Numerical Methods for Poly-Disperse Particles in Circulating Fluidized Beds

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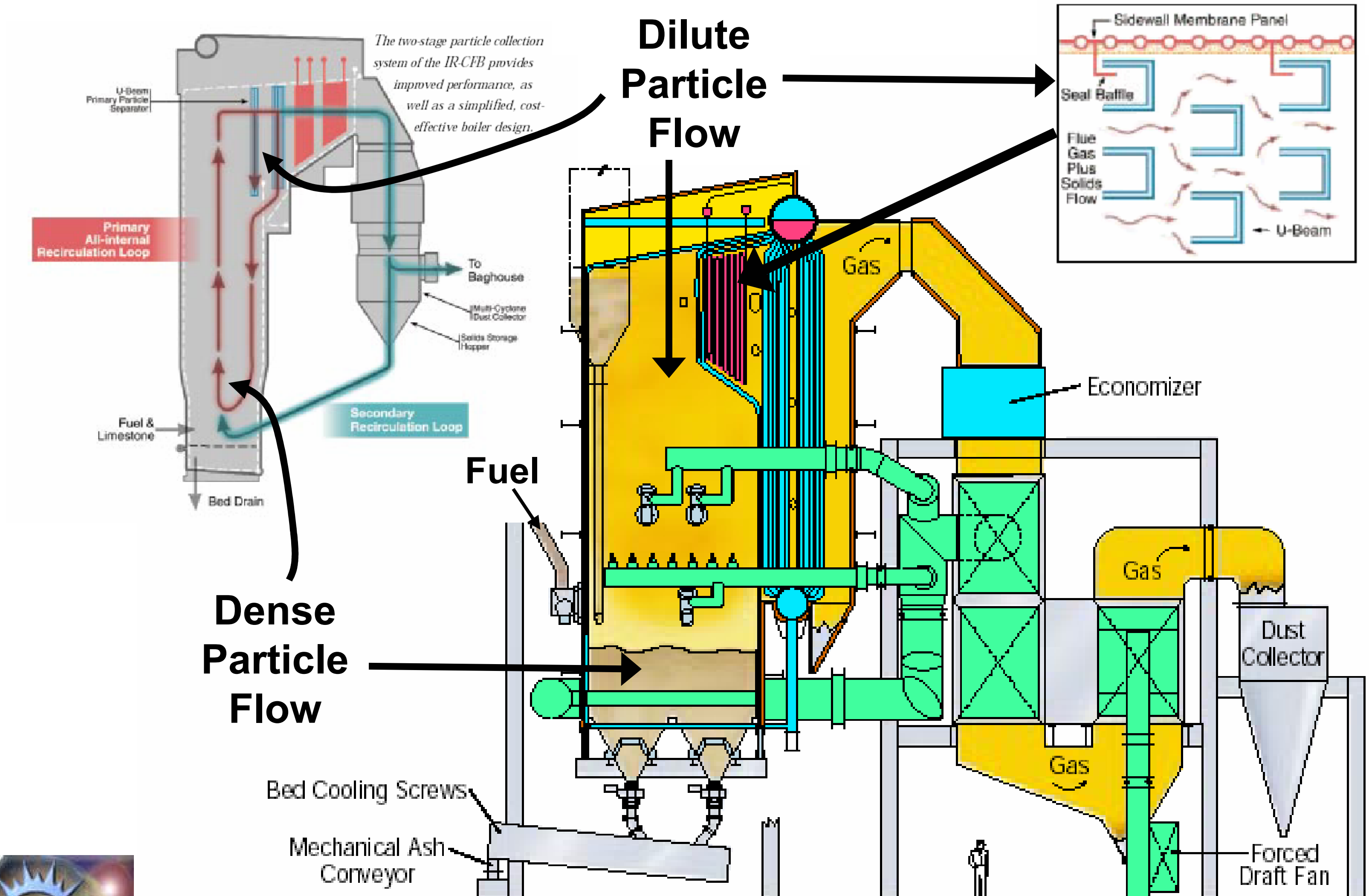
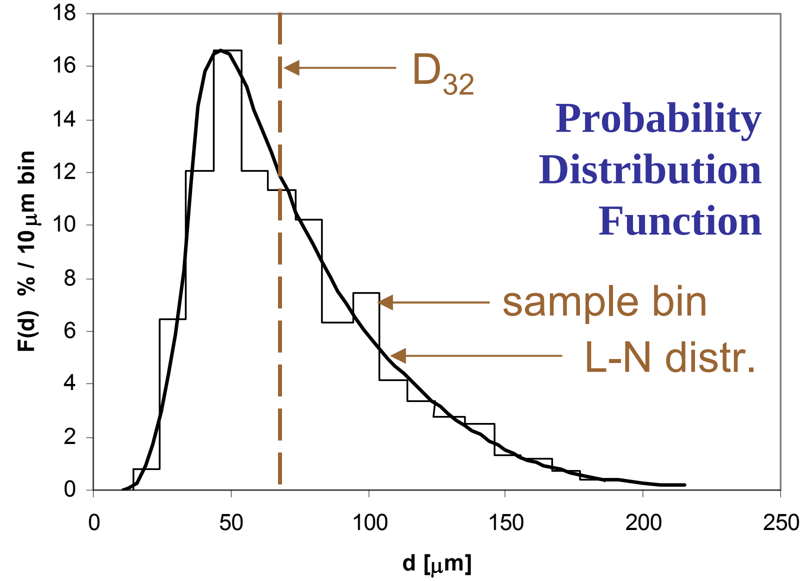
Typical Circulating Fluidized Beds



Dense Flow Issues

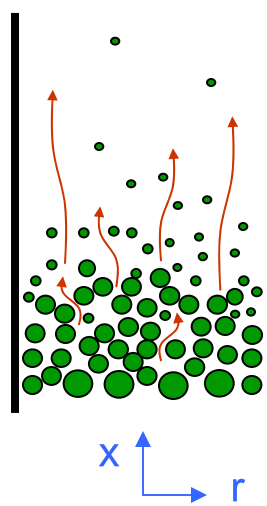
Polydisperse Particle Size Distributions

- Fluidized Beds can have a *wide* distribution of particle sizes, e.g. a range of minimum to maximum diameters of ten or more



- The range of terminal velocities (and thus momentum transfer) typically is even greater such that fully-mixed assumption may not reasonable for many parts of the flow

- In fluidized beds, the particle diameter (and particle relative velocity) can vary significantly with vertical height (x) and radial location (r), and can thus be crucial to local combustion physics and overall performance



MFIX Capabilities

- MFIX is a DOE state-of-the-art continually-developing numerical methodology which uses Partial Differential Equations (PDEs) to describe the unsteady 3-D dynamics of particle collisions, mixing, vaporization, and combustions in a fluidized bed.

- MFIX currently employs two primary techniques to simulate the behavior of a *wide* particle size distributions:

  – Use a single average particle diameter (D_{avg}): this technique is computationally efficient but does *not allow* a prediction of the variation of particle diameter with vertical height or radial distance

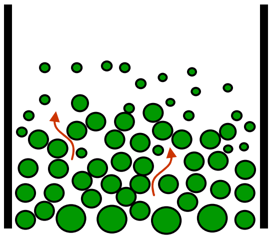
  – Use several particle bins, each with it's own average diameter: this technique *does allow* prediction of particle diameter variation with vertical height and radial distance, but is not typically used due to computational expense as *each* bin typically requires the inclusion of four new PDEs

Dense Flow Numerical Issues

1) If a single diameter can be used, what is the appropriate mean particle diameter in terms of relative velocity, evaporation, and combustion?

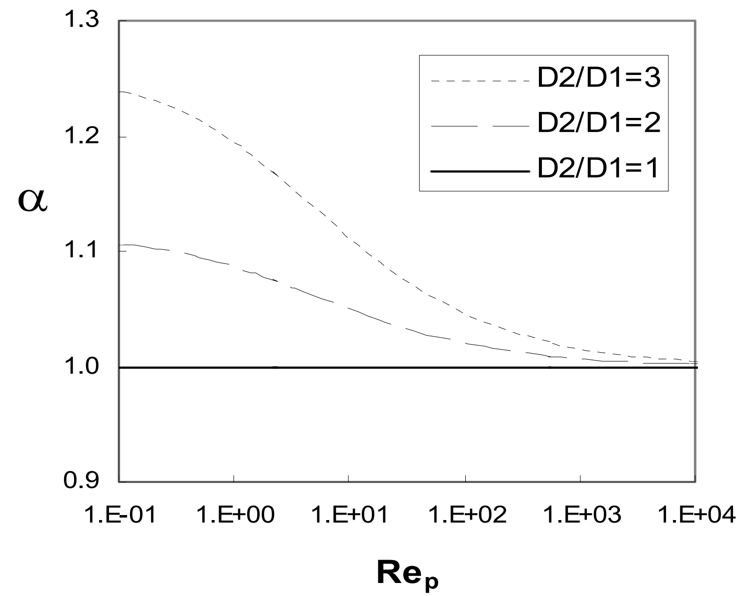
2) Under what conditions is the use of a single average diameter unreasonable, i.e. when are the bin-based techniques appropriate and how many bins are needed for a required accuracy?

3) Are there new numerical techniques which can provide the accuracy of multiple-bin methods but at significantly lower computational costs?



Appropriate Mean Particle Diameter

- Recent research by Loth, O'Brien, Syamlal & Cantero (2003) has shown that the correct average diameter (D_{avg}) based on group relative velocity is a function of particle Reynolds number and width of size distribution. The results were experimentally validated and yield the following limits:
  - $D_{avg} = D_{32}$, i.e. Sauter mean diameter, for large particles, e.g. D > 4000 μm
  - $D_{avg} = D_{31}$, i.e. volume-width diameter, for small particles, e.g. D < 100 μm



Ratio of particle terminal velocity computed with Sauter Mean Diameter vs. computed with correct diameter (binary mixture with D2 and D1 sizes)

- Similar analysis can be conducted to determine the average diameter based on group evaporation and combustion rate

Method of Moments & PDF Transport Method

- **QUADRATURE METHOD OF MOMENTS** was recently developed by Fox (Iowa State) to be compatible with MFIX type of codes. It considers a finite number of moments ($N_{moments}$) to describe the PDF where each moment has it's own transport equations, and in this sense is similar to the conventional bin-based methods (for which void fraction and momentum equations are used for each particle size). However, the number of moments needed to accurately described the PDF evolution is generally much smaller than that required by bin-based methods, e.g. 4-5 are typically needed.

- **PDF TRANSPORT METHOD** employs an assumed PDF shaped (e.g. Log-Normal distribution) and yields two additional transport equations to quantify this distribution: one for a mean diameter (e.g. D_{32}) and one for the variance about this mean (σ). The resulting transport equations yields correct drag-gravity balance and reactive mass-transfer balance as long as presribed PDF shape is reasonably representative of distribution.

Poly-disperseTechniques	Coded?	D(x,r)?	# of PDEs (3-D)
Effective Mean Diameter	yes	no	5
Bin-Based Method	yes	yes	$5N_{bins}$
Method of Moments	~ yes	yes	$5N_{moments}$
PDF Transport Method	no	yes	7

Potential Plan Forward: Dense Flows

- Select a typical fluidized bed with various particle size distributions and apply current MFIX approach with both the average diameter method and the bin-based method (e.g. resolutions of N_{bin} from 2-10) and:
  - Simulate 1-D steady flow and compare w/ 1-D exact solution
  - Simulate 2-D steady & unsteady flow and compare with above & exp. data
  - Simulate 3-D unsteady flow and compare with above

- From this, examine the effect of bin resolution & flow dimensionality on:
  - Accuracy of predicting overall bed expansion for a given gas flow rate
  - Accuracy of predicting mean vertical and radial distributions of particle size
  - Accuracy of predicting evaporation and combustion rates as a function of vertical and radial coordinates
  - Typical CPU and memory requirements (w/ & w/o parallel computing)

- Develop and employ a PDF transport method (perhaps also employ the Quadrature Method of Moments) to examine as above; in particular, examine potential improvements on accuracy and computer requirements

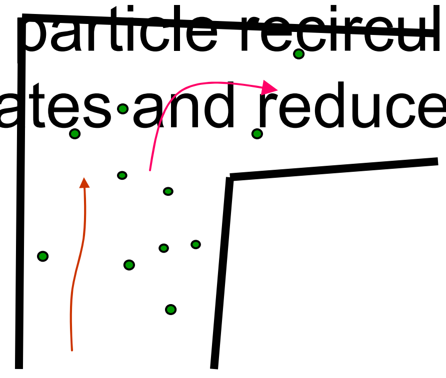
Dilute Flow Issues

Dilute Flow Numerical Issues

1) What is the dilute (above the fluidized bed) particle diameter variation in space for regions such as risers, heat exchangers and particle separators, where gas flow turbulence dominates particle distributions and particle deposition?

2) How do wall collisions and particle separators (e.g. U-beam) affect particle size distribution?

3) Are there geometries (e.g. non-uniform U-beam designs or counter-swirl column shapes) that can improve the efficiency of particle recirculation to allow increased through-flow rates and reduced pollutants?



Turbulent Diffusion of Particles

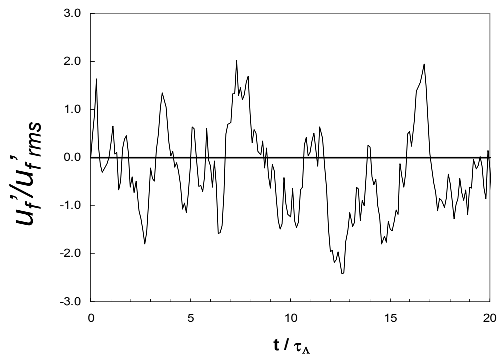
Bocksell & Loth (2002) have developed numerical methods to predict particle diffusion based on stochastic random walk techniques:

$$u_{fi} = \overline{u_{fi}} + u_{fi}'$$

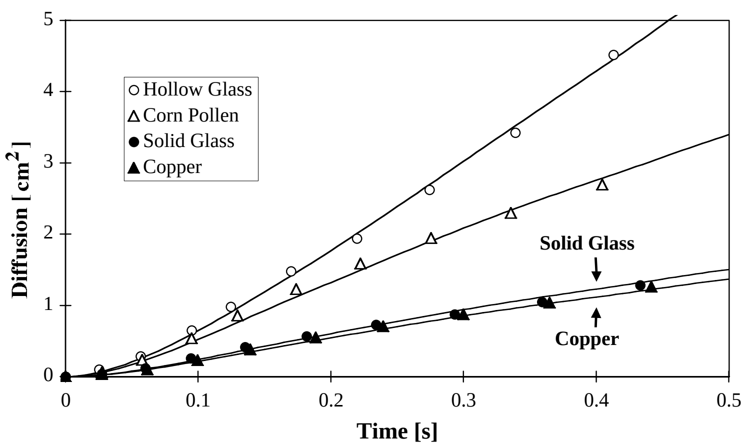
RNG

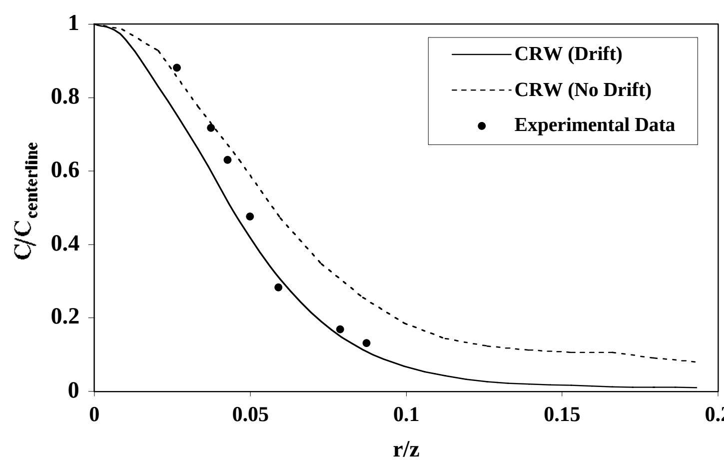
$$u'_{fi}(t+\Delta t) = \alpha_i u'_{fi}(t) + \left\{\left(\delta_{ji} - \alpha_{ij}^2\right)\sigma_{ij}^2\right\}^{1/2}\varphi_i + \delta\overline{u'_{fi}}$$

$$\delta\overline{u'_{f_j}} = \Delta t\left(\frac{\partial\overline{u'_{f_j}u'_{f_i}}}{\partial x_j}\right) \qquad \sigma_{u_j} = u'_{rms,j} = \left(\frac{2}{3}k\right)^{1/2} \qquad \alpha_i = \exp\left(-\Delta t/\tau_\Lambda\right)$$



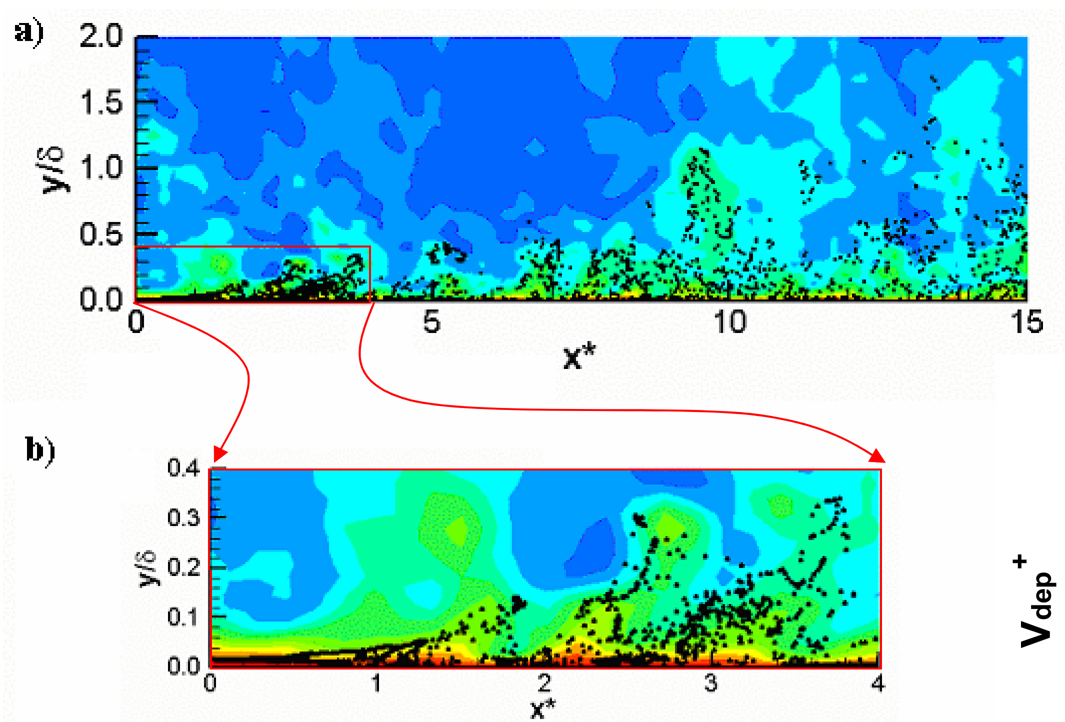
Particle diffusion accurately predicted for channel flow and jet flow:

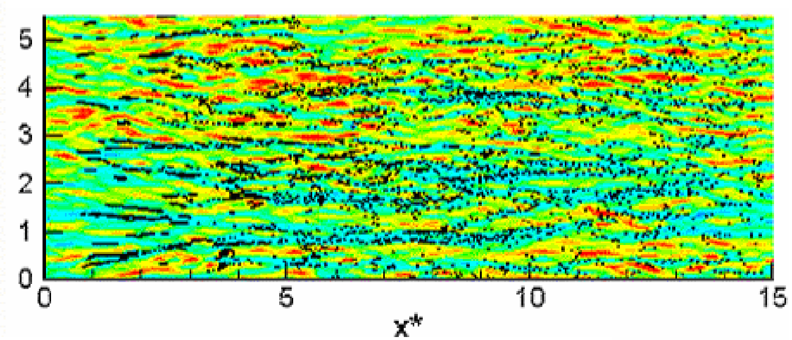


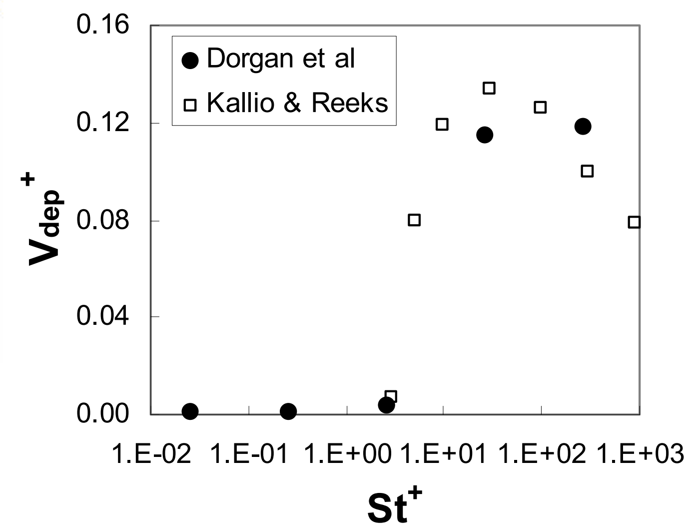


Boundary Layer Simulations with Particles

Dorgan & Loth (2003) have simulated particles in the near-wall region and developed technique to model wall-collisions and turbophoresis effects (important since gradients in turbulence are high)







KEY: particle locations (dots) and streamwise velocity (color contours)

Potential Plan Forward: Dilute Flows

- Use a relevant riser flow with various particle size distributions and apply current MFIX approach with both the average diameter method and the bin-based method (with various resolutions e.g. N_{bin}= 2-10) to:
  - Simulate 2-D steady flow and compare with available experimental data
  - Simulate 3-D unsteady flow and compare with above

- From this, examine the effect of bin resolution & flow dimensionality on:
  - *Accuracy* of predicting *particle-wall collisions and deposition rates*
  - Accuracy of predicting mean spatial distributions of particle size
  - Accuracy of predicting *particle separation effects*
  - Typical CPU and memory requirements (w/ & w/o parallel computing)

- Employ our Stochastic Particle Dynamics method (with and without LES) for the above studies to note its potential improvements on accuracy and computer requirements

- Consider possible changes to riser/separator geometries for improved particle recirculation, flow mixing, particle separation, etc.