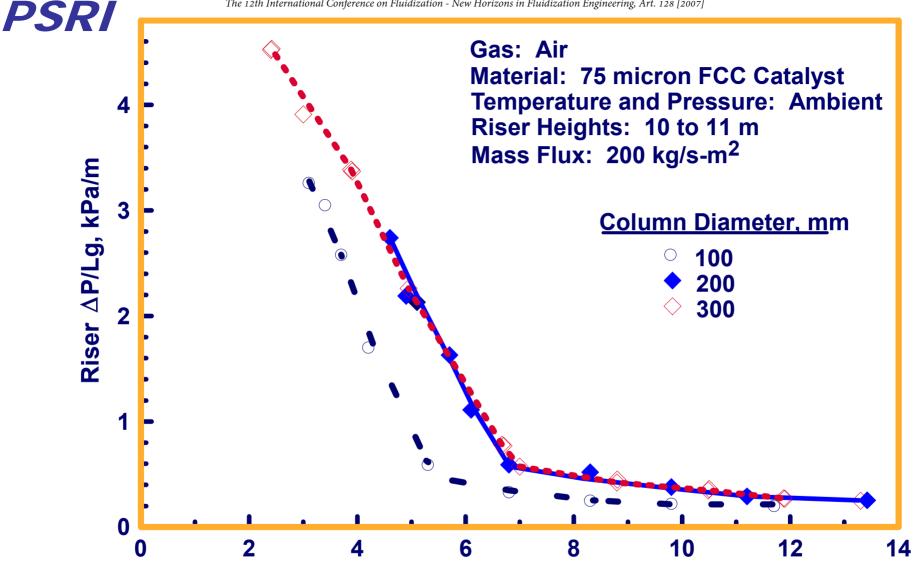
Diameter





 Measurements Have Indicated That This Asymptotic Diameter is Approximately 200 mm for Risers Operating With Group A Material

 Therefore, It is Recommended That Measurements for Scale-Up Should be Conducted in Risers of 200 mm Diameter or Larger



Superficial Gas Velocity in Riser, m/s

Effect of Column Diameter on Riser Holdup http://dc.engconfintl.org/fluidization_xii/128



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Solids Holdup (1 - \varepsilon)
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Solids Holdup is the Most Important Hydrodynamic Parameter to Predict

If Not Estimated Accurately, Yields and Selectivities Will Not be Predicted Correctly

Radial Solids Holdup

The Radial Distribution of the Solids Across the Riser can be Correlated/Predicted by a Power Law Expression Such as:

$$\frac{1-\varepsilon}{1-\varepsilon_{avg}} = \frac{q+2}{q+2f} \left[1+(f-1)\left(\frac{r}{R}\right)^{q} \right]$$

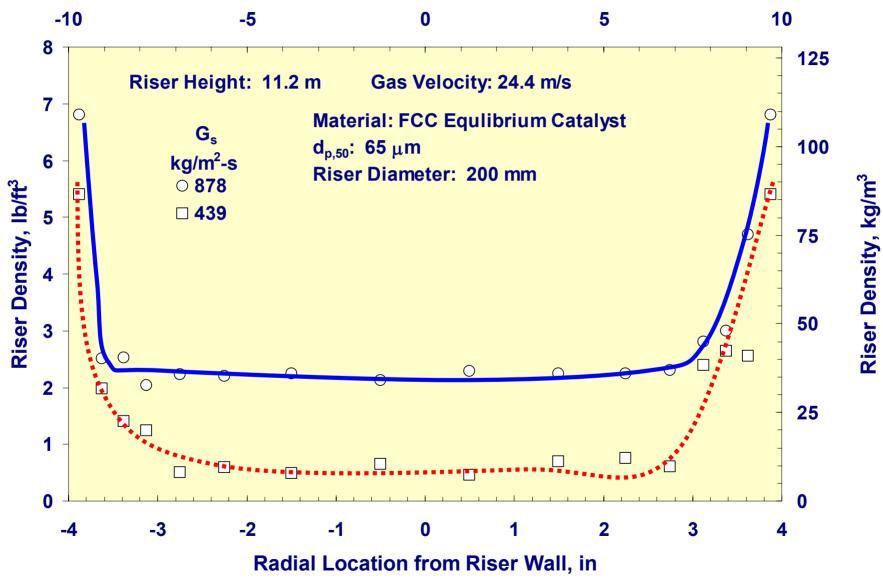
 Where f is the Ratio of the Solids Volume Fraction at the Wall Divided by That in the Center, and q is the Power Law Exponent



Radial Solids Holdup

f and q can be Determined from Data Obtained from an Optical Probe That Has Been Traversed Across the Diameter of the Riser

Radial Location from Riser Wall, cm





Axial Solids Holdup

- ΔP/Lg Measurements at Several Axial Locations in the Cold Model can be Used to Measure the Riser Slip Factor and (1 - ε)
- The Measured Slip Factors can Then be Used to Predict the Slip Factor (and (1 - ε)) in the Commercial Riser
- Alternatively, the Slip Factor can be Calculated from Correlations

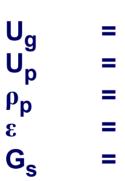


Slip Factor

Riser Slip Factor, ψ *:*

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

where:



Superficial Gas Velocity, m/s Particle Velocity, m/s Particle Density, kg/m³ Voidage, (-) Solids Mass Flux, kg/s-m²



Slip Factor

PATIENCE et al. Correlation for Slip Factor (P. Tech, <u>72</u>, 31, 1992):

$$\psi = 1.0 + \frac{5.6}{Fr} + 0.47 (Fr)_t^{0.41}$$

where: Fr = Froude Number, $U_g / (gD)^{0.5}$ Fr_t = Froude Number, $U_t / (gD)^{0.5}$ U_t = Terminal Velocity, m/s

This Correlation Calculates Slip Factor as a Function of Gas Velocity and Riser Diameter

Velocity Profiles

- Investigators Have Shown That Solid Velocity Profiles in a Riser (CFB) are Often Parabolic
- The Gas Velocity Profile Approximates the Solids Velocity Profile and:
 - 1) May be Barely Parabolic (Close to Uniform Across the Diameter) at Low Solid Mass Fluxes
 - 2) Parabolic for Moderate Solid Mass Fluxes
 - 3) Nearly Triangular/Parabolic for High Solid Mass Fluxes



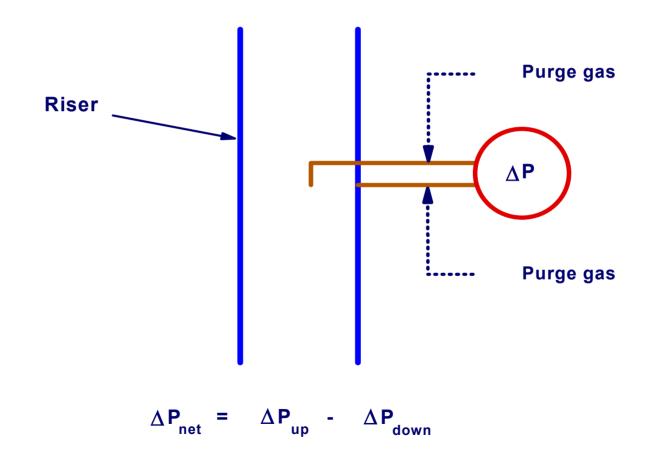
Velocity Profiles

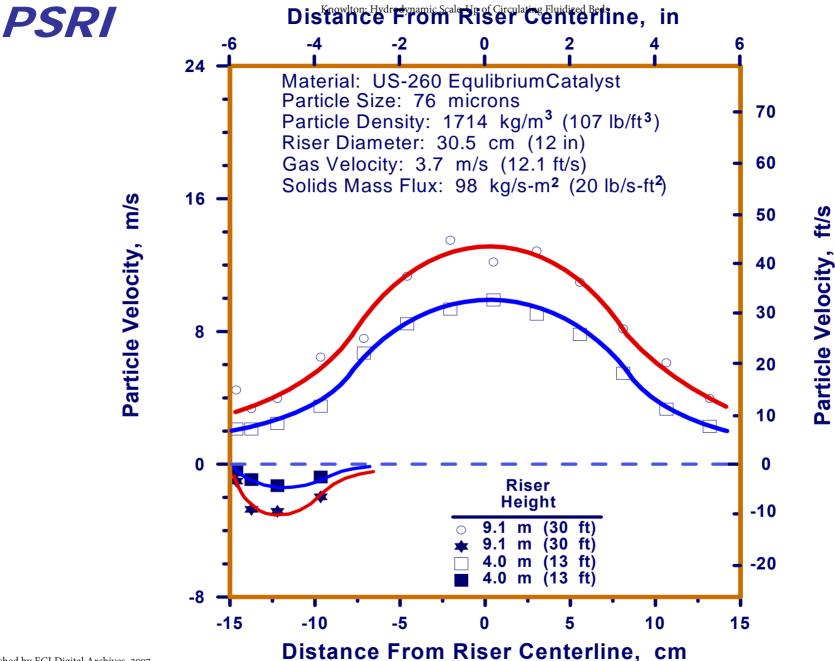
- The Local Slip Factor (at a particular radial position) is Usually Very Close to 1 in a Riser (riser solids are usually small, and the difference between the gas velocity and solids velocity is also small)
- This is Why a Pitot Tube (which measures the solids particle velocity) Can be Used to Infer the Gas Velocity Profile From the Solids Velocity Profile (An Optical Probe can Also be Used to Determine the Solids Velocity Profile)



Radial Distribution of Particle Velocity

• Determined With Purged Pitot Tube







Velocity Profiles

 The Shape of the Velocity Profile for the Solids Mass Flux and Gas Velocity Ranges Anticipated in the Commercial Riser can be Approximated in a Riser Cold Model and Measured



Axial Dispersion Coefficient

• The Axial Peclet Number is Given by:

$$Pe_x = \frac{UL}{D_x}$$

 Axial Dispersion Coefficients (D_x) Have Been Reported in the Literature to be of the Order of 0.3 to 1 m²/s



Axial Dispersion Coefficient

- The Values of D_x in a CFB are Low, Giving Rise to Large Values of the Peclet Number (of the order of several hundreds for tall CFB risers)
- Thus, Axial Mixing is Small Compared to Riser Convection (Werther et al, Martin et al) and Radial Dispersion is the Primary Mechanism Limiting the Plug Flow of the Gas
- Therefore, Axial Dispersion is Generally Considered to be Negligible in Risers

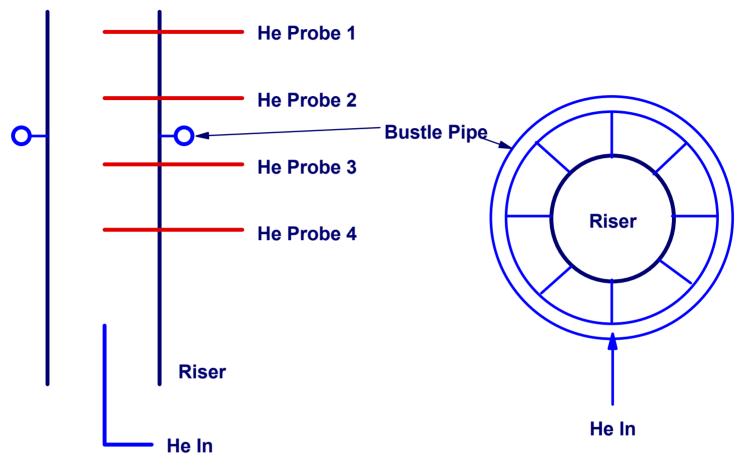
PSRI Radial Dispersion Coefficient

- Radial Dispersion Coefficients in Risers are Determined by Injecting a Continuous Tracer Gas (He, CO₂, etc.) into the Center of the Riser
- The Gas Should be Injected at a Velocity Approximately Equal to the Gas Velocity in the Center of the Riser
- Sampling Probes are Then Traversed Radially at Several Axial Locations to Measure the Tracer Concentration as a Function of Radial Position
- Knowing the Shape of the Gas Velocity Profile (determined previously) the Radial Dispersion Coefficient can be Obtained



- The Tracer Gas Can Also be Injected Circumferentially at the Wall of the Riser
- This Allows the Determination of the Amount of Gas Backmixing if the Annulus Solids Flow Downward Along the Wall
- Gas Sampling Probes are Traversed Radially Above and Below the Gas Tracer Injection Point
- The Tracer is Injected Slowly to Ensure That the Gas Stays Near the Wall (and doesn't jet into the center of the bed)





Tracer Gas Test Configurations



Typical Values of the Radial Dispersion Coefficients in CFB's

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



 Many if Not Most Workers Have Determined the Radial Dispersion Coefficients in Risers Using the Klinkenberg et al Analytic Solution

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

Where

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



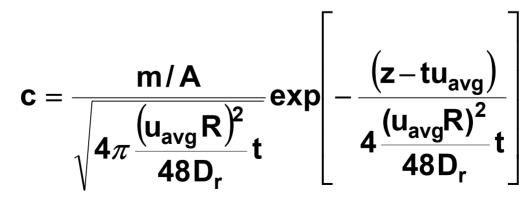
- The Klinkenberg et al Analytic Solution Employs an Average Riser Gas Velocity
- For a Non-Flat Velocity Profile, there are Two Approaches That Can be Used for Calculating/Fitting the Tracer Concentration Profile in the Riser
 - **1)** Assume a Parabolic Velocity Profile (Generally the Case in a Riser)
 - 2) Use a General or Arbitrary Velocity Profile Approach



 If a Parabolic Profile is Assumed, Then the Governing Equation is:

$$\frac{\partial \mathbf{c}}{\partial t} = \frac{\mathbf{D}_{\mathbf{r}}}{\mathbf{r}} \frac{\partial}{\partial \mathbf{r}} \left(\mathbf{r} \frac{\partial \mathbf{c}}{\partial \mathbf{r}} \right) - 2\mathbf{u}_{avg} \left(1 - \left(\frac{\mathbf{r}}{\mathbf{R}} \right)^2 \right) \frac{\partial \mathbf{c}}{\partial \mathbf{z}}$$

• The Solution to This Equation is:





 For the Arbitrary Velocity Case, the Parabolic Velocity Profile Can be Replaced by the General Ostwald-de Waele Velocity Profile

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

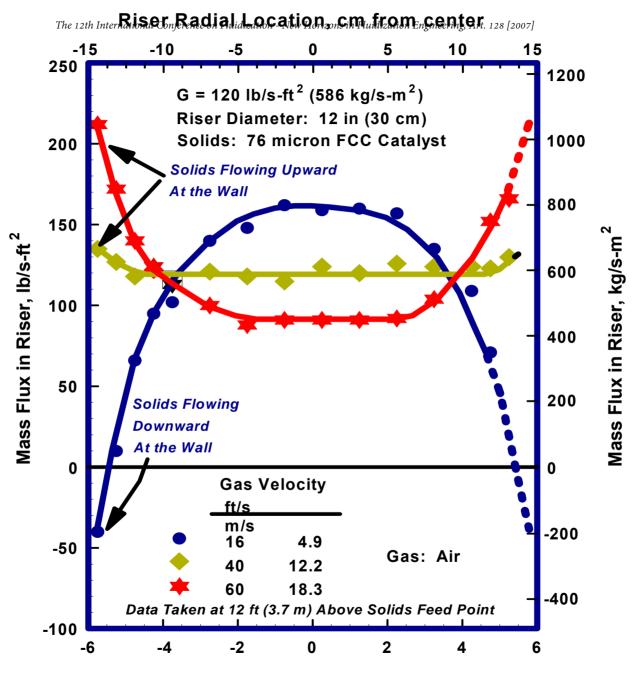
 For n = 1, the Oswald-de Waele Model Reduces to a Parabolic Velocity Profile



- The Previous Expression for the Ostwald-de Waele Velocity Profile Cannot be Applied if the Gas Velocity Profile is Negative (i.e., when the solids flow down at the wall)
- Therefore, the Following Modification to the Ostwald-de Waele Velocity Profile Has Been Proposed That Allows for Negative Components to the Gas Velocity Profile When k < 0

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

PSRI



Riser Radial Location, inches from center



• Arena Has Shown That the Axial Peclet Number is Related to the Radial Peclet Number Through the Expression:

$$Pe_x = \frac{1}{\beta Pe_r} \frac{L}{D}$$

 Where β is a Dimensionless Constant That Describes the Uniformity of the Gas Profile in a Riser



- The Value of β Changes With the Shape of the Gas Velocity Profile
- β is 1/192 for a Parabolic Velocity Profile and if the Gas Profile is Parabolic, the Expression for Pe_x Becomes:

$$Pe_x = \frac{192}{Pe_r} \frac{L}{D}$$



$$Pe_x = \frac{192}{Pe_r} \frac{L}{D}$$

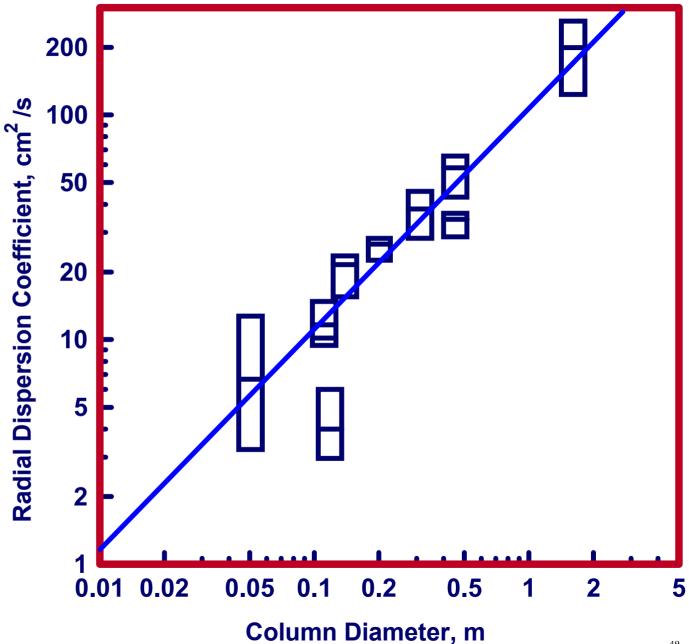
- For Plug Flow: $Pe_x \rightarrow \infty$ For Fully Backmixed Flow: $Pe_x \rightarrow 0$
- A Low Radial Peclet Number is Desired IF Plug flow is Wanted in a Riser
- Increasing D_r (Which Decreases the Value of Pe_r) is also Desired if Plug Flow is Wanted



- Namkung and Kim Presented a Log-Log Plot Indicating That the Radial Dispersion Coefficient Increased (Approximately Linearly) with Reactor Diameter
- This Suggests That the Radial Peclet Number is Relatively Constant Within the CFB Flow Regime, and also That Radial Dispersion Will Increase at the Same Rate That the Riser Diameter Increases



Radial Dispersion Coefficient vs. Riser Diameter (Namkung and Kim)





 Log-Log Plots Can Often Mask the True Variability in a Parameter

 Therefore, it is Recommended That the Radial Dispersion Coefficient be Measured With the Actual Solids Over the Same Gas Velocity and Solids Mass Flux Ranges to be Used in the Commercial Riser



Overall Approach

• A General Combined Hydrodynamic and Kinetic Model in Dimensionless Form is:

$$\frac{\partial \mathbf{c}_{i}}{\partial t} = \frac{1}{\mathbf{P}\mathbf{e}_{r}} \frac{1}{\xi} \frac{\partial}{\partial \xi} \left[\xi \frac{\partial \mathbf{c}_{i}}{\partial \xi} \right] - \frac{\mathbf{u}}{\mathbf{u}_{avg}} (\xi) \frac{\partial \mathbf{c}_{i}}{\partial \eta} + \mathbf{R}_{i} (\mathbf{T}, \mathbf{P}, \varepsilon (\xi))$$

$$\tau = \frac{\mathsf{U}_{\mathsf{avg}} \mathsf{t}}{\mathsf{R}} \qquad \xi = \frac{\mathsf{r}}{\mathsf{R}} \qquad \eta = \frac{\mathsf{z}}{\mathsf{R}}$$

Overall Approach

- The Zero and Negative Values Prevent a Direct Integration of the Steady-State Form of the Equation
- The Three Parameters: Pe_r, U(r), and (1 ε(r)) are Functions of Gas Velocity, Solids Mass Flux and Riser Diameter
- The Relative Order of Importance of Variables Affecting the Riser is:
 - 1. Gas Velocity
 - 2. Solids Mass Flux
 - 3. Tube Diameter



- The Model Incorporates:
 - 1) The Radial Peclet Number, Per
 - 2) The Velocity Profile, [U(r)]
 - 3) Solids Radial Distribution, [1 ε (r)]
 - 4) A Reaction Term, R_i
- A Non- Steady State Model is Necessary for a Riser Because the Gas Velocity Profile May Have Negative or Zero Values (i.e., if the solids in the annulus flow downward along the wall)
- Although the Scale-Up Methods and Modeling Strategies are General, the Values of the Pe_r, [U(r)], and [1 - ε(r)], Must be Determined for the Particular Riser In Question