Parameter Calibration and Uncertainty Quantification via Surrogate Model Optimization for CFD-DEM Modelling of a Small-Scale Slugging Bed

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Cover Illustration: Snapshot of CFD-DEM simulation of the poppy seed fluidized bed with time averaged concentration profiles compared to experimental data.


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Parameter Calibration and Uncertainty Quantification via Surrogate Model Optimization for CFD-DEM Modelling of a Small-Scale Slugging Bed

William D. Fullmer¹, Justin Weber², Dirk VanEssendelft²

¹ U.S. Department of Energy, National Energy Technology Laboratory, AECOM, 3610 Collins Ferry Road, Morgantown, WV 26507
² U.S. Department of Energy, National Energy Technology Laboratory, 3610 Collins Ferry Road, Morgantown, WV 26507

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NETL Contacts:
William Rogers, Principal Investigator
Jonathan Lekse, Technical Portfolio Lead
Bryan Morreale, Executive Director, Research & Innovation Center
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<th>Description</th>
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<tbody>
<tr>
<td>ARS</td>
<td>Advanced Reaction Systems</td>
</tr>
<tr>
<td>BC</td>
<td>Boundary condition</td>
</tr>
<tr>
<td>BVK</td>
<td>Beetstra, van der Hoef and Kuipers (drag law)</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational fluid dynamics</td>
</tr>
<tr>
<td>CI</td>
<td>Confidence interval</td>
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<tr>
<td>DEM</td>
<td>Discrete element method</td>
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<tr>
<td>DOE</td>
<td>Design of Experiments</td>
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<tr>
<td>GP</td>
<td>Gaussian Process</td>
</tr>
<tr>
<td>GUI</td>
<td>Graphical User Interface</td>
</tr>
<tr>
<td>LHS</td>
<td>Latin Hypercube</td>
</tr>
<tr>
<td>MRI</td>
<td>Magnetic resonance imaging</td>
</tr>
<tr>
<td>NETL</td>
<td>National Energy Technology Laboratory</td>
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<tr>
<td>OT</td>
<td>Optimization toolset</td>
</tr>
<tr>
<td>QoI</td>
<td>Quantity of interest</td>
</tr>
<tr>
<td>RMS</td>
<td>Response surface model (surrogate model)</td>
</tr>
<tr>
<td>UQ</td>
<td>Uncertainty quantification</td>
</tr>
</tbody>
</table>
Acknowledgments

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The authors would like to thank Tingwen Li and Jordan Musser for providing the initial MFix input decks used in this work and Terry Jordan and Kyle Buchheit for Nodeworks support.
ABSTRACT

An optimization toolset (OT) was recently developed to help facilitate computational fluid dynamics (CFD)-aided design processes. The basic workflow of the OT is: sweep a parameter space with a Design of Experiments (DOE), run CFD simulations at DOE points, create Response Surface Model (RSM) to act as a surrogate for the full CFD model, and optimize the surrogate model. This report shows how this basic framework can be applied to other CFD problems beyond design optimization. The Müller experiment (Müller et al., 2009) is used as the case of interest: rectangular, desktop-scale bubbling/slugging bed of poppy seeds. The first study used the OT to calibrate five unknown input parameters, particle-particle and particle-wall restitution, and friction coefficients and particle sphericity. The calibrated values correspond to a minimum in error in the predicted void fraction profiles to the experimentally measured profiles. Unfortunately, the optimized values are no better than reasonable but arbitrarily selected “baseline” values. The failure of the calibration stems largely from the fact that output response is largely insensitive to the inputs, even though a relatively wide range of input parameters is studied. In a second study, the simulation results are repurposed for an uncertainty quantification (UQ) study. The uncertainty in the epistemic (interval valued) input parameters are propagated through the CFD-discrete element method (DEM) model to quantify the resulting uncertainty in the interval valued output (void fraction profiles). It was promising that the UQ study was largely able to bound the experimental data. However, the lower bound near the center of the channel was found to be overly conservative when the RSM was forced to extrapolate to corners of the input parameter phase space with little support data. Consequently, this study contains more failures than successes, some of which can hopefully be built on in future work as lessons learned.
1. INTRODUCTION

The optimization toolset (OT) was developed in the Nodeworks graphical processing framework as part of the Advanced Reaction Systems (ARS) project during the FY2017. The OT seamlessly interfaces with the National Energy Technology Laboratories’ (NETL) open-source computational fluid dynamics (CFD) code MFiX through the recently developed MFiX-Graphical User Interface (GUI). The primary purpose of the OT is to aid in the development of novel reactor designs by using CFD to sweep parameter spaces and identifying ideal (optimal) design configurations or operating conditions.

However, the essential process is incredibly powerful and can be extended well beyond design optimization. This brief report attempts to show some of the potential analyses that can be carried out with the OT: i) parameter calibration and ii) uncertainty quantification (UQ). Both analyses consider a set of parameters to be unknown and the former attempts to identify specific parameter conditions which give best results, while the latter attempts to quantify the resulting uncertainty in the CFD prediction due to the uncertainty in the input parameters. Both example problems will utilize the Müller et al. (2009) experiment as the simulation conditions of interest which is described in the next section. Then, the numerical model, MFiX CFD-discrete element method (DEM), is overviewed including a description of the simulation time and the baseline results. The results of the parameter calibration and UQ through surrogate model optimization are presented in the following sections before concluding with a summary and future outlook.
2. MÜLLER EXPERIMENT

The experiments of Müller et al. (2009), hereafter referred to as the Müller experiment, was originally undertaken to generate CFD-DEM validation data and has already been considered in the MFiX-DEM validation process (Li et al., 2012). The experimental unit is a relatively small, lab-scale bubbling fluidized bed constructed of clear Perspex with dimensions 4.4-cm wide by 1.0-cm deep and 1.5 m-tall (although a shortened height is typically assumed for modeling purposes). At the bottom of bed is a porous plate distributor. The fluidizing gas is ambient air which is humidified to reduce electrostatic effects.

Poppy seeds are used as the fluidizing material which are reported (Müller et al. 2009) to have an average particle diameter and density of \( d_p = 0.12 \) cm and \( \rho_p = 1.0 \) g/cm\(^3\), which places the seeds at the intersection of Group B (sand-like) and Group D (spoutable) on the Geldart chart (1973). The minimum fluidization velocity was reported to be \( U_{mf} = 30 \) cm/s and data was collected at 60 and 90 cm/s (2\( U_{mf} \) and 3\( U_{mf} \)). The particle-particle and particle-wall interaction coefficients that need to be specified for DEM models were not directly measured. In MFiX, these four coefficients are the restitution coefficient, \( e_{pp} \) and \( e_{pw} \), and the kinetic friction coefficient, \( \mu_{pp} \) and \( \mu_{pw} \). (Rolling friction is not part of the default MFiX model and it is not included here, essentially making rolling friction coefficients of zero a modeling choice.) Directly measuring these parameters in isolated experiments would be difficult owing to the irregularity of the seeds as displayed in Figure 1. Furthermore, the particles are noticeably aspherical which, in addition to the relatively large microstructure on the surface of the seeds, makes the application of traditional (smooth, spherical particle) drag laws questionable. The impact of the particle shape on the drag will be modeled by a single scalar quantity known as sphericity, \( \psi \).

![Figure 1: Poppy seeds (USDA, 2007), the type of particles used in the Müller experiment. (Steve Hurst @ USDA-NRCS PLANTS Database)](image)

Magnetic resonance imaging (MRI) is used to image the bed in the \( z \)-direction, i.e., perpendicular to the \( xy \)-plane, and extract concentration contours gridded into a 32 × 32 pixel image corresponding to a 60 mm × 70 mm field of view. The gas void (volume) fraction, \( \varepsilon_g \), is reported at two elevations: \( y_1 = 1.64 \) cm and \( y_2 = 3.12 \) cm. Each profile, \( \varepsilon_g(x, y_j = y_1, 2) \), contains 22 discrete (pixelated) values. The \( x \)-locations of the data can be calculated directly from the reported pixel-to-cm ratio. The void fraction at each \( x \)-location is extracted with the web-based
digitizer Web Plot Digitizer (http://arohatgi.info/WebPlotDigitizer/). The digitized data is summarized in Table 1.

### Table 1: Summary of digitized data from Müller et al. (2009)

<table>
<thead>
<tr>
<th></th>
<th>$U = 60$ (cm/s)</th>
<th>$U = 90$ (cm/s)</th>
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<tr>
<td></td>
<td>$x$ (cm)</td>
<td>$y = 1.64$ (cm)</td>
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<tr>
<td>2.8125E+01</td>
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<tr>
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3. CFD-DEM

3.1 MODEL DESCRIPTION

The Müller experiment is modeled with MFiX CFD-DEM. The governing equations are presented in Garg et al. (2012a, 2012b) and are not repeated here. The linear spring dashpot model is used with spring constants of $2 \times 10^5$ g/s² for both particle-particle and particle-wall collisions. Both tangential damping factors are set to $1/2$. Particle time advancement is first order Eulerian. To improve computational speed, the DEM time step is increased to $\tau_{\text{coll}} / 20$ from the default value of $\tau_{\text{coll}} / 50$. The maximum CFD time step is limited to $1.5 \times 10^{-4}$ s which is approximately $\tau_{\text{coll}}$, depending on value of the restitution coefficient, a free variable in this study. The grid-coupled GARG_2012 interpolation scheme is used to transfer discrete particle information to the Eulerian CFD grid and vice versa.

The DNS-based BVK drag law of Beetstra et al. (2007) is applied. All other interfacial momentum transfer terms are neglected as well as the energy equations and interfacial mass transfer. The CFD time stepping is first order Eulerian and adaptive. The spatial discretization scheme applies the Superbee flux-limiter. The total iterative residual is $10^{-3}$ with the NORM_G=0 normalization option enabled. The MFiX default linear equation solver settings are not adjusted. The physical width and depth of the bed are used, i.e., $L_x = 4.4$ cm, $L_z = 1.0$ cm; however, a shortened height of only $L_y = 18$ cm is considered. The shortened height reduces the computational cost, but is tall enough that particles are not ejected through the pressure outlet during bubbling. The CFD grid is $N_x = 18$, $N_z = 4$, and $N_y = 72$ giving a non-dimensional grid size, $\Delta^* \equiv (L_x \times L_y \times L_z / N_x \times N_y \times N_z)^{1/3} / \rho_p$, of approximately 2. The front and back walls are set as free slip boundaries; the left and right walls as no slip. At the exit of the domain is a uniform pressure outflow boundary condition (BC). A uniform inflow BC at the inlet of the domain sets the single-phase distributor velocity to either 60 cm/s or 90 cm/s. No flow is initially prescribed in the bed domain and the pressure is hydrostatic at initialization. The gas-phase is treated as incompressible with a constant, uniform density and material viscosity of $1.2 \times 10^{-3}$ and $1.8 \times 10^{-4}$ g/cm-s. No turbulence modeling is explicitly considered.

Following the simulations of Müller et al. (2009), the bed is assumed to contain 9,240 particles. The particles are initialized in a random array in the lower half of the unit with a small, zero-mean thermal speed. The remaining particle properties needed to close the DEM model are the particle diameter, $d_p$, and material density, $\rho_p$, and restitution and kinetic friction coefficients for both particle-particle and particle-wall interactions. Only the first two of these input parameters have been reported. While almost certainly approximate (i.e., the associated uncertainties are unknown), the reported value of $d_p = 0.12$ cm and $\rho_p = 1.0$ g/cm³ will be treated here as exact. There is a large degree of uncertainty in what values the remaining input parameters should take. Here, $e_{pp}$, $e_{pw}$, $\mu_{pp}$ and $\mu_{pw}$ are treated as uncertain input parameters. One additional parameter is added to the list which, by default, is not a required input of the MFiX CFD-DEM model. Owing to the irregular shape and surface structure of the particles, see Figure 1, the particle sphericity, $\psi$, is included as a fifth uncertain input parameter. The sphericity quantifies how aspherical a particle is and essentially amounts to the transformation $d_p \rightarrow \psi d_p$, wherever $d_p$ is used in the drag law (LaMarche et al., 2015).
### 3.2 TIME AVERAGING WINDOW

The bubbling/slugging of the bed is an inherently dynamic, transient process. The MRI void fraction data are time averaged and an appropriate time averaging window must be used for each simulation considered in the parameter optimization. The simulation time was minimized as much as reasonably possible. Fortunately, the original simulations reported in Müller et al. (2009) indicate that the void fraction profiles converge relatively quickly. The case $U = 2U_{mf}$ (60 cm/s) was considered to determine an appropriate time averaging window.

In order to determine how short of a simulation can be carried out, the unknown parameters must be set to some values. Here, seemingly reasonable values $e_{pp} = e_{pw} = 0.8$, $\mu_{pp} = \mu_{pw} = 0.2$ and $\psi = 0.92$ were selected which will become the baseline values moving forward. Rather than comparing the statistics of the $2 \times 22$ locations where the data was collected, a simplified integral output is sought which will, hopefully, serve as a good indicator of the transient statistics for the depth averaged concentration profiles at elevations $y = y_1$ and $y_2$. This test uses $DP_{12}$, the cross-sectional averaged pressure drop between the elevations of $y_1$ and $y_2$, as the single quantity of interest (QoI).

A single baseline simulation is run for 55 s which took approximately 3 days of wall clock time on a single core. The pressure drop is displayed in Figure 2, showing the full transient on the left and the first 5 s on the right. It is apparent that the frequency of oscillation, which is related to the bubbling/slugging frequency (Boyce et al., 2014), is very high, in the vicinity of $\sim 7$ Hz, which explains why the statistics converge to stable values relatively quickly. The right panel of Figure 2 also indicates that the statistically steady state is reached rather quickly and only the first 2 s of the simulation are discarded as transient data. Figure 3 shows a running average of the pressure drop which also oscillates with a shrinking amplitude. Averages within $\pm 0.5\%$ (dashed lines) of the full 2 s to 55 s average (solid red line) are attained within a few seconds. As a compromise between simulation time and (statistical) accuracy, a time averaging window of 10 s from 2 to 12 s was selected.

![Figure 2: Cross-sectional area-averaged bed pressure drop between data measurement locations in the baseline simulation.](image-url)
Another simple way to quantify the error in this time-average is to bin the full window into shorter segments and calculate the average in each segment. The mean of the ensemble gives the original full-window time-average. The standard deviation among the ensemble of time averages, $\sigma_e$, can be used to give a confidence interval (CI) $\pm t_{0.025}(N_s-1)\sigma_e/N_s^{1/2}$ about mean, where $N_s$ is the number of segments (samples) and $t_{0.025}$ is the t-test statistic corresponding to a 95% degree of confidence. This is interpreted as 95% confidence that the true population mean, in this case the time-averaged value in the limit of an infinite window, lies within the interval around the sample mean. Binning the 10 s window of the $DP_{12}$ signal into 10 1.0 s segments, the 95%-CI is 0.585 or just over 1%. A benefit of this simple method is that it can be applied to other cases without running a longer simulation.

### 3.3 BASELINE RESULTS

Before considering the uncertainty in the input parameters, the baseline results were first compared to the Müller data. The series of images in Figure 4 shows the qualitative features of the simulated bubbling/slugging behavior. Interpolation of the CFD-grid centroid based void fraction field is used for quantitative comparison to the experimental data. Neither of the two $y$-elevations nor the 22 $x$-locations of the data match with the locations of the CFD-grid of the computational model. Therefore bi-linear interpolation is used to estimate the void fraction at the same 44 ($x,y$) locations as the Müller data. The void fraction is also averaged across the $z$-depth of the bed before bi-linear interpolation from the neighboring four CFD-grid points. The resulting depth-averaged, interpolated profiles are compared to the Müller data for the case $U = 2U_{mf}$ in Figure 5. It is almost unfortunate (for purpose of this study) that the comparison is already very good, leaving little room for improvement.
Figure 4: Snapshots of the bubbling bed in the baseline simulation at $U = 2U_{mf}$. Particles are colored by normalized vertical velocity.

Figure 5: Baseline results at $y_1$ (left) and $y_2$ (right) compared to the Müller data at $U = 2U_{mf}$. 
4. CALIBRATION

In order to perform parameter calibration, the following needs to be specified: i) the range possible values for the five particle parameters, and ii) the objective function or functions which will be optimized. For the former, Gel et al. (in press) recently conducted a survey of subject matter experts in the field of CFD-DEM. Their recommendations of $0.0 \leq \mu_{pp}, \mu_{pw} \leq 1.0$ and $0.20 \leq e_{pp}, e_{pw} \leq 0.99$ will be adopted here. The particles considered in the study of Gel et al. (in press) were quite spherical, therefore sphericity was not considered. Using a purely geometrical assumption, a sphericity range $0.80 \leq \psi \leq 1.0$ is applied here.

Next the values of $(e_{pp}, e_{pw}, \mu_{pp}, \mu_{pw}, \psi)$ are optimized within the given constraints (ranges) by minimizing the error between the predicted solution and the experimental data. Strictly speaking, there is a 44-QoI optimization problem (considering only void fraction data at one superficial velocity). Advanced multi-objective optimization methods do exist, e.g., Sandia National Laboratories Dakota software (dakota.sandia.gov), which accept multiple QoIs as inputs. However, many multi-objective problems are reformulated into a single QoI through a suitable weighting function. In this case, the most obvious objective function is a global error estimator, which is taken as the weighted square error:

$$E = \sum_{i=1}^{2} \sum_{j=1}^{22} w_{i,j} \left( e_{g}^{\text{exp}}(i,j) - e_{g}^{\text{sim}}(i,j) \right)^2,$$

where

$$w_{i,j} = W_{i,j}/\sum_{j=1}^{22} W_{i,j}.$$

Based on the baseline results in Figure 5, it might be desirable to consider a spatial weighting which gives more importance to near-wall data. Two weightings were tested: i) uniform, $W_{ij} = 1$, and ii) near-wall, $W_{ij} = (x_i - L_x/2)^2$. However, the global error estimates, $E$, resulting from both weightings showed a largely linear relationship indicating both contain essentially the same information. Therefore, uniform weighting is used throughout for simplicity.
In order to create a surrogate model mapping the uncertain input variables to the model error, $E$, sample simulations are run to fit a response surface model (RSM). To randomly and efficiently sample the 5-dimensional input space, the space filling Latin Hyper Cube (LHS) sampling available within the OT’s Design of Experiments (DOE) node is used. For UQ sampling, Oberkampf and Roy (2010) recommend a minimum of $n_e^3 + 2$ samples for LHS where $n_e$ is the number of epistemic or interval valued variables, i.e., no associated likelihood distributions. (All five variables are considered epistemic in this case unless supplementary experimental measurements were taken.) Although this recommendation is for sampling a model directly, it is applied here for the sampling to support the creation of a surrogate model. A simulation campaign of 127 runs is undertaken. The coverage of the input sampling is shown in Figure 6, comparing each input variable against every other. The points in Figure 6 give the quantities of $(e_{pp}, e_{pw}, \mu_{pp}, \mu_{pw}, \psi)$ for a unique CFD-DEM simulation.

TheMFIX input deck creation and job launching of each case is automated when the OT is accessed from the Nodeworks-MFiX-GUI, as was done in this case. A user defined function compiled into MFIX code interpolated the void fraction to the 44 spatial locations after each CFD time step and added a vector containing the running averages (from 2 to 12 s). At the end of the simulation, the uniform weighting is applied to the 10 s average and the final error estimate, $E$, is printed to a file in the local run directory of each simulation. Following an example from the Nodeworks documentation, a simple code node is added in the Nodeworks-MFiX-GUI which loops over each directory and reads the file containing the value of $E$. The directory loop ensures
that each output is associated with the correct input variables of the DOE table. The global response of $E$ as a function of each input variable is qualitatively shown as a scatter plot in Figure 7. The two variables which appear to show the most variation are the particle-particle restitution coefficient and the sphericity. This observation was confirmed by the Sobol’ sensitivity index calculation from the RSM (below). The third most important parameter is the particle-wall restitution coefficient which was largely due to second order (cross-correlation) effects with other variables.

![Figure 7: Scatter plots showing relationship between the input variables from the DOE and the system response, $E$ (output).](image1)

Next, a RSM surrogate model is built for analysis which is more suitable to analysis because it is continuous and helps to smooth out some of the noise in the results, e.g., from the finite time-average of the results. To construct the RSM, the OT’s squared exponential Gaussian Process (GP) model is used with $\theta_0 = 0.1, \theta_L = 0.001$ and $\theta_U = 1.0$. The nugget size was varied from 1.0 down to $10^{-7}$. It was determined that 0.001 gives a good compromise between uniformity (under-tuned) and noise (over-tuned).

![Figure 8: Gaussian Process surrogate model for $E$. RSM evaluated at $e_{pw} = 0.21, \mu_{pp} = \mu_{pw} = 0.01$.](image2)
The resulting GP surrogate model is shown in Figure 8 as a function $e_{pp}$ (des_en_input) and $\psi$ (c). (Note: The quantities in parentheses which appear in the axes of Figure 8 are the MFiX input variable names.) Optimization of the RSM is straightforward: in a plotting tab similar to Figure 8, the region of local minima is visually found, a point near the minima selected and then used as the starting point for a gradient based optimal calculation. The OT found a minimal error of $E = -0.0004228053721997713$ at $(e_{pp}, e_{pw}, \mu_{pp}, \mu_{pw}, \psi) = (0.98540814645931252, 0.20542187293944492, 0.0075981647927730323, 0.0068266141701654459, 0.99256176591850387)$. Rounding the two most important input quantities to six significant figures and the remainder to only two, $\psi = 0.992562$, $e_{pp} = 0.985408$, $e_{pw} = 0.21$, and $\mu_{pp} = \mu_{pw} = 0.01$ are taken as the calibrated optimal input parameters, i.e., the set of input parameters which minimize the error estimate $E$.

Figure 9: Optimized and baseline results at $y_1$ (left) and $y_2$ (right) compared to the Müller experimental data at $U = 2U_{mf}$. 

![Graphs showing optimized and baseline results compared to experimental data.](image-url)
Since no simulation was run exactly at the optimal condition, an additional simulation was run with these settings. The calibrated results with the optimized input parameters are compared to the original baseline results in Figure 9. The results are rather dissatisfying; in fact, $E$ has slightly increased with the calibrated parameters. As another test of the calibration, the optimized and baseline parameters were also used for simulations of the higher flow $3U_{mf}$ case, the results of which are shown in Figure 10. At $U = 3U_{mf}$, the calibrated parameters actually give a lower global error although not in a desired fashion. While quantitative, the estimator $E$ is lower for the calibrated parameters, it does so by missing most of the trends in the data and simply splitting the difference.

In the end, the failure is not that of MFiX or the OT, but the challenges (or lack thereof) with this problem. As noted in the previous section, randomly selecting plausible values for five input variables gave relatively good results to begin with. Furthermore, even casting a relatively wide net over the input space did not cause terribly wide scatter in the output which can be seen in the RSM, Figure 8, which only varies in global squared void fraction error from 0 to approximately 0.1%. While it may be possible to further improve these predictions (particularly at $3U_{mf}$), the parameter in need of calibration does not appear to be in the list of uncertain parameters, and, further, may not even be an MFiX input parameter, at least in the traditional sense, e.g., rolling friction coefficient (Li et al., 2012).
5. **UNCERTAINTY QUANTIFICATION**

Uncertainty quantification (UQ) traces some similar steps to the previous calibration study; however, the target analysis seeks to answer a more encompassing question. Rather than finding the set of input values give the best output results, UQ attempts to determine the range and/or probability distribution of output results given a range and/or probability distribution of uncertain input parameters. Specifically, this simple study is only concerned with the model input UQ. A full UQ study should also consider numerical uncertainties and (for true prediction, i.e., no experimental data for given conditions) model form error (Oberkampf and Roy, 2010).

To save computational resources for this exploratory study, the UQ analysis piggybacks on the existing results from the calibration study. In addition to printing the weighted error, $E$, the MFIX user defined function also printed the 10s-time averaged void fraction at the 44 experimental locations. In this case, all variables are epistemic in nature. That is, none of the input variables were experimentally measured properties and thus are treated as interval valued quantities with no underlying likelihood or probability distribution. Since any value within the interval is equally valid, the UQ study reduces to finding the minimum and maximum possible void fraction at each of the 44 locations. Rather than running many, many MFIX simulations to resolve the output extremes, a surrogate model will be built and optimized (maximized and minimized). The only significant difference between this process and the previous calibration study is that $\varepsilon_{\text{g}}(i,j)$ is used directly instead of $E$ and that 44 surrogate models are needed rather than just one. The same OT setup and the GP RSM properties used previously are used here to help automate the 44-surrogate model analysis (processed sequentially). The results of the bounding (epistemic only) UQ study are show in Figure 11 for the two void fraction profiles. Some key takeaways from this brief study are summarized below.

- It is promising that almost all of the data points can be bound by the input uncertainty propagated through the MFIX CFD-DEM model. Most of the data not bound by the UQ curves (left wall side of elevation $y_2$) are not side-to-side symmetric which could indicate irregularities in the test section, which would be very difficult to reproduce computationally—and frankly would be better grouped into model form uncertainty, i.e., discrepancies between experiment and prediction that are (presumably) from physics that are not considered in the model.
The top and bottom curves look quite different. This is because most of the DOE simulations over the input parameter phase space predict a center peaked void fraction profile similar to the baseline and optimized results of the previous section. However, some conditions predict a double peaked profile which actually has a (local) minima in the center of the channel. These curves are contributing more to the lower bound. At least one of these double peaked profiles was checked and found to have likely unphysical parameters, e.g., $\mu_{pw} >> \mu_{pp}$. Some of these cases could probably be thrown out; however, since absolutely no information is known for these input parameters, the best conservative practice is to consider all possible combinations of the input parameters.

The profiles may be overly conservative due to the treatment of each data point as a separate QoI, in each case simply looking for the maximum and minimum possible values. In some instances, the conditions along a bounding curve would change drastically from one point to another which disagrees with the physical intuition of how these input parameters should be treated. (For instance, between the 17th and 18th points along the $y_1$ lower bounding profile $e_{pp}$ jumped from \(~0.2~(lower~bound)\) to 0.99 (upper bound). There does not appear to be a straightforward solution to this concern; most UQ studies restrict their focus to a small set of integral or extrema valued system quantities.

The minima at the center of the lower bound profiles is too low. While many of the identified extrema in the RSMs were within the parameter bounds, some (specifically in this region) were identified to be at the limit of one or more parameters. In this case there is little simulation data support in the RSM and it is forced to make an extrapolation rather than an interpolation (which is much less reliable for GP RSMs). Figure 12 shows one such instance at point ($x_1$, $y_2$) where the identified minima was near the lower limit of $e_{pp}$ and upper limit of $\psi$. The RSM projects a minimum from the surrounding points within the input parameter space which is much less than any simulated value. In some instances, this problem could be alleviated by resampling near the region of interest. A
more practical solution may be to simply sample a wider phase space than eventually considered in the optimization step of the constructed RSM. However, this would also require the addition of constrained optimization techniques which may be considered for future development of the OT.

- Finally, the interval valued UQ (finding maxima and minima of RSMs) was only applied here because all uncertain input parameters were considered epistemic. If at least one parameter were aleatory (known distribution), the RSM would need to be sampled with that distribution and a probability box (p-box) constructed for each point to find the observed extrema. The OT has this capability for approximately normal distributions. It would be interesting to test this capability in the future; however, a better set of experiments needs to be identified where (at least some of) these properties have been measured.

![Figure 12: Identified minimum in RSM of void fraction point (x12, y2).](image)
6. SUMMARY AND FUTURE OUTLOOK

This brief work presented two studies using the basic framework of the OT toolset which extend the scope of the original OT analysis methods. In the first test, five uncertain input parameters were calibrated through optimization of an objective function estimating the global error between the simulations and the experimental data. This effort largely failed because the problem was simply not very sensitive to—even to a very wide range of—the five input parameters. In a second take, the uncertainty in the epistemic (interval valued) input parameters were propagated through the CFD-DEM model to quantify the resulting uncertainty in the interval valued output (void fraction profiles). The UQ study was largely able to bound the experimental data; however, some outstanding issues caused overly conservative bounds in some regions of the domain (lower bound, center of channel). In the end, what was found to be most lacking in this study was the selected problem, the Müller experiment (Müller et al., 2009). An ideal system for a follow up study would:

- Have a more sensitive response to the unknown input parameters
- Have some measurements of the input parameters allowing mixed (epistemic-aleatory) UQ
- Keep a similarly low particle count
- Include error estimates of the experimental data

Of course, finding or constructing such an ideal system is a considerable challenge in itself. Some possible ideas for future development of the OT resulting from this work are:

- Constrained optimization
- DOE methods that allow resampling
- Ability to sample RSM with empirical distributions
7. REFERENCES


http://plants.usda.gov/java/nameSearch?keywordquery=Papaver+somniferum&mode=scientific&name&submit.x=11&submit.y=5
Sean Plasynski, Ph.D.
Director (Acting)
National Energy Technology Laboratory
U.S. Department of Energy

John Wimer
Associate Director
Strategic Planning
Science & Technology Strategic Plans & Programs
National Energy Technology Laboratory
U.S. Department of Energy

Brian Morreale
Executive Director
Research & Innovation Center
National Energy Technology Laboratory
U.S. Department of Energy