Using Solid Particles as Heat Transfer Fluid for use in Concentrating Solar Power (CSP) Plants

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Prof. Christine Hrenya University of Colorado (PI)
Dr. Zhiwen Ma NREL (co-PI)
Dr. Aaron Morris University of Colorado (post-doc)
Dr. Sreekanth Pannala ORNL (co-PI)
Dr. Tom O’Brien retired NETL (co-PI)
Team Members

Christine Hrenya
University of Colorado
Continuum and DEM models of solids flows

Zhiwen Ma
NREL
Concentrating Solar Power (CSP) plants

Aaron Morris
University of Colorado
High-performance computing, Gas-solid modeling (beginning 3/15/13)

Tom O’Brien
Consultant (retired NETL)
MFIX multiphase models

Sreekanth Pannala
ORNL
High-performance computing, including MFIX
**BRIDGE Project**

**Objective**

*Fundamental modeling tool that can be used for design of particle receiver: understanding and prediction of heat transfer in solids flows, including radiation*

**Why fundamental (no empirical / adjustable parameters)?**

Previous findings:
(i) for rotating heated tumblers, high-heat capacity particles are heated faster for lower conductivities of the interstitial medium [1]
(ii) for shear flows along an unbounded, inclined plate, the thermal conductivity of dilute flows increases with shear rate [2] while the opposite occurs for denser flows [3]

⇒ non-intuitive behavior call for first-principles models
  - empiricism is costly and time-consuming
  - empiricism not reliable for extrapolation
Modeling Approaches: Various Scales

Two-fluid Model (TFM)
- Gas = continuum
  (averaged over many particles)
- Solids = continuum

\[
\frac{\partial}{\partial t} \left( \varepsilon_s \rho_s \mathbf{V}_s \right) + \nabla \cdot \left( \varepsilon_s \rho_s \mathbf{V}_s \mathbf{V}_s \right) = \nabla \cdot \mathbf{\tau}_s + \varepsilon_s \rho_s \mathbf{g} + \mathbf{F}_{\text{drag}}
\]

Discrete Element Model (DEM)
- Gas = continuum
- Solids = discrete

\[
m_i \frac{dV_{si}}{dt} = m_i \mathbf{g} + \mathbf{F}_{ci} + \mathbf{F}_{\text{drag},i}
\]

Typical CPU times for DEM
Serial processor: \(O(10^5 \text{ particles})\)
Parallel processors: \(O(10^8 \text{ particles})\)

<table>
<thead>
<tr>
<th>(d_p)</th>
<th>(N_p) in 1 cup</th>
</tr>
</thead>
<tbody>
<tr>
<td>100 (\mu)m (sand)</td>
<td></td>
</tr>
<tr>
<td>50 (\mu)m</td>
<td></td>
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Less CPU time
More detail, Fewer closures

ORNL facility
MFIX DEM (and continuum): parallelized
**Model Development for Solar Collector**

**Our Approach**
- Use DEM simulations as “Ideal Experiment” to test continuum theory

**Computational Tool: MFIX** (*Multiphase Flow with Interface eXchanges*)
- Public, cost-free, open-source code from DOE NETL
- DEM model: conduction, convection and radiation (part-part only)
- Continuum model: conduction and convection

**Continuum Models: State of the Art**
- No validation to date for conduction, convection, or radiation
- Caveat 1: flow instabilities difficult to deal with (similar to turbulence)
- Caveat 2: possible large gradients in solids flow variables (requires higher-order model)

**Steps**
- Single-tube system, no radiation: generation of DEM validation data, and comparison with continuum predictions
- Two-tube system, with radiation: generation of DEM validation data, and comparison with continuum predictions
- Prototype receiver, with radiation: assess relative importance of radiation on particle absorber heat transfer
Tasks

1. Model Verification / Validation for Non-Radiative Heat Transfer (BP1)

2. Initial Assessment of MFIX Radiation Model (BP1)

3. Verification of DEM Radiation Model and Generation of DEM validation data (BP2)

4. Implementation, Verification, and Validation of Continuum Radiation Model (BP2)

5. Simulation of Prototype Particle Receiver with Radiative Heat Transfer (BP3)

Note: The end date for Year 1 has recently been updated by DOE from 11/15/13 to 2/14/14.
Current MFIX Modeling Efforts

- Fully coupled two-phase flow.
- Solid phase modeled by either continuum or DEM solver.
- Heat transfer models for solid and fluid phases.
  - Particle-particle conduction.
  - Particle-fluid-particle conduction.
  - Particle-fluid convection.
  - Particle-particle radiation.
- Parallelized for supercomputers.
Current Modeling Efforts

Preliminary DEM Simulations

- Fluidized bed with central jet.
  - Fully coupled phases, no heat transfer.
### Univ. Colorado and ORNL Supercomputing Facilities

<table>
<thead>
<tr>
<th>Janus (Univ. Colorado)</th>
<th>Titan (ORNL)</th>
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</thead>
<tbody>
<tr>
<td>16,416 cores</td>
<td>299,008 cores</td>
</tr>
<tr>
<td>Hex-core 2.8Ghz Intel Westmere processors</td>
<td>16-core AMD Opteron 6274 processors + GPUs</td>
</tr>
<tr>
<td>24GB RAM per node</td>
<td>32GB + 6GB RAM per node</td>
</tr>
<tr>
<td>184 teraflops</td>
<td>20 petaflops</td>
</tr>
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</table>
Parallel Supercomputing on MFIX

DEM

• Parallelization is a new addition (Gopalakrishnan and Tafti, 2013)
• Strong scalability and can simulate millions of particles.

Continuum

Current Modeling Efforts

Preliminary DEM Simulations

- Fluidized bed with central jet.
  - Fully coupled phases.
  - No heat transfer.

- Bubbling bed parallel speed-up test on Janus supercomputer.
  - Simulated 140,400 particles
    » 2.56 mil particles in
  - 30 minutes to simulate 0.1s with 24 processors.
  - Approx. half a cup of 1mm diameter particles.
  - Approx. 1 tablespoon for 500 µm particles.

Current Modeling Efforts: Single-Tube System

DEM Solution with Heat Transfer

- Identify relative importance of various heat transfer mechanisms.
- Determine heat transfer coefficients and distribution of particle temps.
- Comparison to particle flow/heat transfer experiments.
- Verification of future continuum model.
Progress Towards Single Tube DEM

MFIX Modifications

- Need to implement hot wall B.C. (MFIX currently has only adiabatic walls for DEM).
- Cutcell algorithm for flow over internal geometries is still under development.

Input Parameters

- Tube size, shape, heat flux, particle properties

Gas only
Vorticity field

Solids only
Heat Transfer Mechanisms in MFIX

**Particle-Particle Conduction**
- Cond. across contact area.
- Small Biot numbers
- Normally not important bc collisions are brief and contact areas are small.
- Collision duration is important

**Particle-Fluid-Particle Conduction**
- Conduction across interstitial fluid in gap.
- Assumes heat transfer is in direction along axis connecting part. centers.
- Polydispersity
Heat Transfer Mechanisms in MFIX

Particle-Fluid Convection

• MFIX Uses Nusselt number correlations (1952).
• Correlations were derived from single particle systems and should be improved when the particle volume fraction is high.
• Can use LBM or Gunn’s correlations for improved Nusselt number at higher volume fractions.
• Expected to be significant heat transfer mechanism.

\[
\langle \text{Nu} \rangle = \frac{h_{\text{conv}}}{\kappa_g / 2R_p} \\
\text{Re} = \frac{\rho_g \varepsilon_g \| V_g - V_p \| 2R_p}{\mu_g}
\]
Heat Transfer Mechanisms in MFIX

Particle-Particle Radiation

- Best approach would compute view factors between all particles/walls with all other particles and solve radiative balance equations.
  - Computationally expensive – MFIX uses simplified model
- Defines region where radiation occurs and uses a correlation to compute an environment temperature.
- Radius of radiation sub-domain $= 1.5D_p$
- Environment temperature is average temperature of particles within region.
Summary

- Scalability of parallel MFIX DEM increases with # particles
- Preliminary DEM simulations around single, unheated tube qualitatively correct
- Reviewed heat transfer mechanisms in MFIX
  - Particle-particle conduction
  - Particle-gas-particle conduction
  - Particle-gas convection
  - Particle-particle radiation
Next Steps…

• DEM prediction of particle trajectories in flow domain
• Extension of DEM heat transfer to particle-wall contacts
• Single-tube DEM simulation with heat transfer
• Single-tube continuum simulation