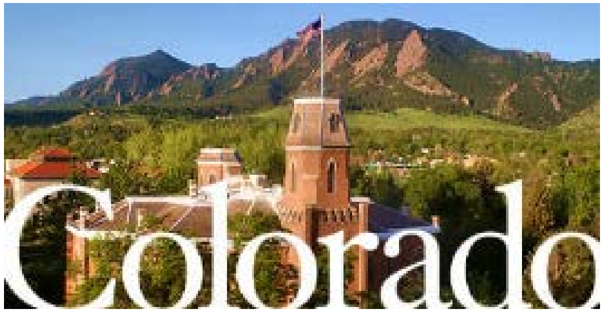
MFIX-DEM Enhancement for Industry-Relevant Flows

PSRI



NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Annual Project Review Meeting for Crosscutting, Rare Earth Elements, Gasification and Transformative Power Generation

Pittsburgh, PA
April 2019

Project leads

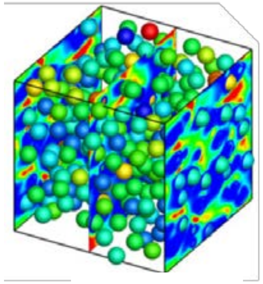
Dr. Ray Cocco (PSRI, co-PI)
Dr. Ray Grout (NREL, co-PI)
Prof. Thomas Hauser (Univ. CO, co-PI)
Prof. Christine Hrenya (Univ. CO, PI)

Funding

NETL
NATIONAL ENERGY TECHNOLOGY LABORATORY

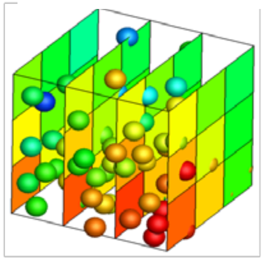
Background: Numerical Methods for Studying Gas-solid Flows

Tenneti & Subramaniam (2016)



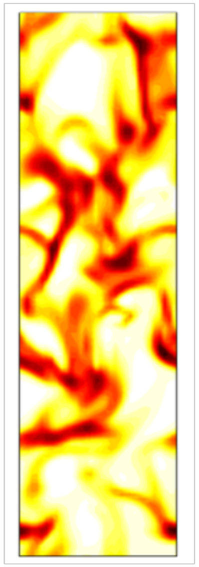
DNS

CFD-DEM



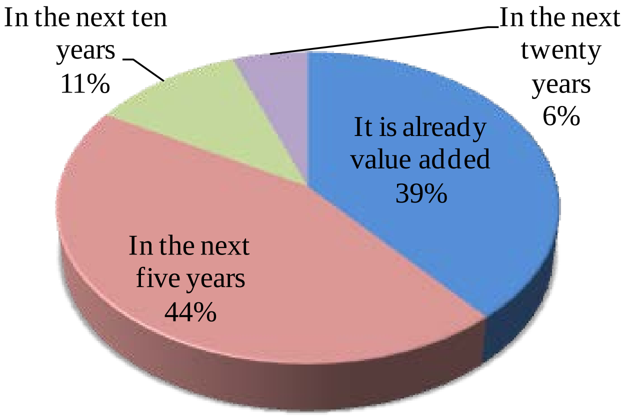
In-house

Two-Fluid Model (TFM)



In-house

Expected value added through DEM



PSRI Industrial Survey
(Cocco et al., *Chem. Eng. Prog.*, 2017)

More detail, fewer closures

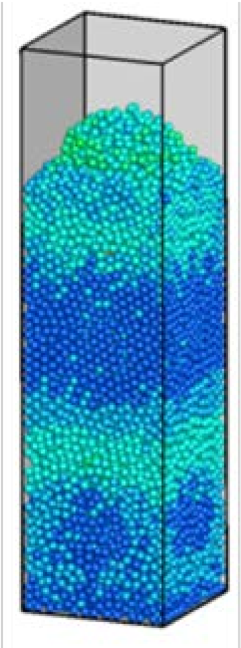
Less CPU time

DEM:

a balance between computational overhead and sources of uncertainty

Fullmer and Hrenya
(*Ann. Rev. Fluid Mech.*, 2017)

Motivation: Big picture



CFD-DEM

$N_p \sim 10^5$ - 10^7

Laboratory

$N_p \sim 10^9$ - 10^{10}

Industry

$N_p \sim 10^{14}$

Goal: DEM application toward industrially relevant flows

Challenges

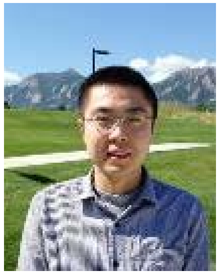
- Speed ⇒ Optimization & Algorithms (this talk)
- Results reliability ⇒ Validation & **Uncertainty Quantification (this talk)**

Team

University of Colorado
Chemical & Biological Engineering
DEM modeling of granular and gas-solid flows, MFIX


Prof. Christine Hrenya


Dr. William Fullmer (now at NETL)


Dr. Peiyuan Liu


Dr. Steven Dahl

University of Colorado
Research Computing
High-performance computing, CFD


Prof. Thomas Hauser

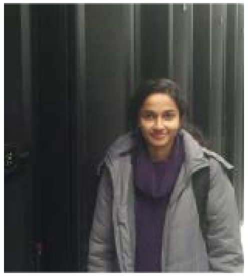

Shadong Lao


Aaron Holt

NREL
Computational Science
High-performance computing, CFD


Dr. Ray Grout


Dr. Hari Sitaraman


Deepthi Vaidhynathan

PSRI
Industrial Application and Experiments of Particle Flows

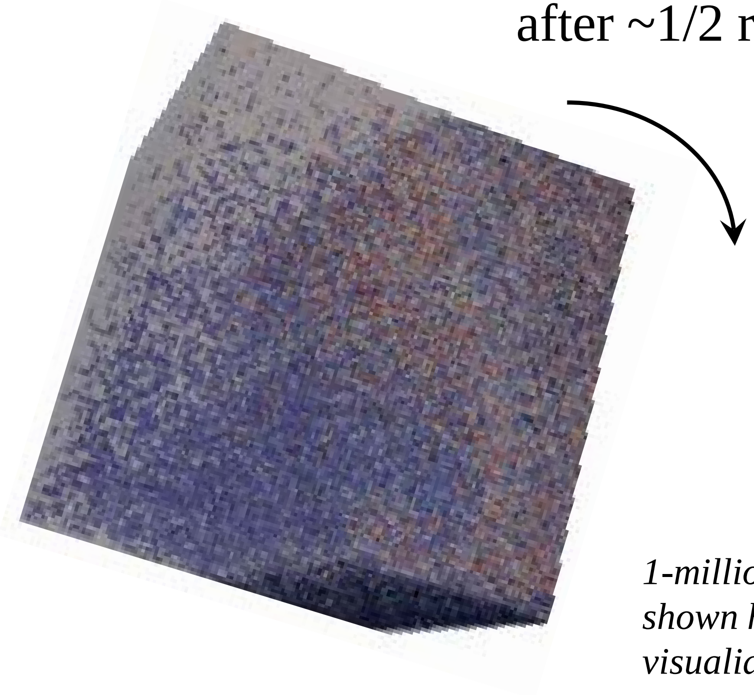

Dr. Ray Cocco


Dr. Casey LaMarche

Recent Accomplishment: 1-billion particle case

Rotating square tumbler

- Gaussian PSD (250-750 μm)
- Domain: 0.72m x 0.72m x 0.72 m
- Simulation time: 1 sec (1 full rotation)



after ~1/2 rotation

1-million particle case shown here for easier visualiation

Background

Computer models are often deterministic

- One set of inputs → one set of outputs

Most real-world problems include input uncertainty

- Measurement precision
- Natural variability (e.g., particle size distribution)

State-of-the-art Uncertainty Quantification (*Full UQ*)

- Direct sampling over the entire phase-space of uncertain inputs
- Establishes range and likelihood of possible outcomes
- Often exceedingly expensive (thousands of simulations; many more than validation)

Need to reduce computational expense to apply UQ to CFD-DEM

- *Reduced UQ*
    - Identify and propagate uncertainties for key input parameters only

CFD-DEM Small-Scale Experiments: Prior Work

Common system

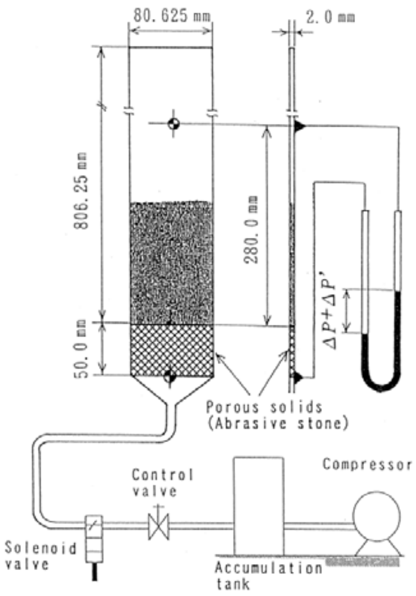
- *Small rectangular FB*
- *Group D particles*
- $N_p \sim 10^5$

Metrics to compare

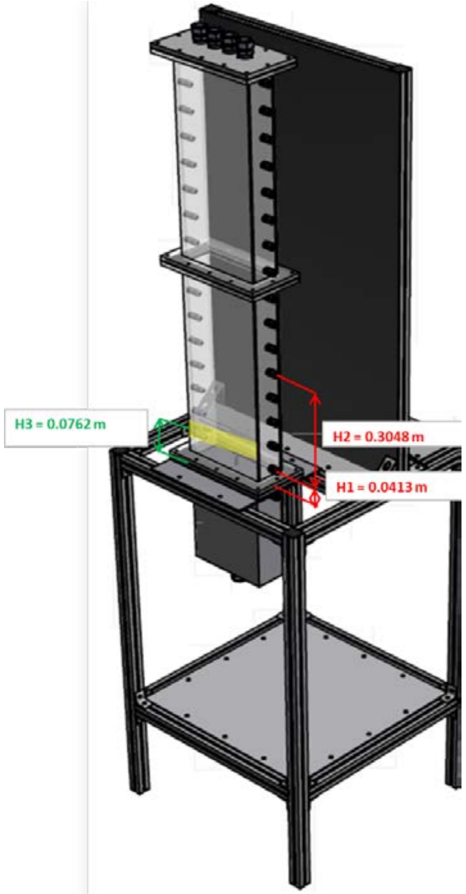
- *Flow patterns*
- *Pressure drop*
- *Velocity profiles*

Objective

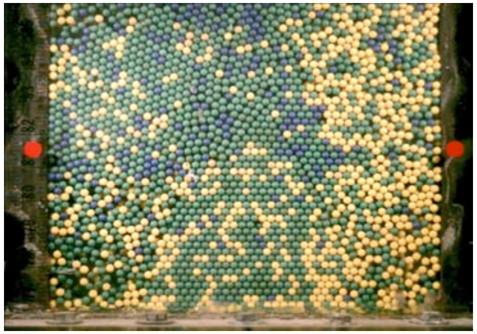
- *Code Validation*



(Yuu et al., *Powder Tech.*, 2000)



NETL Small-Scale Challenge (SSCP) Problem I
(Gopalan et al., *Powder Tech.*, 2016)



Semi-circular bed with Horizontal Jets
(Fullmer, LaMarche, Issangya, Liu, Cocco & Hrenya , *AIChE J.*, 2018)

Motivation and Objective: UQ effort

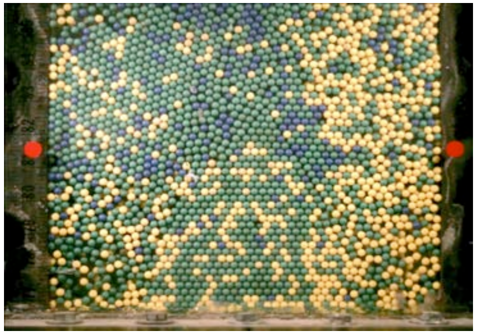
Full UQ

Epistemic Uncertainty – Unknown

- sample N^3+2 epistemic uncertainties

Aleatoric Uncertainty – Measured

- 100 samples/epistemic sample



- 60,000 particles
- 192 cpu hrs/simulation
- 5 epistemic uncertainties
  → 12,700 Simulations

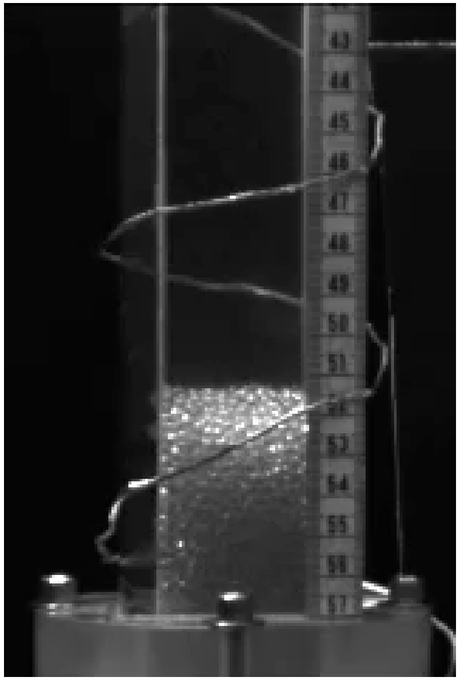
To date, full UQ of CFD-DEM prohibitive

Current Objectives

1. Design experiment in which Full and Reduced UQ can be performed
2. Directly test Full UQ vs. Reduced UQ using MFiX DEM

Experimental Design

Target: Very-very small scale challenge problem (VVSSCP) with simulation times < 8 hours on a single CPU

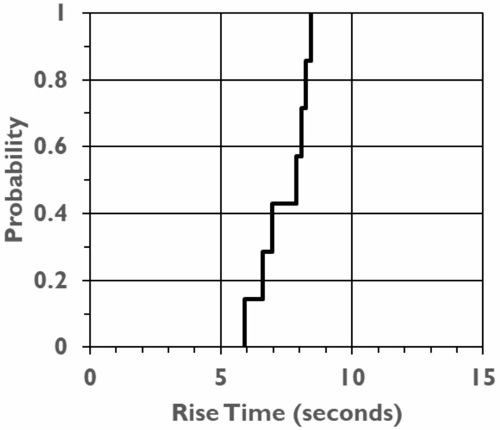


Important Considerations:

- Fast experiment: ~10 s or less
- Small # of particles: *O*(1,000) particles
- Careful characterization: *input uncertainty*
- Robustness
  - Particle-particle interaction important
  - Particle-fluid interaction important
  - Experimental results sensitive to some inputs

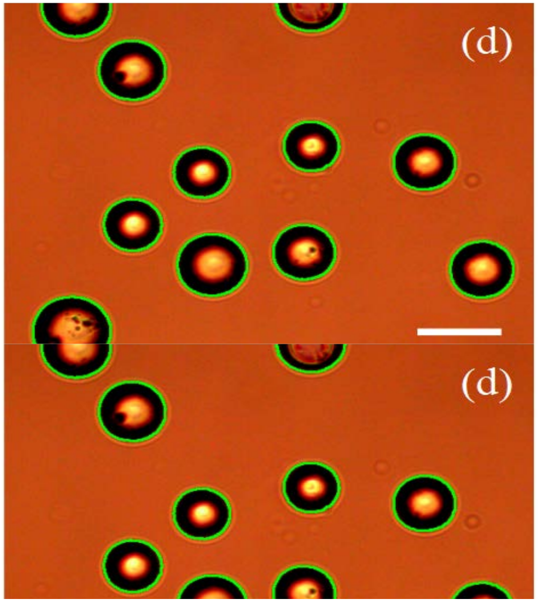
System: Segregating Bed

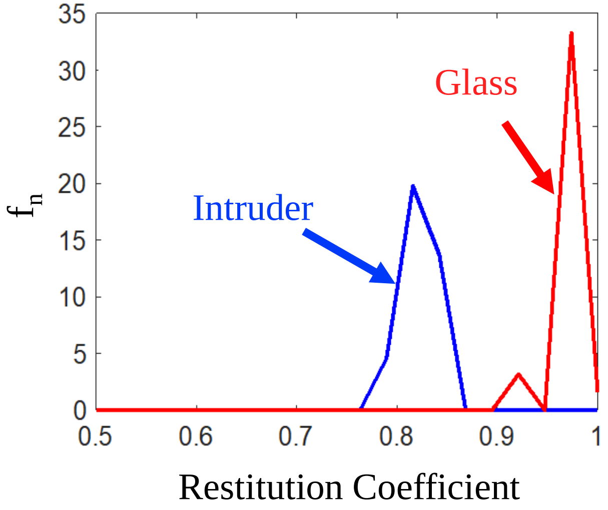
- Glass particles in bed (~4300, ~3.1 mm dia.)
- HDPE particle (~9.4 mm dia.)
- Measurement: rise time
- Repeats to establish *output uncertainty*



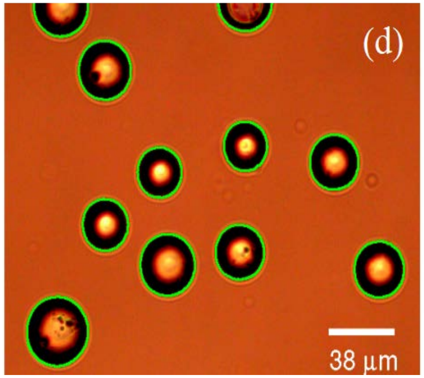
Experiments: Aleatory Uncertainty (Particle Characterization)

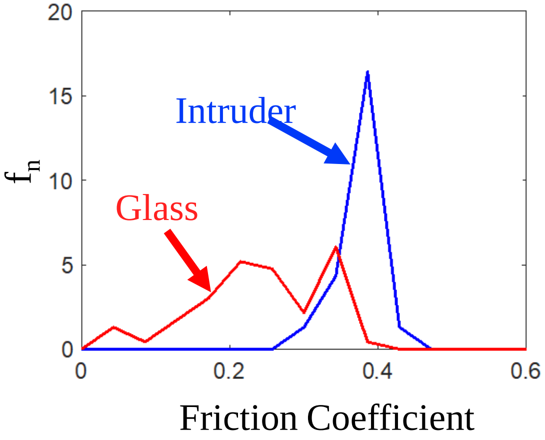
Coefficient of Restitution



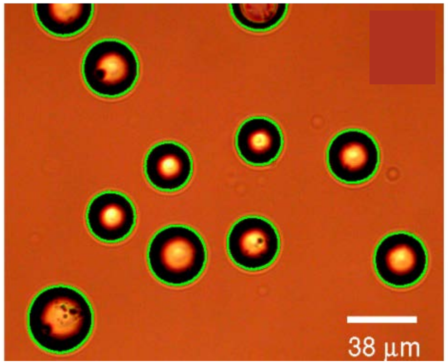


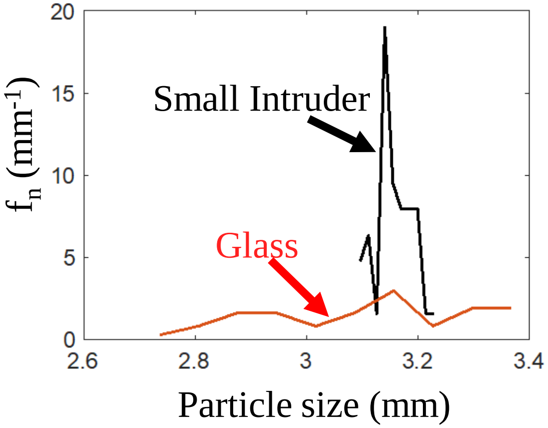
Coefficient of Friction





Size and shape





LaMarche et al. (2017) *Chem Eng J*

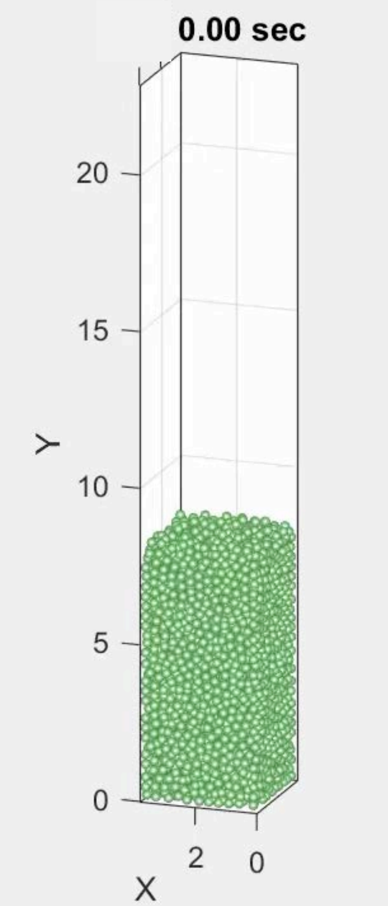
Effort 1 – Segregating Bed

Objective

- Replicate experiments with CFD-DEM
- Apply *Full UQ* and *Reduced UQ* techniques

MFiX

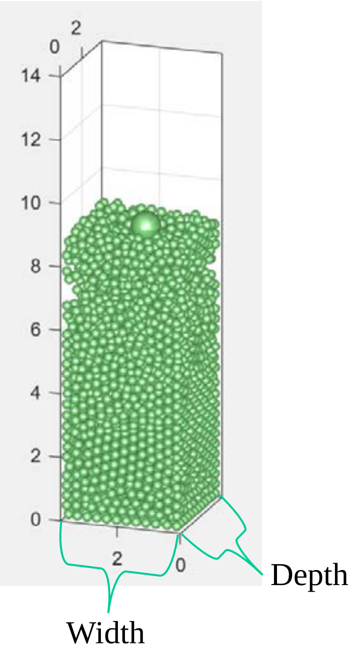
- Release 2016.1
- CFD-DEM
  - Soft-sphere
  - Free-slip wall (gas phase)
  - Rectangular grid
- Segregation time as key output



Effort 1 – Uncertain Model Inputs

Sources of uncertainty

Particle-phase Properties	
HDPE diameter	A
HDPE material density	E
Glass diameter	A
Glass material density	E
Glass-glass coefficient of restitution	A
Glass-wall coefficient of restitution	A
Glass-HDPE coefficient of restitution	A
Sphericity	A
Particle-particle coefficient of friction	A
Particle-wall coefficient of friction	A



Gas-phase Properties	
Gas rate variance	E
Outlet gas pressure	E
Inlet gas temperature	E

Dependent or Known Inputs

- Gas viscosity (via temperature)
- Nominal gas rate (via temp, pressure, nominal gauge readings)
- Total mass of glass particles (known)
- Bed depth & width (known)

Aleatory = Natural variation, characterized by the measured CDF curve

Epistemic = Measurement precision, characterized as uniform probability between measured min & max

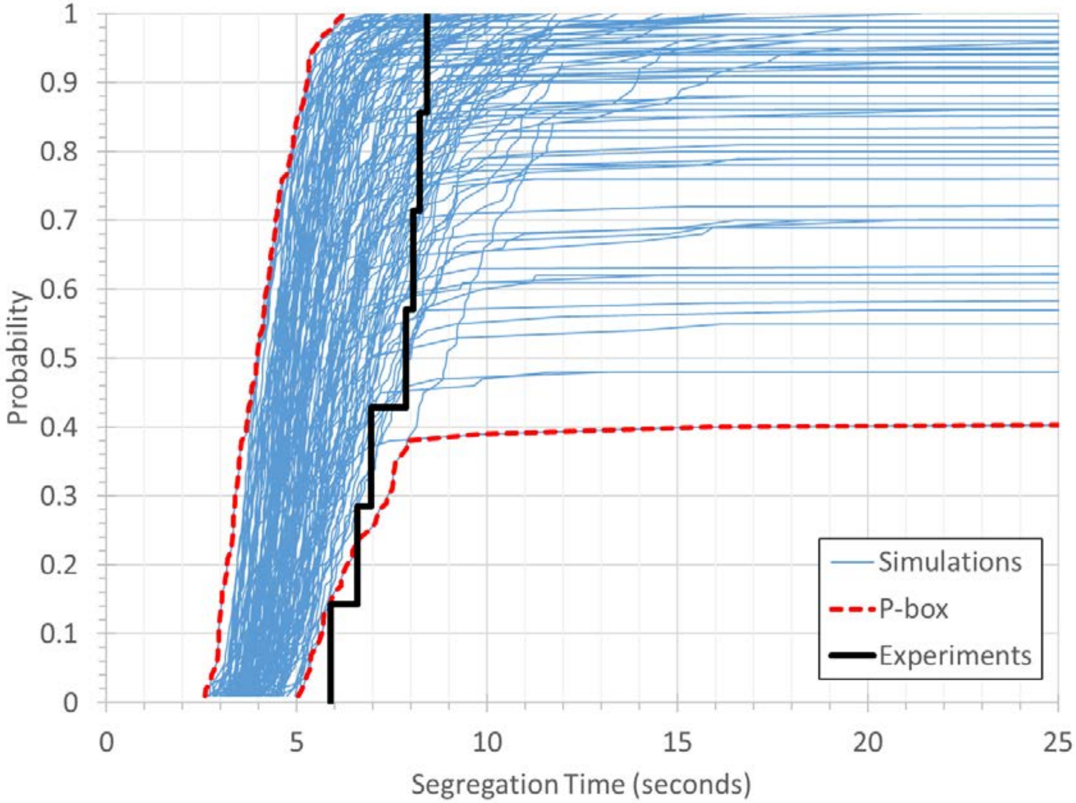
Effort 1 – Full UQ

Full UQ input uncertainty propagation

- All input variables
- 127 epistemic points sampled
- 100 aleatory samples / epistemic point
- 12,700 simulations total

Results vs experiments

- Bias is for faster segregation in simulations



Effort 1 – *Reduced UQ*

Sensitivity analysis

- Run base case
- Test high and low bounds for each input; hold others fixed
- Identify parameters that change output by >5%
- Eliminate others from forward propagation

Investment

- 270 runs, 27 runs with 10 repeats of each to account for variation in initial conditions

Uncertainty propagation

- Only influential variables
- 29 epistemic points sampled
- 100 aleatory samples / epistemic point
- 2,900 simulations total

Particle-phase Properties	
~~HDPE diameter~~	~~A~~
~~HDPE material density~~	~~E~~
Glass diameter	A
Glass material density	E
~~Glass-glass coefficient of restitution~~	~~A~~
~~Glass-wall coefficient of restitution~~	~~A~~
~~Glass-HDPE coefficient of restitution~~	~~A~~
Sphericity	A
Particle-particle coefficient of friction	A
~~Particle-wall coefficient of friction~~	~~A~~

Gas-phase Properties	
Gas rate variance	E
~~Outlet gas pressure~~	~~E~~
Inlet gas temperature	E

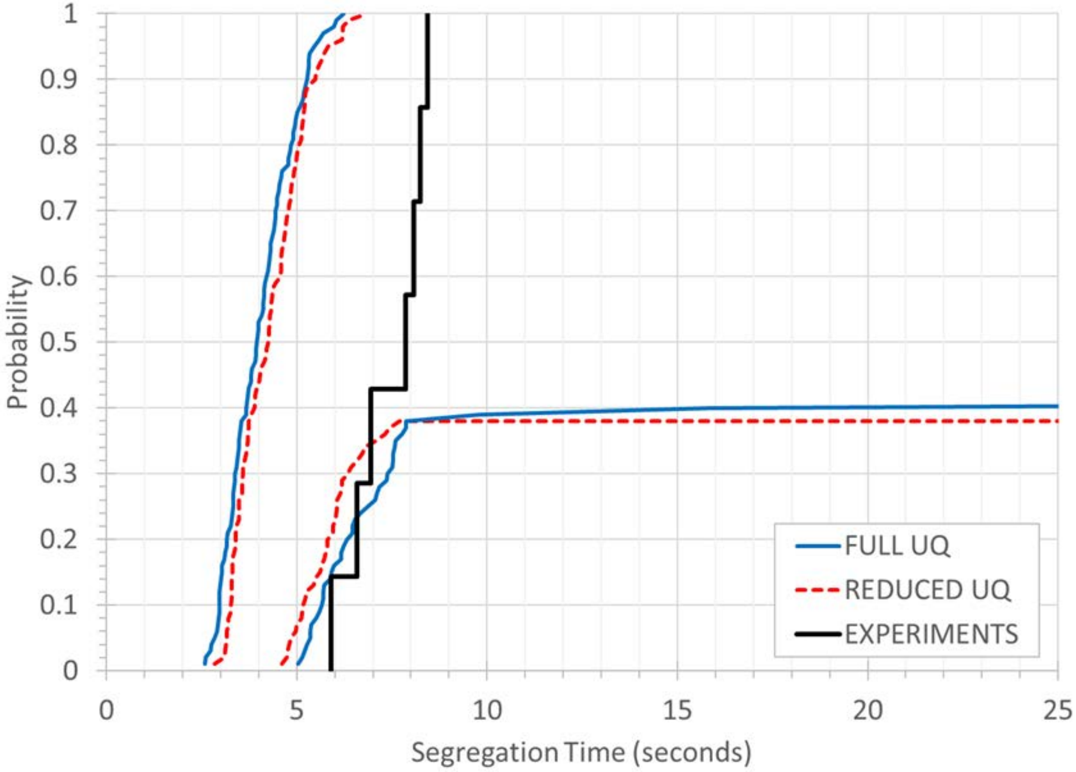
Aleatory = Natural variation

Epistemic = Measurement precision

Effort 1 – *Full UQ* vs *Reduced UQ*

Direct comparison of forward propagation techniques

- *Full UQ*
  - 5 Epistemic variables
  - 8 Aleatory variables
  - 12,700 runs
- *Reduced UQ*
  - 3 Epistemic variables
  - 3 Aleatory variables
  - 3,170 runs
- Good agreement
  - 75% reduction in computational expense

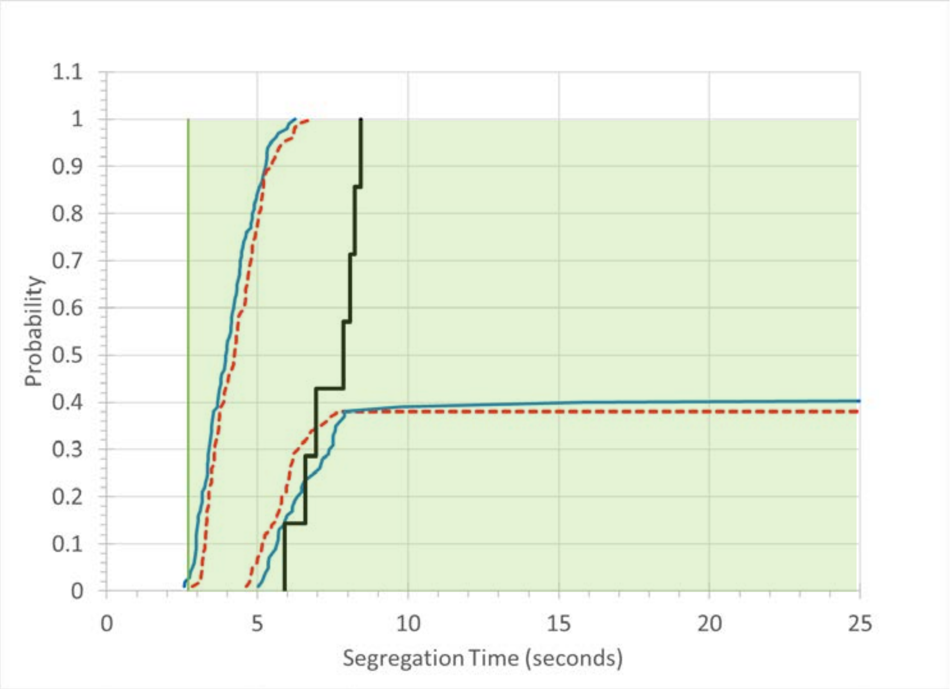


Effort 1 – *Conservative UQ*

What happens if we just attempt to capture the extremes?

- *Conservative UQ*
  - Use directional influence observed in sensitivity analysis (270 runs).
  - Select combinations that should yield fastest and slowest segregation.
  - 20 runs (2 points, with 10 repeats of each to account for initial conditions)

Method	**Result**	**Runs**
Conservative UQ	2.7 sec +	290
Reduced UQ	2.83 sec +	3170
Full UQ	2.58 sec +	12700



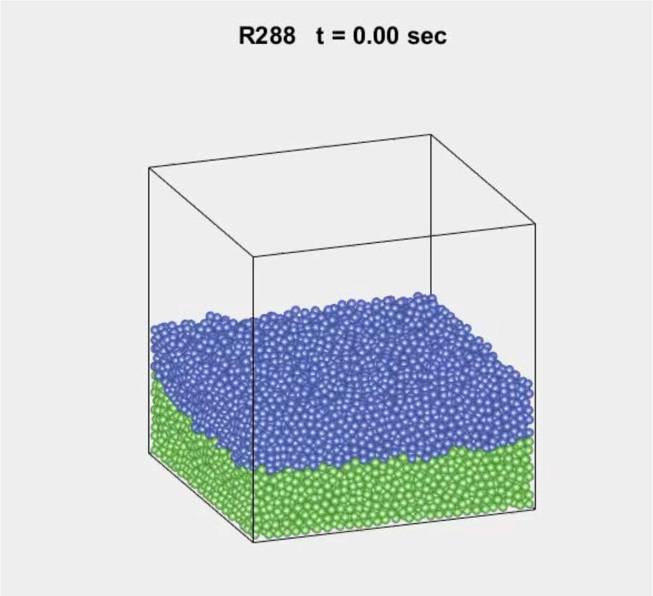
Effort 2 – Mixing in Tumbler

Objective

- Extend analysis to a second system with different physics

MFiX

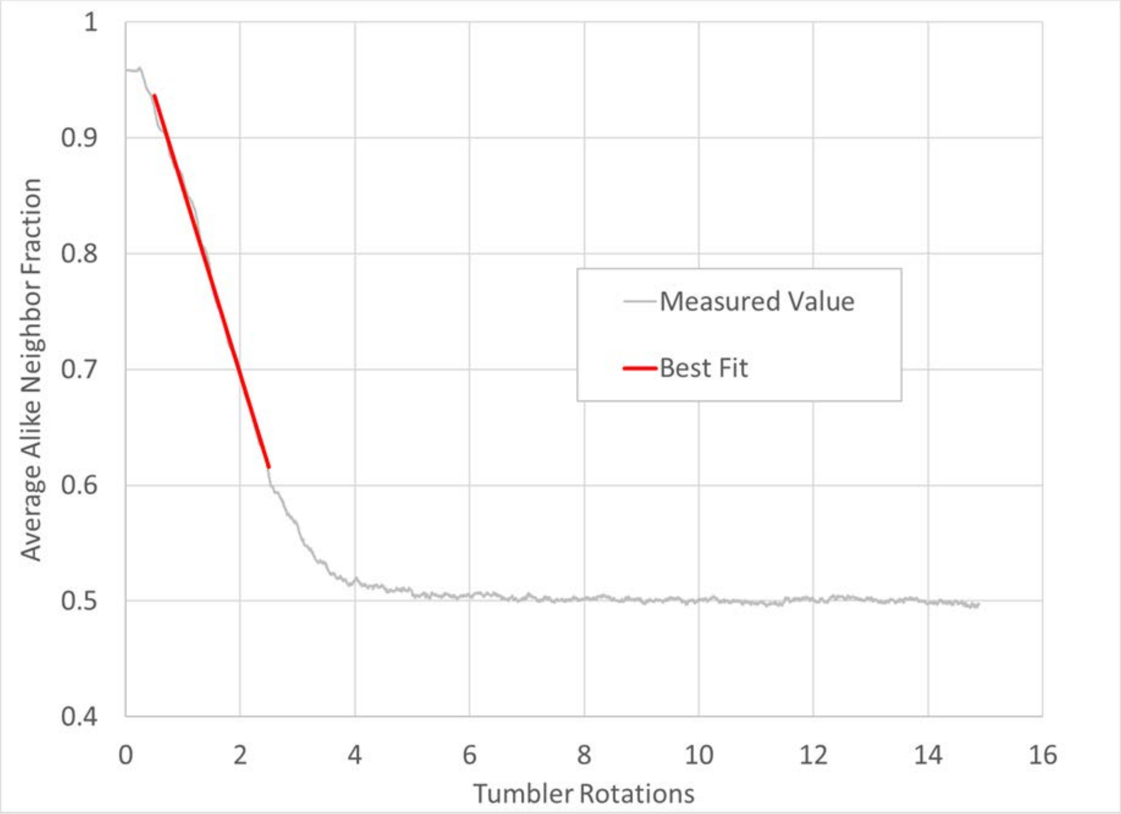
  - Release 2016.1
  - **DEM-only**
    - Soft-sphere
    - Rotating tumbler
    - Identical particles
    - Only color is different



Effort 2 – Mixing in Tumbler

Key output → initial rate of mixing

- Calculate “Alike Neighbor Fraction” (ANF) for each particle
- Calculate average ANF (including all particles with four or more neighbors)
- Focus on slope of best-fit line between 0.5- and 2.5- rotations.



Effort 2 – Uncertain Model Inputs

Known Inputs
Tumbler dimensions
Total mass of glass particles
Acceleration due to gravity

Full UQ

Uncertain Inputs	
Rotation rate	E
Glass diameter	A
Glass material density	E
Glass-glass coefficient of restitution	A
Glass-wall coefficient of restitution	A
Particle-particle coefficient of friction	A
Particle-wall coefficient of friction	A

Reduced UQ

Uncertain Inputs	
~~Rotation rate~~	~~E~~
~~Glass diameter~~	~~A~~
Glass material density	E
Glass-glass coefficient of restitution	A
~~Glass-wall coefficient of restitution~~	~~A~~
Particle-particle coefficient of friction	A
Particle-wall coefficient of friction	A

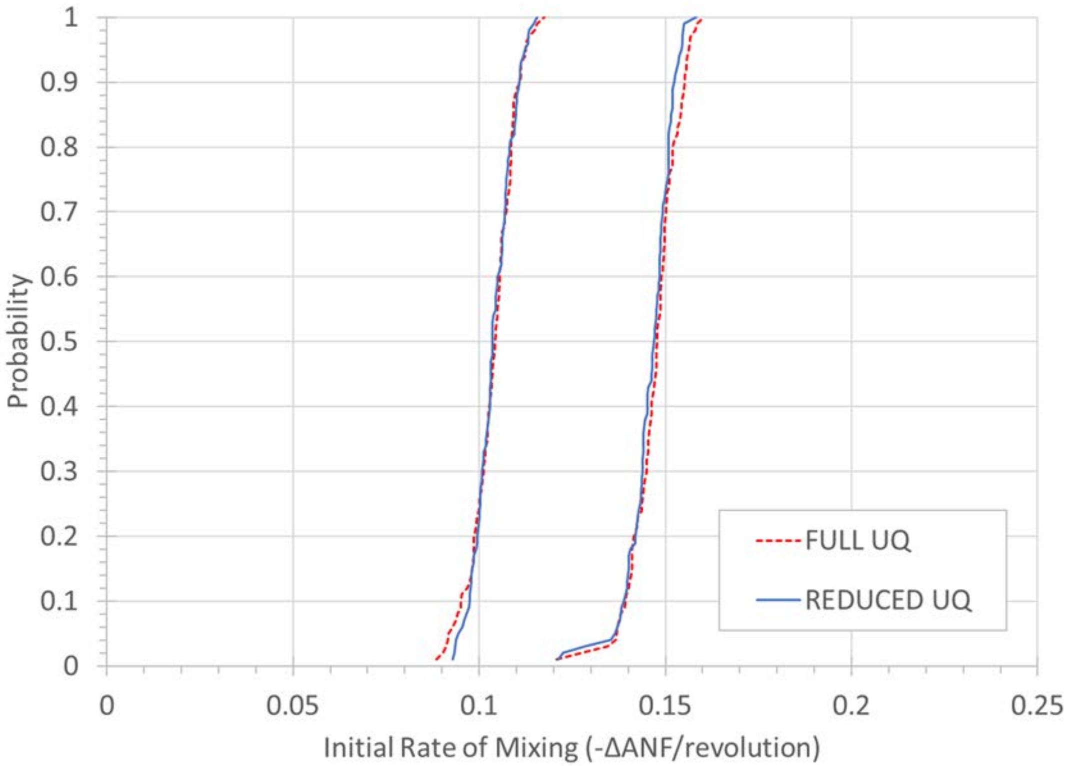
Aleatory = Natural variation, characterized by the measured CDF curve

Epistemic = Measurement precision, characterized as uniform probability between measured min & max

Effort 2 – *Full UQ* vs *Reduced UQ*

Direct comparison of forward propagation techniques

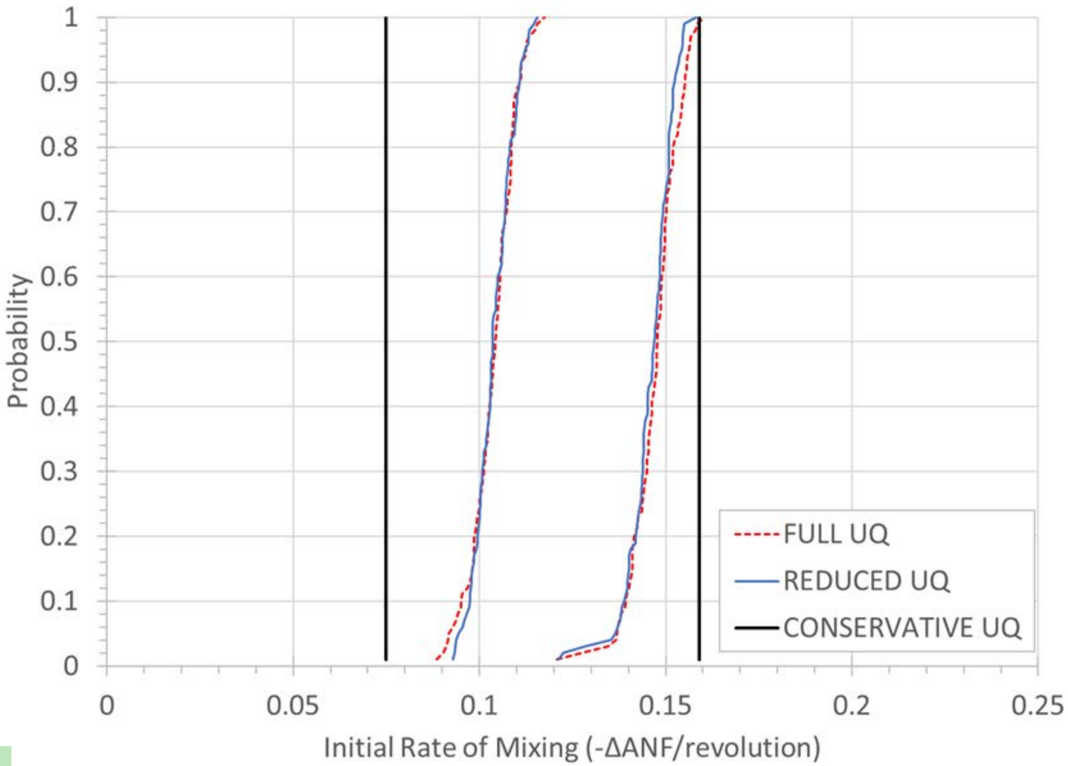
- *Full UQ*
  - 2 Epistemic variables
  - 5 Aleatory variables
  - 1000 runs
- *Reduced UQ*
  - 1 Epistemic variable
  - 3 Aleatory variables
  - 345 runs
- Good agreement
  - 65% reduction in computational expense



Effort 2 – *Conservative UQ*

What happens if we just attempt to capture the extremes?

- *Conservative UQ*
  - Use directional influence observed in sensitivity analysis (45 runs).
  - Select combinations that should yield fastest and slowest mixing.
  - 6 runs (2 points, with 3 repeats of each to account for initial conditions)



Method	**Runs**
Conservative UQ	51
Reduced UQ	345
Full UQ	1000

Summary

Reduced UQ

- Performing a sensitivity analysis to eliminate insignificant input uncertainties can significantly reduce computational burden
    - NOTE: Systems in which all epistemic uncertainties are important would not benefit from a sensitivity-analysis since primary computational gains of *Reduced UQ* come from reducing epistemic uncertainties
- agreed well with *Full UQ* at 65%-75% computational savings

Conservative UQ

- If only min/max output bounds are desired, using sensitivity analysis to guide inputs for min/max cases is promising
- agreed well with *Full UQ* for both efforts at a 95% computational savings