Gravity-based percolation of small particles through an assembly of large particles

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**Context: Chemical-Looping Combustion**

### Coal-fueled Options

- **Syngas-CLC**
  - Air reactor → Fuel reactor → Gasifier → Reduced Oxygen Carrier → Ash, CO₂, H₂O
  - Air → syngas → Coal → H₂O → CO₂

### In-Situ Gasification-CLC

- Air reactor → Fuel reactor → Gasifier → Reduced Oxygen Carrier
- Air → CO₂ + H₂O → H₂O → CO₂

### In-Situ Coal Gasification and Waste (Ash) Removal

- Oxygen Carrier → CO₂, H₂O → Ash
- Coal → Aeration → Reduced Oxygen Carrier
- Aeration

### NETL Cold Moving Bed: Fluidization-Based Percolation

- Oxygen Carrier
- Ash, CO₂, H₂O
- Coal → Aeration → Reduced Oxygen Carrier
Solid-Fueled Moving Bed Operation

**Hydrodynamics**
- Transport/Separation (by Elutriation): carrier-fuel/waste
  - Flow regimes, Dispersion, Transit time, ...etc.
- Packed bed pressure drop

**Heat and Mass transfers**
- Temperature distribution
- Reaction rates

➤ Get insight first with “simple” flows: Gravity-based percolation
Outline

   o “Simple” mono-disperse intruder flow

2. Discrete Element Method Simulations of Lomine & Oger’s Exp.
   o Goal: Gain Understanding to be fed into KTGF Models

3. Preliminary assessments of Poly-disperse KTGF models
   o e.g. Syamlal’s Friction-based Poly-disperse Particle-Particle Drag (1987)

4. Conclusion – Future plans
What measurements were performed?

1. Collect intruder with respect to time (scale) ➔ Mean transit time (➔ mean velocity)
2. Intruder total mass in each cell of collecting box ➔ Position variance (➔ dispersion coefficients)

Objective: Describe flow behavior using Advection-Dispersion model

\[
\frac{\partial C(r, t)}{\partial t} + U \cdot \nabla C(r, t) = \frac{D_\parallel}{\partial r_\parallel^2} + \frac{D_\perp}{\partial r_\perp^2}
\]

Mean velocity  
Longitudinal & Transverse dispersion coefficients
Cooperative Percolation Flow Regimes

Flow Regimes (from Mean Transit Time)

- Faster-Collective (Gravity-dominated)
- Steady (Equilibrium Gravity-Collision)
- Slower-Positive (Collision-dominated)

- (May be) useful to guide, design and operation of the moving bed solid-fueled reactors
- How well can the flow regimes be captured with DEM models?
- What mechanisms control these flow regimes? (useful for the KTGF models)
  - Intruder-Intruder interactions (dispersion)
  - Intruder-Fixed bed interactions (dispersion)
  - Pore jamming
  - Bed dispersivity (local structure arrangement)

Packed Bed Generation

Lagrangian DEM-based Gravitational Settling

(release and settling of large amount of particles in larger container → cut to match domain of interest)

Average porosity = 0.435

(Lominé & Oger reported bed porosity around 0.4)

(The effects) Pore distribution, Tortuosity, Spatial randomness etc. ... have not been investigated yet

Modified Lubachevsky-Stillinger\(^1\) algorithm

(Random Sequential Addition init., Particle grow, Hard Sphere Coll, Solid Pressure → cut to match domain of interest)

Average porosity = 0.376

Steady Percolation Dynamics

(4 beds constructed from the same parent)

<table>
<thead>
<tr>
<th>H/D</th>
<th>5.04</th>
<th>7.57</th>
<th>8.84</th>
<th>10.0</th>
<th>11.37</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number large particle</td>
<td>1428</td>
<td>2152</td>
<td>2523</td>
<td>2851</td>
<td>3257</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.438</td>
<td>0.436</td>
<td>0.434</td>
<td>0.435</td>
<td>0.432</td>
</tr>
</tbody>
</table>

(3 amounts of intruder particles)

<table>
<thead>
<tr>
<th>Number of intruder: N [-]</th>
<th>500</th>
<th>10,000</th>
<th>70,000</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensionless number: N_p[-]</td>
<td>3.8</td>
<td>77.0</td>
<td>538.4</td>
</tr>
</tbody>
</table>

- Predictions within exp. uncertainties ➔ porous medium geometrical structures seem adequately captured
- Mean transit velocity is constant regardless bed height
Flow Regime Predictions

- Percolation dynamics appears quite dependent on the inter-particle interaction models (especially for the collision-dominated regime).

- The dependence of the restitution coefficient to impact velocity with Hertz model force calculations (contrary to the Linear Spring-Dashpot) may have been critical in the predictions for that regime.

Animation (Intruder: \(N=95,404\) or \(N_p=734\))

- **Linear Spring-Dashpot**
- **Hertz**

(colored by the magnitude of the intruder velocities)

- The intruder particles percolate through the porous medium by remaining a bulb
- Intruder scattering is wider at the bed with L.S.-D. compared to Hertz
Dispersion Coefficients

Transverse Dispersion

Longitudinal Dispersion

→ Wider spreading found with L.S-D. versus Hertz model: decrease of the probability of Intruder-Intruder interactions with L.S-D. model

→ Intruder bed expands more vertically with Hertz model as in the experiments

Uncertainty due to Bed Porosity

Flow regime predictions appear independent of the uncertainty in the bed porosity, even though the denser bed unsurprisingly slowed down the intruder particles.
Larger size intruders transited slowly but percolation dynamics (in terms of flow regime) appears independent of the diameter ratio (at least using the Linear Spring-Dashpot force calculation).

\[ N_p \left( N, \frac{d_p}{D} \right) \approx 31.5N \left( \frac{d_p}{D} \right)^3 \]
Preliminary assessments of KTGF models

**Kinetic Theory-based Poly-Disperse Model**

- Syamlal (1987): translational-based motion, friction between particles
- Maximum packing: Yu & Standish (1987)
- Constant restitution and friction coefficients (interaction between particles by collisions)

\[ t = 0.00 \text{s} \]

**Influence of the Fixed Bed Height: 10,000 small particles**

<table>
<thead>
<tr>
<th>H/D</th>
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<th>7.57</th>
<th>8.84</th>
<th>11.37</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transit time [s]</td>
<td>0.471</td>
<td>0.599</td>
<td>0.724</td>
<td>0.806</td>
</tr>
<tr>
<td>( \langle (\Delta r)^2 \rangle [\text{cm}^2] )</td>
<td>-</td>
<td>2.915</td>
<td>-</td>
<td>4.023</td>
</tr>
<tr>
<td>( D_1 [\text{cm}^2/\text{s}] )</td>
<td>-</td>
<td>1.217</td>
<td>-</td>
<td>1.248</td>
</tr>
<tr>
<td>( \langle (\Delta z)^2 \rangle [\text{cm}^2] )</td>
<td>-</td>
<td>1.687</td>
<td>-</td>
<td>2.826</td>
</tr>
<tr>
<td>( D_2 [\text{cm}^2/\text{s}] )</td>
<td>5.312</td>
<td>1.409</td>
<td>-</td>
<td>1.753</td>
</tr>
</tbody>
</table>

\[ \Rightarrow \text{Relatively small errors in the prediction of mean transit time} \]
\[ (27\%, 11\%, 1\% \text{ and } -11\%) \]

\[ \Rightarrow \text{Low scattering and expansion of intruder particles} \]

**Despite:**

- Constant restitution, friction coefficients
- Translational-based motion Kinetic theory-based model (Syamlal, 1987) assuming:
  - Dirac velocity distribution function \( \Rightarrow \text{momentum transfer doesn’t account for agitation of the particles} \)
  - Energy redistribution due to inter-particle collisions between different particle phases
- Additional dispersion induced by the porous medium assembly \( \Rightarrow \text{dispersivity not accounted in the kinetic theory model (local structure of the arrangement)} \)
Conclusion – Future works

• **Conclusions:**
  • Hertz model (in contrast) to LS-D predicts the experimentally measured variation in the mean transit time (intruder velocity) with respect to the intruder concentration.
  • Hertz under-predicts the transverse and axial dispersion
  • LS-D over-predicts the transfer and under-predicts the axial dispersion
  • Predicted sensitivity of the transit time with respective to material properties is consistent with experimental observations

• **Future**
  • Trajectory/collision analysis
  • Hertz model parameters sensitivity
  • Continuum/large scale modeling
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Back-up: Steady Percolation Dynamics

Mean transit time

$N_p = 3.8$

$N_p = 538.4$

Particle Small-Small Small-Large
Normal stiffness $10^5$ g/s$^2$
Normal restitution 0.99 0.84
Tangential stiffness $2/7 \times 10^5$ g/s$^2$
Friction coefficient 0.10

(Linear Spring-Dashpot collision parameters)
Back-up: Sensitivity Study (L.S-D.)

- **Restitution Intruder-Intruder**
- **Friction**
- **No Rotation**

- **Mean Transit Time**
  - $t_{mean} = \sqrt{\frac{2h}{g}}$

- **Radial Position Variance**
  - $\Delta r^2 = \frac{1}{N_p}$

Graphs showing the effects of restitution, friction, and no rotation on mean transit time and radial position variance.
Back-up: Post-process (as in experiments)

- **Mean transit time**
  \[
  \tau_{\text{mean}} = \int_0^\infty t \varphi(t) dt \quad \text{with} \quad \varphi(t) = \frac{d}{dt} \left( \frac{m(t)}{\int_0^\infty m(t) dt} \right)
  \]

- **Transverse variance & dispersion (i.e. orthogonal to mean flow)**
  \[
  \langle (\Delta r)^2 \rangle = \sum_i p_i (r_i - \langle r \rangle)^2 = 4D_\perp \tau_{\text{mean}}
  \]
  \[
  p_i = \frac{m_i(x_i, y_i)}{\sum_i m_i(x_i, y_i)}
  \]

- **Longitudinal variance & dispersion (i.e. mean flow direction)**

  **Assumption**: Intruder transport through medium described by advection-dispersion model

  \[
  m(z = H, t) = \frac{m_0}{2} \left[ \exp \left( \frac{zV}{D_\|} \right) \text{erfc} \left( \frac{z + Vt}{\sqrt{4D_\| t}} \right) + \text{erf} \left( \frac{z - Vt}{\sqrt{4D_\| t}} \right) \right]
  \]
  \[
  \langle (\Delta z)^2 \rangle = 2D_\| \tau_{\text{mean}}
  \]

Find $D_\|$ which best fits normalized collected mass (Nonlinear Least Squares minimization algorithm: augmented Gauss-Newton and Levenberg-Marquardt)