# Uncertainty Quantification Tools for Multiphase Flow Simulations using MFIX


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# Outline

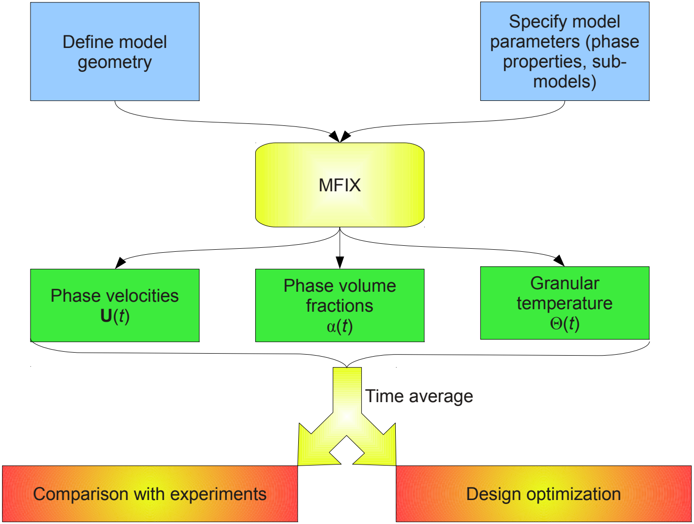
1. Introduction and background
2. Project objectives and milestones
3. Technical progress
4. Future work

# Outline

# Eulerian multiphase models for gas-particle flows

- Widely used in both academia and industry
- Computationally efficient
- Applicable to real-world cases (gasifiers, combustors, ...)
- Directly provide averaged quantities of interest in design and optimization studies
- Implemented into many computational codes
  - Commercial codes, eg. FLUENT
  - Open-source codes, eg. OpenFoam®, MFIX

# Typical steps in a simulation project with MFIX



# Motivations and objectives

## Models and uncertainty

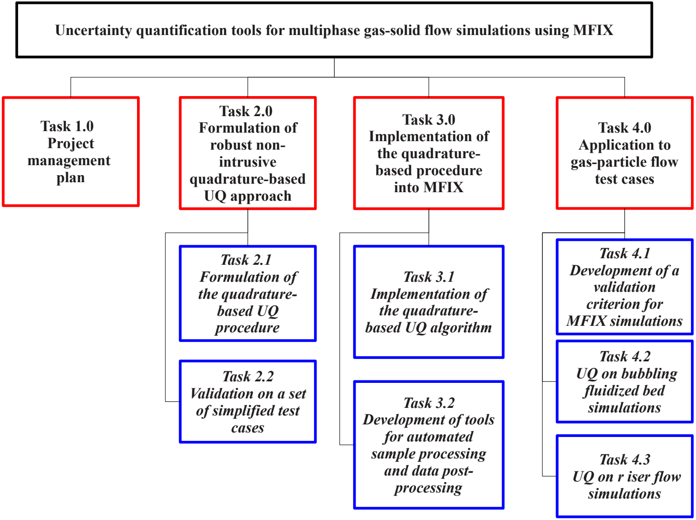
- Models present a strongly non-linear relation between inputs and outputs
- Input parameters are affected by uncertainty
  - Experimental inputs
  - Theoretical assumptions
- Need to quantify the effect of uncertainty on the simulation results

## Main objectives

- Develop an efficient quadrature-based uncertainty quantification (UQ) procedure
- Develop a reconstruction procedure for the probability distribution function (PDF) of the system response
- Apply such a procedure to multiphase gas-particle flow simulations considering parameters of interest in applications

# Outline

# Project tasks



# Project milestones and current status

| Milestone n. | Description | Due on | Status |
|---|---|---|---|
| 1 | Submission of project management plan | Dec. 30, 2011 | Completed |
| 2 | Formulation of the quadrature-based UQ procedure | Jul. 1, 2012 | Completed |
| 3 | Validation of the quadrature-based UQ procedure on simplified test-cases | Oct. 1, 2012 | Completed |
| 4 | Implementation of the quadrature-based UQ algorithm into MFIX | May 31, 2013 | Completed |
| 5 | Development of automated tools for processing input/output data | Oct. 1, 2013 | Completed |
| 6 | Development of a Validation Criterion for MFIX Simulations | Jan. 3, 2014 | Completed |
| 7 | UQ on bubbling fluidized bed simulations | Mar. 31, 2014 | Completed |
| 8 | UQ on riser flow simulations | Sept. 1, 2014 | In progress, on time |
| 9 | Preparation of final report | Sept 31, 2014 | Starts on Sept. 1, 2014 |

# Outline

# Basic concepts

- We study propagation of uncertainty from inputs to outputs
- Sources of uncertainty
  - Domain geometry
  - Initial/boundary conditions
  - Model inputs and parameters
  - Model assumptions
- Non-intrusive approach
  - Sample the space of the uncertain input parameters of the model
  - Obtain simulation results for each sample
  - The moments (statistics) of the model results are the quantity of interest
    - Low-order statistics for practical purposes (mean, variance, ...)
    - Reconstructed PDF of the response

# Quadrature-based UQ procedure – univariate case

- Consider a probability space $\mathcal{P}(\Omega, \mathfrak{F}, P)$
  - A sample space $\Omega$, a $\sigma$-algebra $\mathfrak{F}$, and a probability measure $P$
  - One random variable (uncertain parameter) $\xi$
  - A random process $\kappa(\xi, x)$
- The objective is to compute the moments of the random process:

$$m_n = \int_\Omega \kappa(\xi, x)^n p(\xi) \mathrm{d}\xi$$

## Direct quadrature approach

- Sample $\Omega$ using Gaussian quadrature formulae.
- Evaluate the model for each sample to obtain abscissas.
- Approximate moments directly using quadrature weights and abscissas.

# Quadrature-based UQ procedure – univariate case

- Use Gaussian quadrature formula, the moments about the origin of the response can be approximated as

$$m_n = \int_\Omega \kappa(\xi, x)^n p(\xi) \mathrm{d}\xi \approx \sum_{i=1}^{\mathrm{M}} w_i(x) \left[\kappa(\xi_i, x)\right]^n$$

where

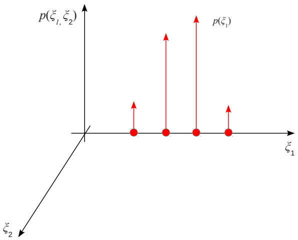
  - M is the number of nodes
  - $w_i(x)$ are the quadrature weights
  - $\xi_i$ are the quadrature nodes

## Weight functions

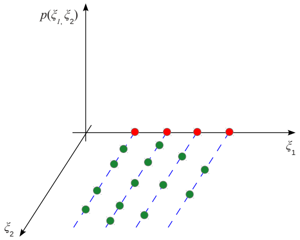
The form of $p(\xi)$ depends on the assumed PDF of the uncertain parameter (uniform, Gaussian, ...)

# Quadrature-based UQ procedure – multivariate case

- Sampling procedure for a bivariate case ($\boldsymbol{\xi} = \xi_1, \xi_2$) using CQMOM




Find weights $w_{l_1}$ and nodes $\xi_{1,l_1}$




Use conditional moments $\langle \xi_2^j \rangle_{l_1}$ to find weights $w_{l_1,l_2}$ and nodes $\xi_{2,l_1,l_2}$

## Moments of the system response

$$\langle \kappa^n(\boldsymbol{\xi}) \rangle = \int_{\mathbb{R}^2} [\kappa(\boldsymbol{\xi})]^n p(\boldsymbol{\xi}) \mathrm{d}\boldsymbol{\xi} \approx \sum_{l_1=1}^{M_1} \sum_{l_2=1}^{M_2} w_{l_1} w_{l_1,l_2} \left[\kappa(\xi_{1,l_1}, \xi_{2,l_1,l_2})\right]^n$$

# Low-order statistics

- Central moments

$$\mu_n = \sum_{i=0}^{n} \binom{n}{j} (-1)^{n-i} m_i \mu^{n-j}$$

- Mean

$$\mu = m_1/m_0$$

- Variance (distance from the mean)

$$\sigma^2 = \frac{m_2}{m_0} - \mu^2$$

- Skewness (symmetry of the distribution)

$$\gamma_1 = \frac{\mu_3}{\sigma^3} = \frac{m_3/m_0 - 3\mu m_2/m_0 + 2\mu^3}{\sigma^3}$$

- Kurtosis (importance of tails)

$$\gamma_2 = \frac{\mu_4}{\sigma^4} = \frac{m_4/m_0 - 4\mu m_3/m_0 + 6\mu^2 m_2/m_0 - 3\mu^4}{\sigma^4}$$

# Reconstruction of the response PDF

- The foundation of extended quadrature method of moments (EQMOM):

$$f_N(\kappa) = \sum_{i=1}^{N} \rho_i \delta_\sigma(\kappa, \kappa_i)$$

  where
  - N is the number of non-negative kernel functions
  - $\rho_i$ is the $i$-th quadrature weight used in the PDF reconstruction
  - $\delta_\sigma(\kappa, \kappa_i)$ is the kernel density function
- The choice of the kernel density function $\delta_\sigma(\kappa, \kappa_i)$
  - Beta distribution: $\kappa$ on bounded interval $[a, b]$
  - Gamma distribution: semi-infinite $\kappa$ on $[a, +\infty)$
  - Gaussian distribution: $\kappa$ on the whole real set

# Beta EQMOM

**Beta kernel function**

$$\delta_\sigma(\kappa,\kappa_i)=\frac{\kappa^{\lambda_i-1}(1-\kappa)^{\phi_i-1}}{B(\lambda_i,\phi_i)},\ \lambda_i=\frac{\kappa_i}{\sigma},\ \phi_i=\frac{1-\kappa_i}{\sigma}$$

↓

**PDF of the response**

$$f_N(\kappa)=\sum_{i=1}^{N}\rho_i\frac{\kappa^{\lambda_i-1}(1-\kappa)^{\phi_i-1}}{B(\lambda_i,\phi_i)}$$

↓

**Integer moments of the kernel**

$$m_n^{(i)}=\frac{\kappa_i+(n-1)\sigma}{1+(n-1)\sigma}m_{n-1}^{(i)}=m_0^{(i)}\prod_{j=0}^{n-1}\frac{\kappa_i+j\sigma}{1+j\sigma}$$

↓

**Integer moments of the PDF**

$$m_n=\sum_{i=1}^{N}\rho_i G_n(\kappa_i,\sigma),\ G_n(\kappa_i,\sigma)=\begin{cases}1 & n=0\\ \prod_{j=0}^{n-1}\frac{\kappa_i+j\sigma}{1+j\sigma} & n\geq 1\end{cases}$$

↓

**Lower triangular system**

$$m_n=\eta_n m_n^*+\eta_{n-1}m_{n-1}^*+\ldots+\eta_1 m_1^*,\ m_n^*=\sum_{i=1}^{N}\rho_i\kappa_i^n$$

# Beta EQMOM

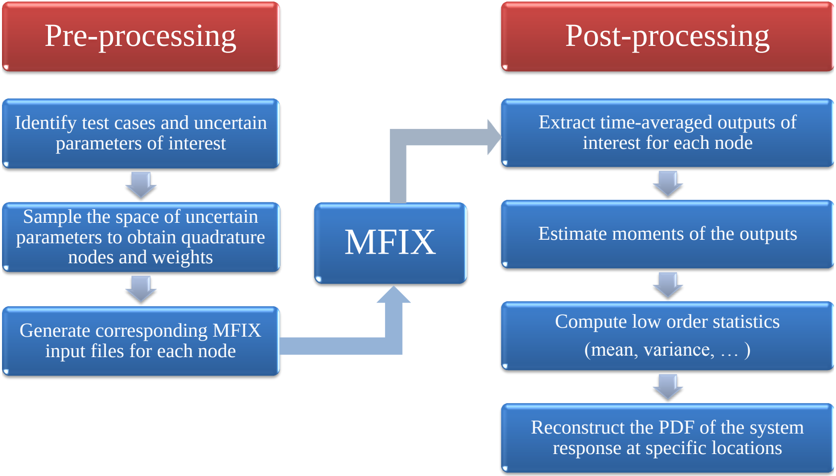
- The algorithm to solve for $\sigma$ is:
  1. Guess $\sigma$
  2. Compute the moments $m_n^*$ from the system $\mathbf{A}(\sigma)\mathbf{m}^* = \mathbf{m}$
  3. Use the Wheeler algorithm to find weights and abscissas from $\mathbf{m}^*$
  4. Compute $m_{2N}^*$ using weights and abscissas
  5. Compute

     $$J_N(\sigma) = m_{2N} - \eta_{2N} m_{2N}^* - \eta_{2N-1} m_{2N-1}^* - \ldots - \eta_1 m_1^*$$

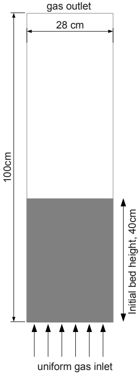
  6. If $J_N(\sigma) \neq 0$, compute a new guess for $\sigma$ and iterate from step 1 until convergence
- The normalized distribution for $\kappa$ on bounded interval $[a, b]$ is

$$f_N(\kappa) = \frac{1}{b-a} \sum_{i=1}^{N} \rho_i \frac{\left(\frac{\kappa-a}{b-a}\right)^{\lambda_i - 1} \left(\frac{b-\kappa}{b-a}\right)^{\phi_i - 1}}{B\left(\lambda_i, \phi_i\right)}$$

# Implementation into MFIX



# Bubbling fluidized bed




- Two fluid model (MFIX)
- Kinetic theory closures

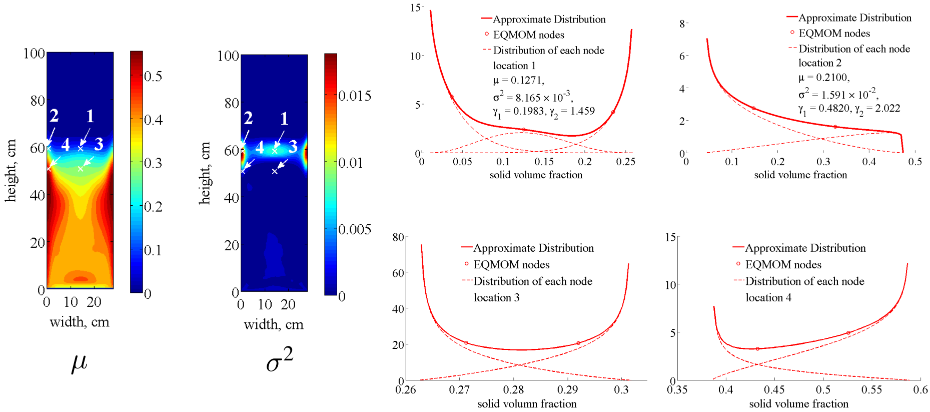
## Properties

- Gas density $\rho_g = 1.225 \text{ kg/m}^3$
- Solid density $\rho_s = 2500 \text{ kg/m}^3$
- Uncertain particle size
  - Mean diameter $d_s = 275\ \mu\text{m}$
  - Uniform distribution
  - Standard deviation $\sigma = 0.3\ d_s$

## Initial and boundary conditions

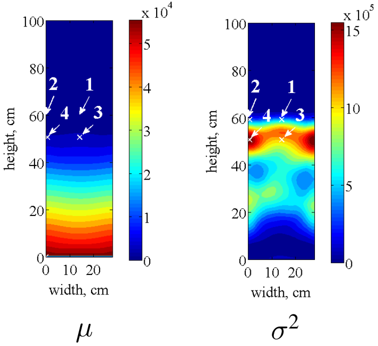
- Bed height: 0.40 m, void fraction: 0.4
- Inlet gas velocity: 0.38 m/s
- Inlet: constant gas inflow
- Outlet: zero gas pressure
- Wall: no-slip boundary condition

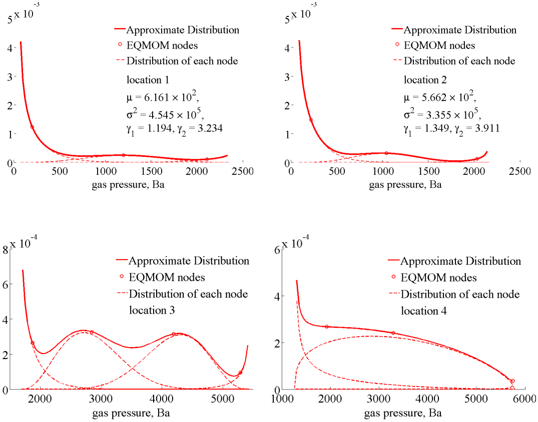
# Solid volume fraction




- The effect of uncertain particle diameter focuses on the interface of the bed, in particular near the wall.

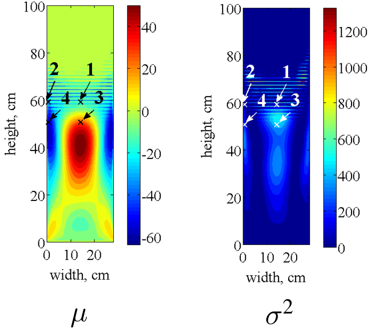
# Gas pressure

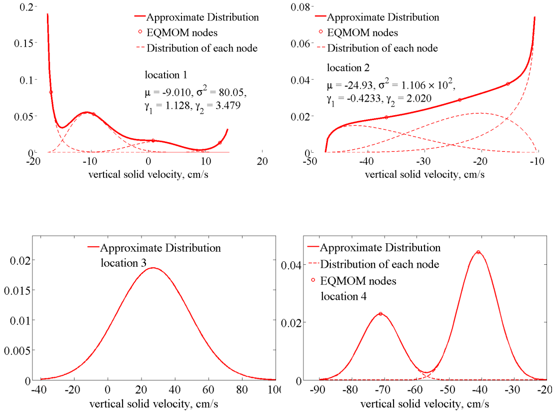



- The effect of uncertain particle diameter focuses on the interface of the bed, especially near the wall.

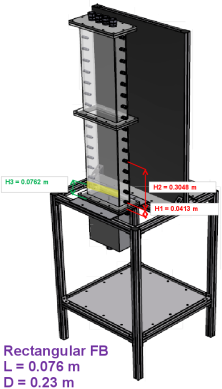
# Vertical solid velocity




- The effect of uncertain particle diameter focuses on the interface of the bed and also near the wall.

# Descriptions of Small Scale Challenge Problem SSCP-I




Rectangular FB
L = 0.076 m
D = 0.23 m
H = 1.22 m

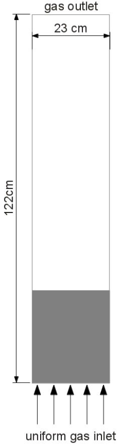
## Properties

- Particle diameter 3256 $\mu$m
- Particle density 1131 $\mathrm{kg/m^3}$
- Sphericity 0.94
- Gas density 1.204 $\mathrm{kg/m^3}$
- Gas viscosity $1.79 \times 10^{-5}$ Pa $\cdot$ s
- Minimum fluidization velocity 1.05 m/s

## Uncertain parameters

- Particle-particle restitution coefficient 0.84
- Particle-wall restitution coefficient 0.92
- Independent variables

# Descriptions of Small Scale Challenge Problem SSCP-I




## Initial conditions

- Bed height 0.163 m
- Void fraction 0.40
- Superfacial gas velocity 2.19 m/s

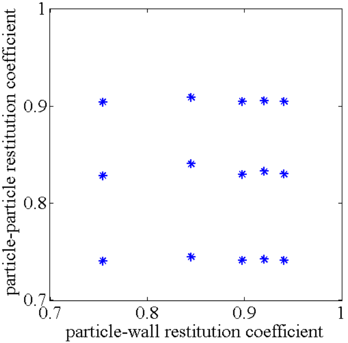
## Boundary conditions

- Inlet: constant inlet velocity
- Outlet: zero gas pressure
- Wall: no-slip (gas)
  Johnson-Jackson (particles)

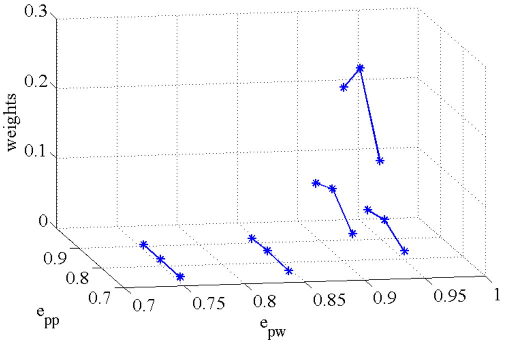
- Two fluid model (MFIX)
- Kinetic theory closures

- Simulation time 90 s
- Convergence criterion $10^{-4}$

# Sampling method: CQMOM

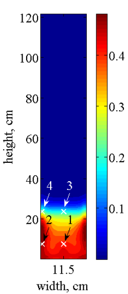



Samples generated by CQMOM

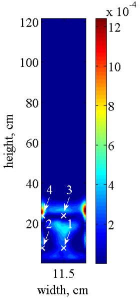



Weights for each sample

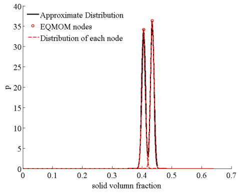
# Solid volume fraction



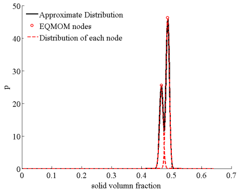

$\mu$



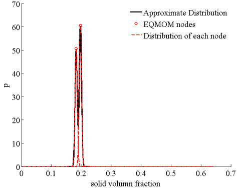

$\sigma^2$



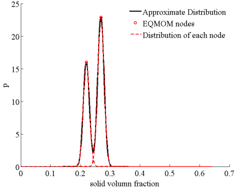

Location 1




Location 2



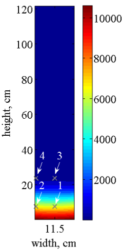

Location 3



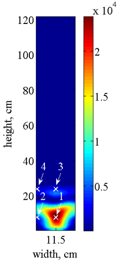

Location 4

- The effect of uncertain parameters focuses on the interface of the bed, in particular near the wall, and also on the center of the bed.

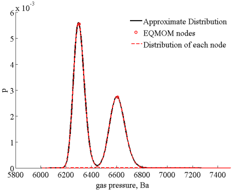
# Gas pressure



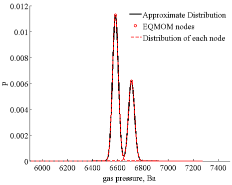

$\mu$



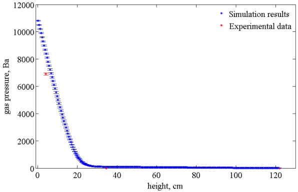

$\sigma^2$

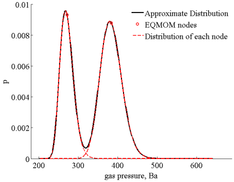



Location 1

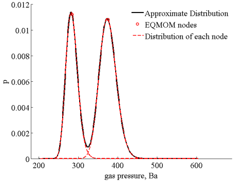



Location 2



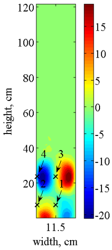

Location 3



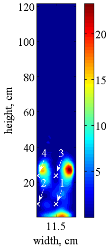

Location 4

- The effect of uncertain parameters focuses on the center of the bed.

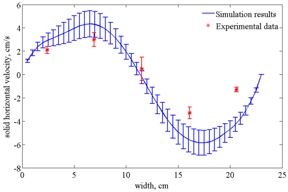
# Solid horizontal velocity

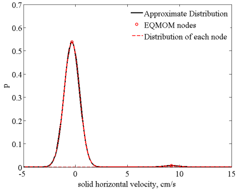



$\mu$




$\sigma^2$

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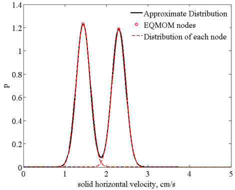
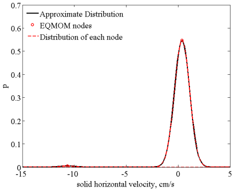
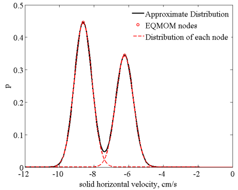



Location 2



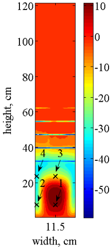

Location 3



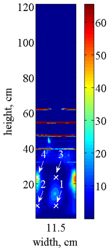

Location 4

- The effect of uncertain parameters focuses on the interface and bottom of the bed.

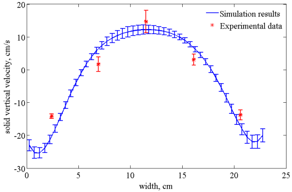
# Solid vertical velocity

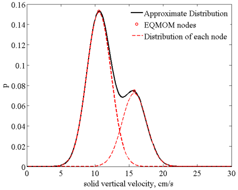



$\mu$

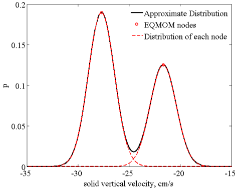



$\sigma^2$

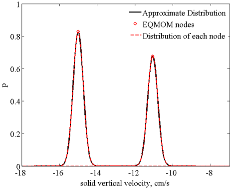


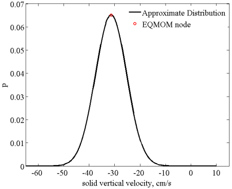

Location 1




Location 2




Location 3




Location 4

- The effect of uncertain parameters focuses on locations near the wall.

# Outline

# Future work

- Apply the developed procedure to gas-particle flow simulations in risers
- Prepare for the final report

# Budget

| DOE UCR – FE0006946<br>Cost plan status | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | | |
| **Baseline Reporting Quarter** | **Budget Period 2** | | | | **Budget Period 3** | | | |
| | **Q3** | | **Q4** | | **Q1** | | **Q2** | |
| | **Apr. 1, 2013 - Jun. 30, 2013** | | **Jul. 1, 2013 - Sept. 30, 2013** | | **Oct 1. 2013 - Dec. 31, 2013** | | **Jan. 1, 2014 - Mar. 31, 2014** | |
| | **Q3** | **Cumulative total** | **Q4** | **Cumulative total** | **Q1** | **Cumulative total** | **Q2** | **Cumulative total** |
| **Baseline cost plan** | | | | | | | | |
| Federal share | 26603.00 | 174123.00 | 22905.00 | 197028.00 | 28347.00 | 225375.00 | 23592.00 | 248967.00 |
| Non-federal share | 1850.00 | 12950.00 | 1850.00 | 14800.00 | 1850.00 | 16650.00 | 1850.00 | 18500.00 |
| Total planned | 28453.00 | 187073.00 | 24755.00 | 211828.00 | 30197.00 | 242025.00 | 25442.00 | 267467.00 |
| **Actual incurred cost** | | | | | | | | |
| Federal share | 31646.29 | 134567.13 | 33777.04 | 168344.17 | 33456.69 | 201800.86 | 29371.87 | 231172.73 |
| Non-federal share | 1850.00 | 12950.00 | 1850.00 | 14800.00 | 1850.00 | 12950.00 | 1850.00 | 14800.00 |
| Total incurred costs | 33496.29 | 147517.13 | 35627.04 | 183144.17 | 35306.69 | 218450.56 | 31221.87 | 249672.73 |
| **Variance** | | | | | | | | |
| Federal share | 5043.29 | -39555.87 | 10872.04 | -28683.83 | 5109.69 | -23574.14 | 5779.87 | -17794.27 |
| Non-federal share | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| Total variance | 5043.29 | -39555.87 | 10872.04 | -28683.83 | 5109.69 | -23574.14 | 5779.87 | -17794.27 |

# Personnel and publications

## Personnel

- 1 Assistant professor (Alberto Passalacqua) from October 2011
- 1 Ph.D. student (Xiaofei Hu) from June 2012

## Publications

- X. Hu, A. Passalacqua, R. O. Fox, P. Vedula, A quadrature-based uncertainty quantification approach with reconstruction of the probability distribution function of the system response, in preparation.
- X. Hu, A. Passalacqua, R. O. Fox, A quadrature-based uncertainty quantification approach with reconstruction of the probability distribution function of the system response in bubbling fluidized beds, 2013 AIChE Annual Meeting, San Francisco, CA, November 3rd – 8th, 2013.
- X. Hu, A. Passalacqua, R. O. Fox, Validation of a quadrature-based uncertainty quantification approach using NETL small scale challenge problem SSCP-I, ASME 2014 Verification and Validation Symposium, Las Vegas, NV, May 7th – 9th, 2014.
- X. Hu, A. Passalacqua, R. O. Fox, A quadrature-based uncertainty quantification approach in a multiphase gas-particle flow simulation in a riser, 2014 AIChE Annual Meeting, Atlanta, GA, November 16th – 21st, 2014, submitted.

Thanks for your attention!

Questions?