Development of a verification, validation and uncertainty quantification roadmap for multiphase flows with preliminary results for hopper bin discharge problem

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Outline

• Development and application of a systematic VVUQ approach for multiphase flows
  • Extension of the existing methodologies
  • Survey of subject matter experts and tollgates for review
  • Systematic simulation campaign and design of experiments

• Benchmark problem and preliminary experiments: Hopper discharge
  • Bench-scale experiments to enable a quick turnaround for Discrete Element Modeling (DEM) simulations
  • Design criteria to ensure mass flow operation mode

• MFIX-DEM simulation campaign
  • Validation of MFIX-DEM linear spring dashpot (LSD) model
  • Sensitivity analysis of model parameters on the quantities of interest
Motivation

• VVUQ standards have been established to quantify the degree of accuracy using CFD solution and experimental data for a specified variable at a specified validation point

• Application to multiphase flow modeling and simulation has encountered several challenges
  • Assessing uncertainty due to numerical discretization
  • Lack of readily available objectively-assessed experimental uncertainty

• Explore the extension of the VVUQ procedures for multiphase flow applications using some demonstrative cases starting with granular discharge through a conical hopper
Extended VVUQ roadmap for multiphase flows - NETL

Define research objectives & general problem classification

Identify and define application specific constraints

Identify Quantities of Interest (QoI)

Query subject matter experts (SMEs)

No

Assess feedback

Tollgate review prior to testing

Yes

Revision

Mathematical model

Computational model setup

Simulation campaign design

Quality assurance (QA) check

Simulation campaign execution

QA & preliminary analysis

Simulation outcomes

Revision

Experimental model

Experiment setup design

Experimental campaign design

Quality assurance (QA) check

Experimental campaign execution

QA & preliminary analysis

Experimental outcomes

Agreement?

Yes

Next research objective

No
Extended VVUQ roadmap for multiphase flows - NETL

1. Define research objectives & general problem classification
2. Identify and define application specific constraints
3. Identify Quantities of Interest (QoIs)
4. Query subject matter experts (SMEs)
   - Assess feedback
   - Tollgate review prior to testing
   - Yes
   - Revision

5. Mathematical model
6. Computational model setup
7. Simulation campaign design
8. Quality assurance (QA) check
9. Simulation campaign execution
10. QA & preliminary analysis
11. Simulation outcomes
12. Experimental outcomes
13. Experimental campaign design
14. Experimental campaign execution
15. Quality assurance (QA) check
16. Qualitative comparison
17. Quantitative comparison
18. Agreement?
   - Yes
   - Next research objective
   - No

Revision

NETL

U.S. DEPARTMENT OF ENERGY
Benchmark problem – Preliminary experiments

• Discharge through conical hopper having pure granular flow commonly seen in industries (chemical, pharmaceutical, food, mining)
• Simplified hydrodynamics to focus on particle-particle and particle-wall interactions. Interfacial gas neglected (High Bagnold number).
• Bench-scale experiments to enable a quick turnaround, 3-D printed geometries to ensure consistency between experiments and simulations
Benchmark problem – Preliminary experiments

• Control variables
  • Orifice diameter
  • Apex angle

• Quantities of interest (QoI)
  • Discharge flow rate
  • Angle of repose

• Material: High density polyethylene (HDPE)
  • Geldart B classification
  • Mean particle diameter: 848 μm
  • Density: 884 kg/m³

<table>
<thead>
<tr>
<th>Index</th>
<th>θ (deg)</th>
<th>h₁ (cm)</th>
<th>h₂ (cm)</th>
<th>D₀ (mm)</th>
<th>D₁ (cm)</th>
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<td>10</td>
<td>2.5</td>
<td>7</td>
<td>9.33</td>
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</table>
Benchmark problem – Simulations

• Increasing demand for DEM simulations with improving computational resources

• Focus on particle properties before including the gas phase

• Solution methodology: Alternating use of Force-displacement law and Newton’s second law of motion. Time step size based on spring stiffness provided by the user (fixed).

• Isolating uncertainties due to model parameters related to particle-particle and particle-wall interactions from the other sources including spatio-temporal discretization
Survey of Subject Matter Experts

- Survey pertaining to experiments and DEM simulations was carried out with the subject matter experts to identify:
  - Quantities of interest (or response variables)
  - Control variables, which are to be varied systematically
  - Held-constant factors for experiments and modeling
  - Known nuisance factors for the experiments

- Based on the feedback, 10 control variables were identified for DEM simulations as important but without any consistent and objective ranking of importance

- Screening study initiated to quantitatively determine the most influential factors on the response variables
Example illustration of survey:
- Identification and Characterization of Control Variables for CFD Simulations:

### Computational model - Rejected Response Variables

<table>
<thead>
<tr>
<th>SME</th>
<th>Rejected response variable</th>
<th>Justification of rejected response variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Particle Size Distribution (PSD) of discharged particles</td>
<td>Computational simulations will be conducted with mono-disperse particles so there is no PSD will be generated of discharged particles</td>
</tr>
<tr>
<td>3</td>
<td>Flow pattern - highest and lowest points in hopper</td>
<td>These are connected to model input parameters, specifically the total number of particles</td>
</tr>
<tr>
<td>4</td>
<td>Particle-wall friction coefficient</td>
<td>This is a model input parameter</td>
</tr>
<tr>
<td>4</td>
<td>Particle-particle restitution coefficient</td>
<td>This is a model input parameter</td>
</tr>
<tr>
<td>4</td>
<td>Particle-particle friction coefficients</td>
<td>This is a model input parameter</td>
</tr>
</tbody>
</table>

### Computational model - Accepted Control Variables

#### Particle-particle coefficient of friction (sliding)

- **Rank: 1 of 10**

<table>
<thead>
<tr>
<th>SME</th>
<th>Rank</th>
<th>Normal</th>
<th>Low</th>
<th>High</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>0.35</td>
<td>0.31</td>
<td>0.39</td>
</tr>
</tbody>
</table>

- **Justification**
  1. I have seen the friction coefficient can be very sensitive to things like humidity. It would be best to measure the friction coefficient in house if possible.

#### Particle-wall coefficient of friction (sliding)

- **Rank: 2 of 10**

<table>
<thead>
<tr>
<th>SME</th>
<th>Rank</th>
<th>Normal</th>
<th>Low</th>
<th>High</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td>0.66</td>
<td>0.45</td>
<td>0.50</td>
</tr>
</tbody>
</table>

- **Justification**
  1. I have seen the friction coefficient can be very sensitive to things like humidity. It would be best to measure the friction coefficient in house if possible.
Screening study

• Morris One-at-a-time (MOAT): Computationally efficient for screening study involving a large parameter space

• Elementary effect: \( d_{ij} = \frac{c_i(k_1,k_2,\ldots,k_{j-1},k_j+\Delta,k_{j+1},\ldots,k_m) - c_i(k_1,k_2,\ldots,k_{j-1},k_j,k_{j+1},\ldots,k_m)}{\Delta} \)

• Global effect: \( \mu_{ij} = \frac{\sum|d_{ij}|}{r}, \quad \sigma^2_{ij} = \frac{r \sum(d_{ij})^2 - (\sum d_{ij})^2}{r(r-1)} \)

• Larger mean (\( \mu_{ij} \)) \( \rightarrow \) more sensitive; larger variance, (\( \sigma^2_{ij} \)) \( \rightarrow \) more non-linearity/interactive effects

• Computational model – Parameters considered based on Subject matter expert (SME) feedback
  - Particle-Particle coefficient of friction
  - Particle-Wall coefficient of friction
  - Particle-Particle coefficient of restitution
  - Particle-Wall coefficient of restitution
  - Particle-Particle LSD normal spring stiffness
  - Particle-Wall LSD normal spring stiffness
  - Particle-Particle LSD tangential spring stiffness coefficient
  - Particle-Wall LSD tangential spring stiffness coefficient
  - Particle-Particle LSD tangential spring stiffness damping coefficient
  - Particle-Wall LSD tangential spring stiffness damping coefficient
Screening study – Sampling

**Scatterplot Matrix**

<table>
<thead>
<tr>
<th>Uncertain input parameter</th>
<th>Lower bound</th>
<th>Upper bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>x1 PP friction coefficient [−]</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>x2 PW friction coefficient [−]</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>x3 PP restitution coefficient [−]</td>
<td>0.2</td>
<td>0.99</td>
</tr>
<tr>
<td>x4 PW restitution coefficient [−]</td>
<td>0.2</td>
<td>0.99</td>
</tr>
<tr>
<td>x5 PP normal spring stiffness [N/m]</td>
<td>1.0E+02</td>
<td>1.0E+06</td>
</tr>
<tr>
<td>x6 PW normal spring stiffness [N/m]</td>
<td>1.0E+02</td>
<td>1.0E+06</td>
</tr>
<tr>
<td>x7 PP tangential spring stiffness coefficient [−]</td>
<td>0.1</td>
<td>0.9</td>
</tr>
<tr>
<td>x8 PW tangential spring stiffness coefficient [−]</td>
<td>0.1</td>
<td>0.9</td>
</tr>
<tr>
<td>x9 PP tangential damping factor [−]</td>
<td>0.1</td>
<td>0.9</td>
</tr>
<tr>
<td>x10 PW tangential damping factor [−]</td>
<td>0.1</td>
<td>0.9</td>
</tr>
</tbody>
</table>

Morris method (MOAT)
No. of input parameters: 10
Preferred sample size: 110
Most conservative sample size: 44
Screening study – Results

Modified Means Plot (bootstrap)

N = 44

N = 55

N = 77

N = 110

<table>
<thead>
<tr>
<th>Rank</th>
<th>N=44</th>
<th>N=55</th>
<th>N=77</th>
<th>N=110</th>
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<td>x4</td>
<td>x6</td>
<td>x6</td>
<td>x10</td>
</tr>
</tbody>
</table>

- Ranking order: 1. $e_{p-p}$, 2. $\mu_{p-p}$, 3. $\mu_{p-w}$, 4. $e_{p-w}$
- Time for completion – 2 days to 2 months depending on $k_n$ which determines $\Delta t$
- $k_n=100$ N/m for global sensitivity analysis based on screening study
Global Sensitivity Analysis (GSA)

- **Question:** What is the extent to which the input parameters or their interactions influence the quantities of interest?

- Top four parameters determined by the screening study were selected for Global Sensitivity Analysis.

- A new set of design of experiments was generated
  - 40 samples having 4 parameters varied systematically.

- The effect of sampling methodology was also investigated
  - Space-filling design based Optimized Latin Hypercube (OLH) sampling (R library)
  - Quasi Monte-Carlo sampling (LPTAU sampling in PSUADE UQ toolkit from LLNL)
Effect of sampling methods on GSA

OLH

LPTAU
Surrogate model for GSA

- Monte Carlo sampling based methods are computationally prohibitive for uncertainty quantification analysis of multiphase flows
- Gaussian process based surrogate model built using the OLH sampling simulation results (40 samples)

Note that other two parameters are kept at mid point settings for the construction of surrogate contour plots
Surrogate model quality

- To assess the quality of the surrogate model perform cross validation
- One sample point outside 1σ
Surrogate model for GSA

• Similar Gaussian process based surrogate model constructed for simulation results obtained through LP TAU sampling

Note that other two parameters are kept at mid point settings for the construction of surrogate contour plots.
Preliminary GSA results

- Preliminary variance based sensitivity analysis: Sobols’ Total Indices Method implemented in PSUADE UQ Toolkit using OLH (40 samples)

- Particle-particle coefficient of restitution is the most influential model parameter

- Analysis of interaction effects in progress
Summary

• Extension of VVUQ methodology with systematic design of experiments and simulations (work in progress)
• Bench-scale experiments to ensure quick turnaround
• 3-D printed geometries to ensure consistency with the simulations
• Survey of subject matter experts for VVUQ methodology input
• Global sensitivity analysis (GSA) shows sampling invariance, possible interaction between model parameters
• Ranking of model parameters for hopper discharge process:
  1. Particle-particle coefficient of restitution
  2. Particle-particle coefficient of friction
  3. Particle-wall coefficient of restitution
  4. Particle-wall coefficient of friction

Thank you for your attention. Questions???