Experimentation, CFD and Reactor Models: Complementary Tools for Resolving Challenging Issues in Fluidization

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Key Steps in Building and Validating Models

1. Initial Experimental Observations
2. Conceptual Model
3. Equations Describing Model
4. Numerical Solutions of Equations
5. Compare Predictions with Experimental Results
   - Acceptable deviations
   - Unacceptable deviations

6. Verification of Numerical Solutions
7. Plan New Experiments
8. Carry out Experiments
Background

It is well understood, though not always acted on, that experimental validation is essential for successful application of CFD codes to difficult multiphase flows like fluidized beds. This presentation will attempt to outline some cases where the interaction can potentially go further, providing information that otherwise would be virtually impossible to gather.
Physical Experiments

Reactor Models

CFD

Tri-Partite Interactions
<table>
<thead>
<tr>
<th>Type</th>
<th>Model Complexity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Purely empirical correlations</td>
<td>Simple; may even lack dimensional consistency</td>
</tr>
<tr>
<td>Empirical correlations based on dimensional analysis</td>
<td>Usually involves multivariate regression.</td>
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<tr>
<td>Semi-empirical: mechanistic plus fitted constant(s)</td>
<td>Usually results in explicit equation or equations.</td>
</tr>
<tr>
<td>Physical “cold models” for dynamically similar expts.</td>
<td>Requires geometric scaling and matching of Π groups</td>
</tr>
<tr>
<td>Fully mechanistic models</td>
<td>Requires solution of set of DEs or algebraic eqns.</td>
</tr>
<tr>
<td>Comprehensive models based on physical laws, balances</td>
<td>Numerical solution, e.g. via CFD codes</td>
</tr>
</tbody>
</table>
1. Experimental Evidence from Axial Gas Mixing Related to Wall Particle Slip Boundary Condition

- Gas backmixing in fluidized beds is important in determining the conversion and selectivity in fluidized bed reactors.
- It is often measured experimentally using a tracer (e.g. helium) injected at one level and then detected upstream:
Axial Gas Mixing in Fluidized Beds

• Consider a steady state back-mixing test as shown below.
• Gas backmixing in fluidized beds is caused by drag by particles descending near the outer walls.
• Commonly this is modelled (erroneously) as axial dispersion (diffusion-like process).

Li Tingwen, Zhang YM, Grace JR and Bi XT, Numerical investigation of gas mixing in gas-solid fluidized beds, AIChE Jl., in press.
Biased Gas Sampling

Fig. 5. Vertical gas concentration profile of regenerator.
* Same numerical scale as gas concentration.
Physical System Modelled

76 mm i.d. x 1.830 m tall column studied by Mason (1950) with 155 µm glass beads and helium tracer injected at $z = 1.05$ m

- CFD Eulerian-Eulerian model
- Kinetic granular theory
- 3-D simulation, ~100,000 grid points
- Fluent 6.3
- Little influence of coefficient of restitution or turbulent diffusivity.
- Johnson & Jackson partial slip B.C. at wall.
Effect of Wall B.C. on Backmixing

Influence of specularity coefficient on lateral profiles of upstream tracer concentration: 2-D simulations

Influence of specularity coefficient on lateral profiles of upstream tracer concentration: 2-D simulations
Axial profiles of mean tracer concentration predicted by 3-D simulations at $r = 0$ for $U_g =$ (a) 0.183 m/s; (b) 0.274 m/s; (c) 0.354 m/s
Axial profiles of mean tracer concentration predicted by 3-D simulations at \( r = 36 \text{ mm} \) for \( U_g = \) (a) 0.183 m/s; (b) 0.274 m/s; (c) 0.354 m/s.
Radial profiles of mean tracer concentration above injection level
Radial profiles of mean tracer concentration at $z = 1.0 \text{ m}$ for $U_g = (a) 0.183 \text{ m/s}; (b) 0.274 \text{ m/s}; (c) 0.354 \text{ m/s}$. 
Radial profiles of mean tracer concentration at $z = 0.9$ m for $U_g =$ (a) 0.183 m/s; (b) 0.274 m/s; (c) 0.354 m/s.
2-D vs 3-D Simulations

Radial profiles of time-average gas vertical velocity and tracer concentration by 2-D and 3-D simulations.
Parametric Studies

2-D simulations were used to conduct parametric studies

– Bed height
– Tracer flow rate
– Particle-particle restitution coefficient
– Turbulence diffusivity
– Wall boundary condition

Lesson: Solid-phase wall boundary condition needs to be specified with great care when modelling mixing. Free slip, partial slip and no-slip boundary conditions give substantially different gas backmixing.
Summary: Effect of Wall B.C.

- Specularity coefficient has a significant impact on the flow hydrodynamics near the wall.

- Since gas backmixing is initiated by drag of the descending particles at the wall, it is sensitive to the specularity coefficient in the range 0 to 0.05.

- Experimental backmixing measurements may then provide a means of specifying the specularity coefficient.
2. How Representative are Two-Dimensional Fluidized Beds?

• Thin fluidized beds, commonly referred to as “two-dimensional”, are often used both as educational tools and to gain quantitative information that might help understand the behaviour of fully three-dimensional columns.

• The idea is that should provide a view of a slice through a fully 3-D column.

• How “two-dimensional” are they?

• Also relevant to the question of whether 2-D simulations can be used for real 3-D columns.
Experiment & Simulation Set-up

• Experiment
  – 2-D bubbling fluidized bed of Laverman et al. 2008
  – Geometry: 0.3 x 0.7 x 0.015 m; $U = 0.27$ & $0.45$ m/s
  – Mean particle diameter: 485 µm

• Simulation:
  – MFIX
  – Johnson and Jackson (1987) B.C.s
  – $e_w = 0.95$; $\varphi = 0, 0.005, 0.05, 0.5$

Numerical Simulation cont’d

- Simulation setup and results
Lateral profile of time-mean voidage at $z = 0.2$ m for $U_g = 2.5U_{mf}$ predicted by 2-D and 3-D simulations. Simulation time: 70 s for 2-D; 10 s for 3-D.
Lateral profile of time-mean vertical solid velocity at $z = 0.2$ m for $U_g = 2.5 U_{mf}$ predicted by 2-D and 3-D simulations. Simulation time: 70 s for 2-D; 10 s for 3-D.
Bubble Diameter Averaging Methods

Equivalent bubble diameter:

• Diameter average:
\[ \overline{D}_{b,eq} = \frac{\sum D_{b,eq}}{N} \quad D_{b,eq} = \sqrt{\frac{4A}{\pi}} \]

• Area average:
\[ \overline{D}_{b,eq} = \sqrt{\frac{4\overline{A}}{\pi}} \quad \overline{A} = \frac{\sum A}{N} \]

where \( A \): void frontal area
and \( N \): total bubble number.
Effect of Averaging Method

Mean bubble diameters calculated by two methods: $U_g = 1.5 U_{mf}$; $e_w = 0.8$; $\phi = 0.05$; $D_{b_{min}} = 2.5$mm; 3-D simulation.
Effect of Bubble Boundary

Mean bubble diameters calculated with different bubble definitions ($U_g = 1.5 U_{mf}$; $\Phi = 0.05$; $D_{b,\text{min}} = 2.5$ mm; 3-D simulation).
Effect of Minimum Bubble Diameter

Mean bubble diameter calculated with different minimum bubble sizes ($U_g = 1.5 U_{mf}$, $\phi = 0.05$; $\varepsilon_{bndy} = 0.8$; 3-D simulation).
Lateral profiles of time-mean solid velocity at (a) $z = 0.105$ m; (b) $z = 0.245$ m for $U_g=2.5U_{mf}$.

Red: 3-D Simulations
Blue: 2-D Simulations
Comparison with Experimental Bubble Diameters

Predicted mean bubble diameters compared with experimental data for (a) $U_g = 1.5U_{mf}$; (b) $U_g = 2.5U_{mf}$ ($\varepsilon_{bndy} = 0.8$; $D_{b,\text{min}} = 5$ mm, diameter average).

Red: 3-D Simulations
Blue: 2-D Simulations
Comparison with Experimental Bubble Rise Velocities

Average bubble rise velocity versus mean bubble diameters for (a) $U_g = 1.5 U_{mf}$; (b) $U_g = U_{mf}$.
Effect of Particle/Wall Restitution Coefficient

Lateral profiles of time-mean (a) voidage, and (b) solid velocity at $z = 0.2$ m for different particle-wall restitution coefficients; 2-D simulations.
Effect of Wall Specularity Coefficient

Lateral profiles of time-mean (a) voidage, and (b) vertical solid velocity at $z = 0.2$ m for different specularity coefficients; 2-D simulations; $U_g = 1.5U_{mf}$
Effect of Wall Specularity Coefficient

Lateral profiles of time-mean (a) voidage, and (b) vertical solid velocity at $z = 0.2$ m for different specularity coefficients by 2-D simulations; $U_g = 2.5U_{mf}$. 
Summary: 2-D vs. 3-D Columns

- Wall boundary solid phase boundary condition again needs to be specified with great care.
- 3-D simulation of 2-D column is needed.
- Many factors, including bubble definition, minimum detectable bubble size, and averaging method, must be considered when comparing simulation predictions with experimental results.
3. Change in Volumetric Flow

- The volumetric flow of gas in fluidized beds reaction may vary with height due to:
  - Chemical reactions: mole change:
    - e.g. \( \text{CH}_4 + 2\text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + 4\text{H}_2; \)
  - Decrease of flow due to gas addition or removal through jets or membranes;
  - Changes in temperature and/or pressure;
  - Change of phase: drying, condensation.
Numerical Model

• 2-D simulation of change of volumetric flow in fluidized bed
  – Drying/condensation and Ozone decomposition reaction \(\text{O}_3 \rightarrow 1.5\text{O}_2\)
  – 485 \(\mu\text{m}\) glass beads, same Laverman et al. column (0.015 x 0.3 x 0.7 m)

• Numerical model
  – Eulerian-Eulerian model
  – MFIX
### Drying and Condensation

#### Simulation conditions

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Cases</th>
<th>Condensation</th>
<th>Base Case</th>
<th>Drying</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U_{g,\text{bottom}}$, m/s</td>
<td>0.24</td>
<td>0.24</td>
<td>0.24</td>
<td>0.24</td>
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<tr>
<td>$U_{g,\text{exit}}$, m/s</td>
<td>0.185</td>
<td>0.24</td>
<td>0.287</td>
<td></td>
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<tr>
<td>$U_{g,\text{exit}}-U_{mf}$, m/s</td>
<td>-0.009</td>
<td>0.046</td>
<td>0.093</td>
<td></td>
</tr>
</tbody>
</table>
Drying and Condensation

Snapshots of voidage contours for condensation (left), base case (middle), and drying (right).
Bubble Characteristics

Variation of average bubble diameter (left) and shape factor (right) with height for base case compared with cases with condensation and drying.
Chemical Reaction

Particle diameter = 0.50 mm

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Cases</th>
<th>$3\text{O}_2\rightarrow2\text{O}_3$</th>
<th>Base case</th>
<th>$2\text{O}_3\rightarrow3\text{O}_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U_g$, bottom, m/s</td>
<td>0.24</td>
<td>0.24</td>
<td>0.24</td>
<td>0.24</td>
</tr>
<tr>
<td>$U_g$, exit, m/s</td>
<td>0.208</td>
<td>0.24</td>
<td>0.277</td>
<td></td>
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<tr>
<td>$U_g$, exit-$U_{mf}$, m/s</td>
<td>0.014</td>
<td>0.046</td>
<td>0.083</td>
<td></td>
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</tbody>
</table>

Particle diameter = 0.20 mm

<table>
<thead>
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<th>Parameters</th>
<th>Cases</th>
<th>$3\text{O}_2\rightarrow2\text{O}_3$</th>
<th>Base case</th>
<th>$2\text{O}_3\rightarrow3\text{O}_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U_g$, bottom, m/s</td>
<td>0.09</td>
<td>0.09</td>
<td>0.09</td>
<td></td>
</tr>
<tr>
<td>$U_g$, exit, m/s</td>
<td>0.077</td>
<td>0.09</td>
<td>0.112</td>
<td></td>
</tr>
<tr>
<td>$U_g$, exit-$U_{mf}$, m/s</td>
<td>0.039</td>
<td>0.052</td>
<td>0.074</td>
<td></td>
</tr>
</tbody>
</table>
Summary: Effect of Volume Change

• For coarse particles, bubble size is predicted to increase or decrease significantly due to volumetric flow changes in the dense phase.
• For fine particles, changes in bubbles size are predicted to be small for volumetric flow changes in the dense phase.
• Defluidization might occur for decreases in volumetric flow, but this needs further study.
• Experimental work is in progress on effect of step changes (up and down) in pressure.
4. Particle Velocity/Travelling Fluidized Bed

Column designed & constructed to travel from location to location. Co-application by a team of researchers from five Canadian universities (UBC, Calgary, Saskatchewan, Western Ontario, Ecole Polytechnique) funded by NSERC.


2. Provide a unique comprehensive database for validation of CFD codes.

3. Provide a method for evaluating probes that can be deployed in industrial units.
Traveling fluidized bed (TFB) column: a) assembled, b) exploded modular view

Example of difference in measured mean particle velocities.
One Dilemma

• Reasonably good agreement with respect to voidage measurements from different techniques
• However, significant differences between particle velocity measurements for:
  ➢ **Radioactive particle tracking**: (Chaouki et al.) follow a single particle trajectory over a very long time period.
  ➢ **Optical probes**: cross-correlate signal from particles passing vertically aligned fibres.

Can CFD help sort out whether the differences are reasonable?
RPT experiment schematic

Lead Shielding

Argon Injection

Nal detector

Optical fibre probe
Other Areas for Complementary Work

• Effect of electrostatics on hydrodynamics and entrainment;
• Non-uniformity of multiphase flow through identical parallel paths;
• Determining bubble properties from pressure fluctuations;
• Distributor: influence of the windbox on hydrodynamics;
• Fluidization of particles of extreme shapes, e.g. biomass particles;
• Dynamics of liquid-fluidization inversion;
• Jets entering fluidized beds;
• Fluidization around baffles, e.g. sheds.
Acknowledgement

- Tingwen Li, Xiaotao Bi, Yongmin Zhang, Andrés Mahecha-Botero, Kristian Dubrawsky

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