Calibration of a Particle-In-Cell Simulation Model for Gravitational Settling Bed Application
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Outline

- Brief Overview of MFiX-PIC
- Representative Problems for the Calibration Study
- Brief Overview of Calibration Methods
- Simulation Campaigns to Construct Surrogate Models
- Assessment of Deterministic Calibration Results
- Concluding Remarks
Brief Overview of MFiX-PIC

Concept: When particles are of equal physical property, they can be grouped together as larger parcels. Multiple particle types can be managed as separate parcel distributions.

Instead of managing each particle with Newtonian physics, parcel motion is influenced by a collisional stress model.

\[ \frac{d\bar{V}_p}{dt} = \beta (\bar{U}_g - \bar{V}_p) - \frac{1}{\rho_p} \nabla p - \frac{1}{\epsilon_p \rho_p} \nabla \tau_p + \ddot{g} \]

\[ \tau_p = \frac{P_p \epsilon_p}{\max(\epsilon_{cp} - \epsilon_p, \delta (1 - \epsilon_p))} \]

Solids stress

A reduced computational load allows the simulations to proceed very rapidly. Lagrange tracking of parcels results in excellent visual graphics of statistically weighted particle motion.
Representative Problems for the Calibration Study

- Cases selected to cover a broad range of flow conditions
  - Particle Settling: $U/U_{mf} < 1.0$ ($P_0 \sim 1$) (Simulation campaign)
  - Bubbling Fluidized bed: $U/U_{mf} \sim 1$ ($P_0 \sim 10$)
  - Circulating Fluidized bed: $U/U_{mf} >> 1.0$ ($P_0 \sim 100$)

- Summary of model parameters used:

<table>
<thead>
<tr>
<th>t1</th>
<th>t2</th>
<th>t3</th>
<th>t4</th>
<th>t5</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1: Particle Settling</td>
<td>[1,20]</td>
<td>[2,5]</td>
<td>[3,20]</td>
<td>[0.35,0.5]</td>
</tr>
<tr>
<td>C2: Fluidization</td>
<td>[1,100]</td>
<td>[2,5]</td>
<td>[10,100]</td>
<td>[0.4,0.5]</td>
</tr>
<tr>
<td>C3: Circulating Fluidized Bed</td>
<td>[1,250]</td>
<td>[2,5]</td>
<td>[4]</td>
<td>[0.4,0.5]</td>
</tr>
</tbody>
</table>

*Parameters selected based on prior sensitivity study

Parcel momentum equation

$$\frac{dV_p}{dt} = \beta \left( V_g - V_p \right) - \frac{1}{\rho_p} V_p - \frac{1}{\varepsilon_p \rho_p} \gamma_p + g$$

$$\tau_p = \frac{P_0 \varepsilon_p^\delta}{\max (\varepsilon_{cp} - \varepsilon_p, \delta(1 - \varepsilon_p))}$$

Hypothetical flow regime map
C1: Particle settling

**Problem setup**

**Control variable: Initial solids concentration**

<table>
<thead>
<tr>
<th>x1: Initial solids concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1: Particle Settling</td>
</tr>
<tr>
<td>[0.05, 0.25]</td>
</tr>
</tbody>
</table>

**Response variable: Location of filling shock (y2)**

CFD results are compared with analytical solutions.

**Control variables: CFD (PIC parameters)**

<table>
<thead>
<tr>
<th></th>
<th>t1 or (θ1): Pressure linear scale factor</th>
<th>t2 or (θ2): Vol. fraction exponential scale factor</th>
<th>t3 or (θ3): Statistical weight</th>
<th>t4 or (θ4): Vol. fraction at maximum packing</th>
<th>t5 or (θ5): Solid slip velocity factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1: Particle Settling</td>
<td>[0.48*, 20]</td>
<td>[2, 5]</td>
<td>[2.96*, 20]</td>
<td>[0.35*, 0.5]</td>
<td>[0.5, 1.0]</td>
</tr>
</tbody>
</table>

* Initial targeted lower bound might be slightly different than actual samples generated as part of Latin Hypercube sampling.

**Analytical Solution:**

Location of shock:

\[
x(t) = -t\left(\frac{\epsilon_s^x \epsilon_s^u u_r - \epsilon_s^x \epsilon_s^u u_r^0}{\epsilon_s^x - \epsilon_s^0}ight)
\]

Relative velocity (Stokes’ drag):

\[
u_r = \frac{g \Delta \rho d_p^2}{18 \mu_g} \epsilon_s^{3.65}
\]
Brief Overview of Calibration Methods

**Deterministic versus Statistical Calibration**

- **Maximize agreement between simulation and experiment target by improving the characterization of model parameters, \( \theta_i \) (e.g., \( P_0, \beta \)) using available data.**

- **Also known as parameter estimation /identification, inverse problem modeling**

- **Calibration ≠ validation**

Two approaches:

- **Deterministic Calibration:**
  - Framed as minimization problem that seeks one or more sets of parameter values that reduce the error between simulation \( s_i(\theta) \) and data \( y_i \), typically in a norm:
    \[
    \min_{\theta} f(\theta) = SSE(\theta) = \sum_{i=1}^{n} [(s_i(\theta) - y_i)^2 = \sum_{i=1}^{n} [T(\theta)]^2
    \]
  - Available in UQ software: DAKOTA (SNL), PSUADE (LLNL), OpenTURNS (Airbus+ONERA), Nodeworks (NETL) with some modifications

- **Statistical calibration (Bayesian):**
  - Instead of standalone parameter values, it seeks a statistical characterization of parameters most consistent with the data.
  - Available in UQ Software: PSUADE (LLNL), DAKOTA (SNL), OT, GPM/SA & SEPIA (LANL)

Source: DAKOTA Software Training: Model Calibration (SAND2015-6813PE)
Deterministic Calibration Procedure

Calibration Proposed Settings for Model Parameters

- Utilize the constructed surrogate model and the set of analytical solutions (used in lieu of experiments) to perform the deterministic calibration.

- Deterministic calibration problem can be reframed as a minimization problem, i.e.,

- find a set of theta values that minimizes the residuals for all experiment data points

\[
\min_{\theta} f(\theta) = SSE(\theta) = \sum_{i=1}^{n} [(s_i(\theta) - y_i)^2 = \sum_{i=1}^{n} [r_i(\theta)]^2
\]

- Utilized PSUADE and DAKOTA UQ toolkits to perform the optimization.
- Recently implemented the workflow in Nodeworks
Deterministic Calibration Procedure

Workflow

1. Identify which model parameters to be calibrated with the lower and upper bound values.
2. Compile the tabular format dataset from observations or experiments, which will be used to guide the calibration.
3. Design and execute simulation campaign based on statistical design of experiments.
4. Post-process simulation campaign results and compile the tabulated input file containing samples and QoIs from simulations.
5. Construct an adequate surrogate model. Perform the optimization for minimization of residuals to determine the calibrated parameter settings.
6. Verify the proposed calibrated model parameter settings by performing samples of simulations and compare the discrepancy with respect to observations with the new settings.

- Multiple step workflow followed for deterministic calibration procedure
- Design of the simulation campaign in Step (3) was carried out with Nodeworks, simulations were performed with MFiX-PIC on Joule 2.0
- Step (5) was performed with PSUAD, DAKOTA and Nodeworks by providing the same tabulated file that contains simulation campaign input and responses.
C1: Particle Settling Simulation Campaigns

Construct Surrogate Model from Simulation Campaign (120 samples)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>m</td>
<td>Mass</td>
</tr>
<tr>
<td>n</td>
<td>Number of particles</td>
</tr>
<tr>
<td>t</td>
<td>Time</td>
</tr>
<tr>
<td>V</td>
<td>Volume</td>
</tr>
<tr>
<td>T</td>
<td>Temperature</td>
</tr>
</tbody>
</table>

### Uncertain Input Parameters/Factors:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>m</td>
<td>1.456</td>
<td>Mass</td>
</tr>
<tr>
<td>n</td>
<td>2.039</td>
<td>Number of particles</td>
</tr>
<tr>
<td>t</td>
<td>2.046</td>
<td>Time</td>
</tr>
<tr>
<td>V</td>
<td>0.180</td>
<td>Volume</td>
</tr>
<tr>
<td>T</td>
<td>0.501</td>
<td>Temperature</td>
</tr>
<tr>
<td>m</td>
<td>0.056</td>
<td>Mass</td>
</tr>
</tbody>
</table>

Scatter matrix plot of the simulation campaign samples, which is used to construct a surrogate model. Only the 5 model parameters are shown.

(a) Design of experiments matrix (first 42 out of 120 samples shown)

(b) Scatter matrix plot of the simulation campaign input dataset

Optimal Latin Hypercube Sampling based Simulation Campaign
C1: Particle Settling Analytical Solution

Available Analytical Solution Used for Deterministic Calibration

To guide the calibration process, analytical solution was used in lieu of actual experiments.

Three different scenarios are employed by computing the analytical solution for $0.05 \leq x_1 \leq 0.25$ range with different number of samples:

- 21 samples
- 11 samples
- 5 samples
C1: Particle Settling Simulation Campaigns

Construct Surrogate Model from Simulation Campaign (120 samples)

3D plot of the data-fitted surrogate model

Sensitivity Analysis using Sobol’ Indices

120 sample-based simulation campaign results.
Illustration of Nodeworks Implementation Workflow

New node used to import experimental dataset and perform residual calculations required as part of the optimization (i.e., minimization of residuals).

Minimization performed by the General Optimizer node for:

\[
\min_{\theta} f(\theta) = \text{SSE}(\theta) = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} r_i(\theta)^2
\]

Optimal set of parameters identified that minimize the residual:
[9.55, 3.44, 9.41, 0.4, 0.69]

For more information on Nodeworks please visit:
https://mfix.netl.doe.gov/products/nodeworks/
or please scan the QR code:
**Comparison of Histograms for % Rel. Error Before & After Bug Fix**

**C1: Verification Simulation Campaigns (n=119)**

<table>
<thead>
<tr>
<th>MFFIX-PIC model Parameter</th>
<th>Default Settings</th>
<th>V&amp;V Manual Settings</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\theta_1$: Pressure linear scale factor</td>
<td>100</td>
<td>10</td>
</tr>
<tr>
<td>$\theta_2$: Vol. fraction exponential scale factor</td>
<td>3.0</td>
<td>3.0</td>
</tr>
<tr>
<td>$\theta_3$: Statistical weight</td>
<td>5.0</td>
<td>5.0</td>
</tr>
<tr>
<td>$\theta_4$: Vol. fraction at maximum packing</td>
<td>0.42</td>
<td>0.4</td>
</tr>
<tr>
<td>$\theta_5$: Solid slip velocity factor</td>
<td>1.0</td>
<td>0.5</td>
</tr>
</tbody>
</table>

### Theta 1 ($\theta_1$): Pressure linear scale factor
- Default (before BugFix) [Graph]
- Default (after BugFix) [Graph]

### Theta 2 ($\theta_2$): Vol. fraction exponential scale factor
- V&V Man (before BugFix) [Graph]
- V&V Man (after BugFix) [Graph]

### Summary Statistics
- Mean
- Std Dev
- Std Err Mean
- Upper 95% Mean
- Lower 95% Mean
C1: Proposed Calibrated Settings

Deterministic calibration with additional simulation campaigns (using 120 samples with different bounds)
## C1: Proposed Calibrated Settings

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Theta1 ( (\theta_1) ): Pressure linear scale factor</td>
<td>100</td>
<td>10</td>
<td>2.71</td>
<td>16.1</td>
<td>3.08</td>
<td>4.2</td>
</tr>
<tr>
<td>Theta2 ( (\theta_2) ): Vol. fraction exponential scale factor</td>
<td>3.0</td>
<td>3.0</td>
<td>3.74</td>
<td>2.04</td>
<td>3.71</td>
<td>2.1</td>
</tr>
<tr>
<td>Theta3 ( (\theta_3) ): Statistical weight</td>
<td>5.0</td>
<td>5.0</td>
<td>8.86</td>
<td>10.51</td>
<td>8.93</td>
<td>8.49</td>
</tr>
<tr>
<td>Theta4 ( (\theta_4) ): Vol. fraction at maxi-mum packing</td>
<td>0.42</td>
<td>0.4</td>
<td>0.4</td>
<td>0.4</td>
<td>0.4</td>
<td>0.38</td>
</tr>
<tr>
<td>Theta5 ( (\theta_5) ): Solid slip velocity factor</td>
<td>1.0</td>
<td>0.5</td>
<td>0.7</td>
<td>0.53</td>
<td>0.69</td>
<td>0.66</td>
</tr>
</tbody>
</table>

### Column Legend:
- **Default Settings**: Settings in MFIX-PIC
- **V&V Manual Settings**: Settings determined by trial-error.
- **PS Exp_n11 [NB]**: Proposed calibrated model parameter settings obtained with **PSUADE** using a surrogate model constructed from the simulation campaign with new bounds and 11 samples of analytical solution to guide calibration
- **PS Exp_n21 [NB]**: Same as above except 21 samples of analytical solution employed.
- **DK Exp_n21 [NB]**: Proposed calibrated model parameter settings obtained with **DAKOTA** using a surrogate model constructed from the simulation campaign with new bounds and 11 samples of analytical solution to guide calibration
- **DK Exp_n21 [OB]**: Same as above except surrogate model constructed from the simulation campaign with original bounds used.

### Note:
- Avg. % Rel. Err. is the % Relative Error calculated by \((\text{Surrogate model evaluation} - \text{Analytical Solln.})/ \text{Analytical Solln.}\)
### C1: Error Assessment of the Proposed Calibrated Settings

#### Comparison of PSUADE and DAKOTA (119 unseen samples for x1)

<table>
<thead>
<tr>
<th>Default (after BugFix)</th>
<th>PSU Exp_n11 (NB)</th>
<th>DAKOTA with 21 analytical samples</th>
<th>PSU Exp_n21 (NB)</th>
<th>DAKOTA with 21 analytical samples</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Quantiles</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>100.0% maximum</td>
<td>37.8%</td>
<td></td>
<td>100.0% maximum</td>
<td>7.09%</td>
</tr>
<tr>
<td>99.5%</td>
<td>37.82%</td>
<td></td>
<td>99.5%</td>
<td>9.66%</td>
</tr>
<tr>
<td>97.5%</td>
<td>35.44%</td>
<td></td>
<td>97.5%</td>
<td>9.66%</td>
</tr>
<tr>
<td>90.0%</td>
<td>28.40%</td>
<td></td>
<td>90.0%</td>
<td>7.01%</td>
</tr>
<tr>
<td>75.0% quartile</td>
<td>-5.42%</td>
<td></td>
<td>75.0% quartile</td>
<td>-1.99%</td>
</tr>
<tr>
<td>50.0% median</td>
<td>-11.46%</td>
<td></td>
<td>50.0% median</td>
<td>-6.44%</td>
</tr>
<tr>
<td>25.0% quartile</td>
<td>-15.47%</td>
<td></td>
<td>25.0% quartile</td>
<td>-14.15%</td>
</tr>
<tr>
<td>10.0%</td>
<td>-17.50%</td>
<td></td>
<td>10.0%</td>
<td>-10.86%</td>
</tr>
<tr>
<td>2.5%</td>
<td>-18.88%</td>
<td></td>
<td>2.5%</td>
<td>-14.15%</td>
</tr>
<tr>
<td>0.5%</td>
<td>-19.95%</td>
<td></td>
<td>0.5%</td>
<td>-10.86%</td>
</tr>
<tr>
<td>0.0% minimum</td>
<td>-19.95%</td>
<td></td>
<td>0.0% minimum</td>
<td>-14.15%</td>
</tr>
<tr>
<td><strong>Summary Statistics</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mean</td>
<td>-0.066134</td>
<td></td>
<td>Mean</td>
<td>-0.022515</td>
</tr>
<tr>
<td>Std Dev</td>
<td>0.144354</td>
<td></td>
<td>Std Dev</td>
<td>0.058876</td>
</tr>
<tr>
<td>Std Err Mean</td>
<td>0.0132577</td>
<td></td>
<td>Std Err Mean</td>
<td>0.0047578</td>
</tr>
<tr>
<td>Upper 95% Mean</td>
<td>-0.03982</td>
<td></td>
<td>Upper 95% Mean</td>
<td>-0.047746</td>
</tr>
<tr>
<td>Lower 95% Mean</td>
<td>-0.002447</td>
<td></td>
<td>Lower 95% Mean</td>
<td>-0.070207</td>
</tr>
<tr>
<td>N</td>
<td>119</td>
<td></td>
<td>N</td>
<td>119</td>
</tr>
</tbody>
</table>

Note: NB: surrogate model constructed from a simulation campaign with new bounds for some of the parameters, OB: simulation campaign with original bounds

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#### Summary

- **PSUADE**:
  - Analytical samples: 119
  - Error Assessment: comparison with analytical solutions

- **DAKOTA**:
  - Analytical samples: 21
  - Error Assessment: comparison with analytical solutions
C1: Proposed Calibration Settings

Visualization of Proposed Settings and Simulation Campaign

Proposed Calibrated Settings

- t1:p0 = 100;
- t5:VelfacCoeff = 1.0

Proposed Calibrated Settings (excl. t1=100, t5=1 for Default Settings)
Concluding Remarks

- MFiX-PIC offers substantial savings in time-to-solution, but the trade-off is accuracy.

- Objective was to employ various calibration techniques to assess the most uncertain model parameters specific to Parcel-in-Cell methodology and observe how they vary across different flow regimes.

- Adopted a systematic calibration procedure to identify optimal model parameter settings to minimize the discrepancy between MFiX-PIC and available experimental/analytical dataset. Started with Deterministic calibration as it is cheaper than Bayesian Calibration.

- Test the performance of calibrated model parameters rigorously. Also assessed the effect of varying sample size in the experiments (analytical solution).

- Explored different UQ toolkits such as PSUADE and DAKOTA and implemented the deterministic calibration capability within Nodeworks.

- When compared with the default settings, demonstrated significant accuracy improvement for Particle Settling case with deterministic calibration.
Future Work

- Perform deterministic calibration and statistical calibration for all selected cases and compare the outcomes from both calibration approaches

Case 1: Particle Settling (Preliminary Bayesian Calibration Results)

Case 3: Circulating Fluidized Bed

Case 2: Fluidization
**Future Work**

- Compare proposed calibrated model parameter settings for different flow regimes and provide best practices guidance to MFix-PIC users on how to set PIC specific parameters based targeted application. For example, for $\theta_3$:

<table>
<thead>
<tr>
<th>Cases / Flow Regimes</th>
<th>$t_1$ or ($\theta_1$): Pressure linear scale factor</th>
<th>$t_2$ or ($\theta_2$): Vol. fraction exponential scale factor</th>
<th>$t_3$ or ($\theta_3$): Statistical weight</th>
<th>$t_4$ or ($\theta_4$): Vol. fraction at maximum packing</th>
<th>$t_5$ or ($\theta_5$): Solid slip velocity factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1: Particle Settling</td>
<td>....</td>
<td>....</td>
<td><img src="image.png" alt="Histogram" /></td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td>C2: Fluidization</td>
<td>....</td>
<td>....</td>
<td><img src="image.png" alt="Histogram" /></td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td>C3: Circulating Fluidized Bed</td>
<td>....</td>
<td>....</td>
<td><img src="image.png" alt="Histogram" /></td>
<td>....</td>
<td>....</td>
</tr>
</tbody>
</table>


Note: QR codes for the URL of the references have been included to facilitate easy access via mobile devices.
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Additional Slides
Deterministic Calibration Procedure

Illustration of Nodeworks Implementation Workflow
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