NATIONAL ENERGY TECHNOLOGY LABORATORY

Overview of Multiphase Flow Science at NETL

M. Syamlal

National Energy Technology Laboratory

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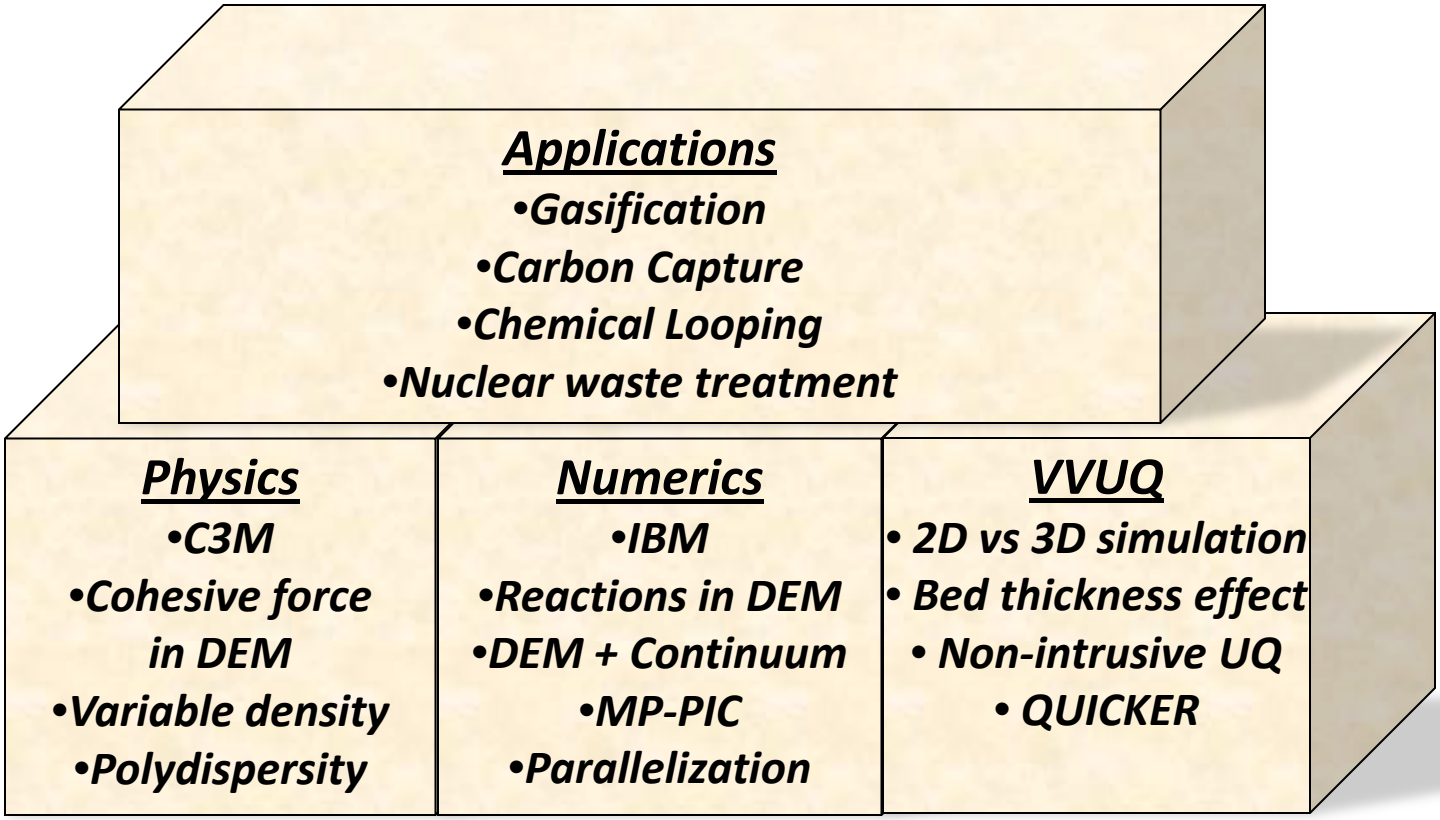
NETL 2012 Workshop on Multiphase Flow Science, NRCCE Conference Center, Morgantown, WV, May 22-24, 2012

Advancing multiphase flow science in support of energy applications



Gasifier Modeling: Assessing Commercial Readiness

Models

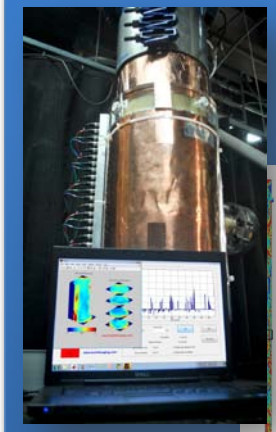
C3M™ Carbonaceous Chemistry for Computational Modeling

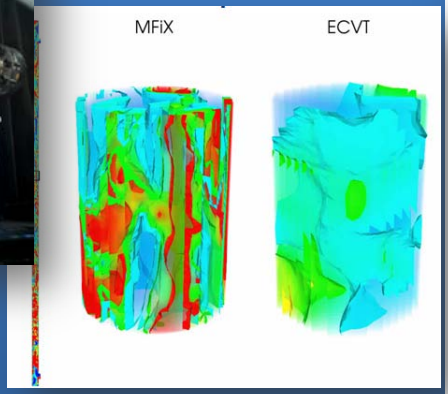
MFiX

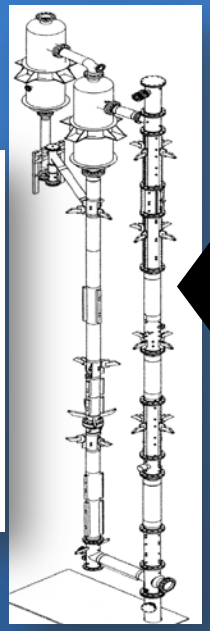
BARRACUDA

ANSYS FLUENT®

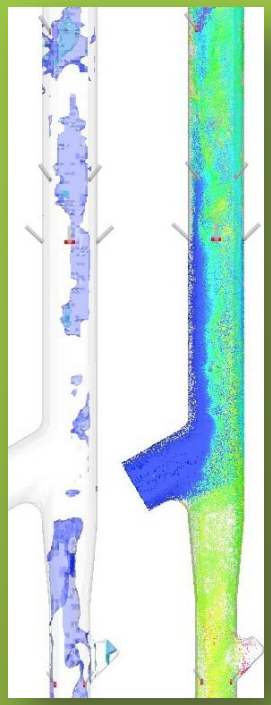
Experiments

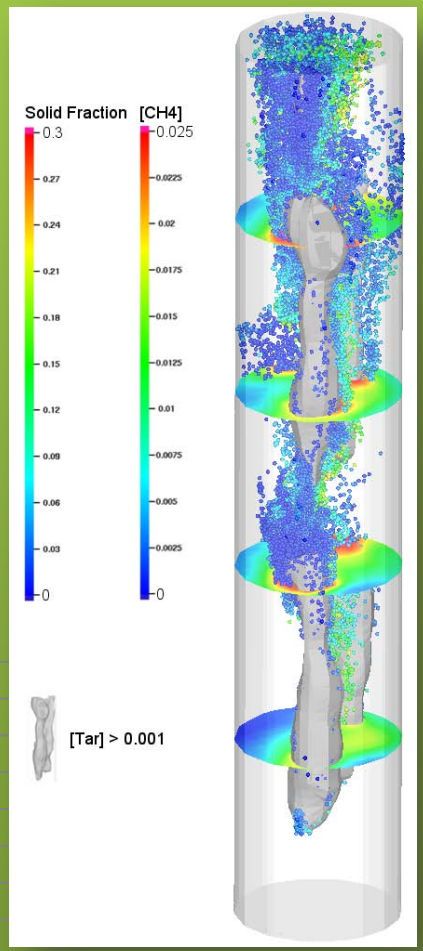






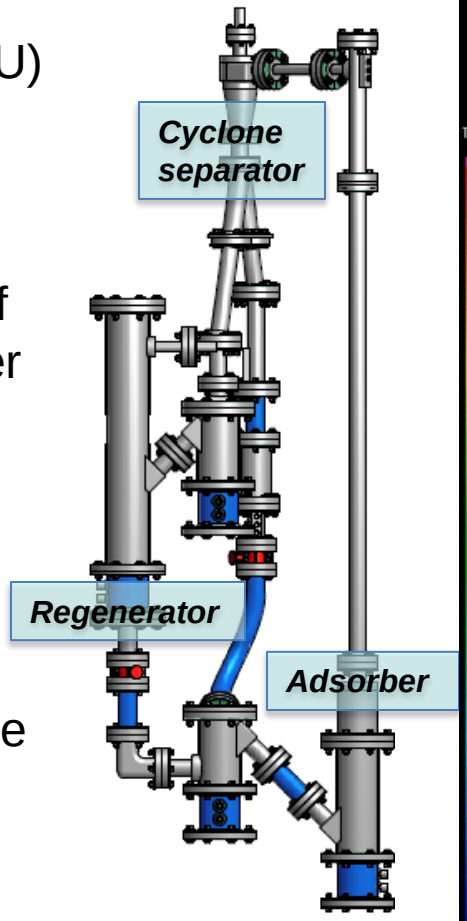
Results

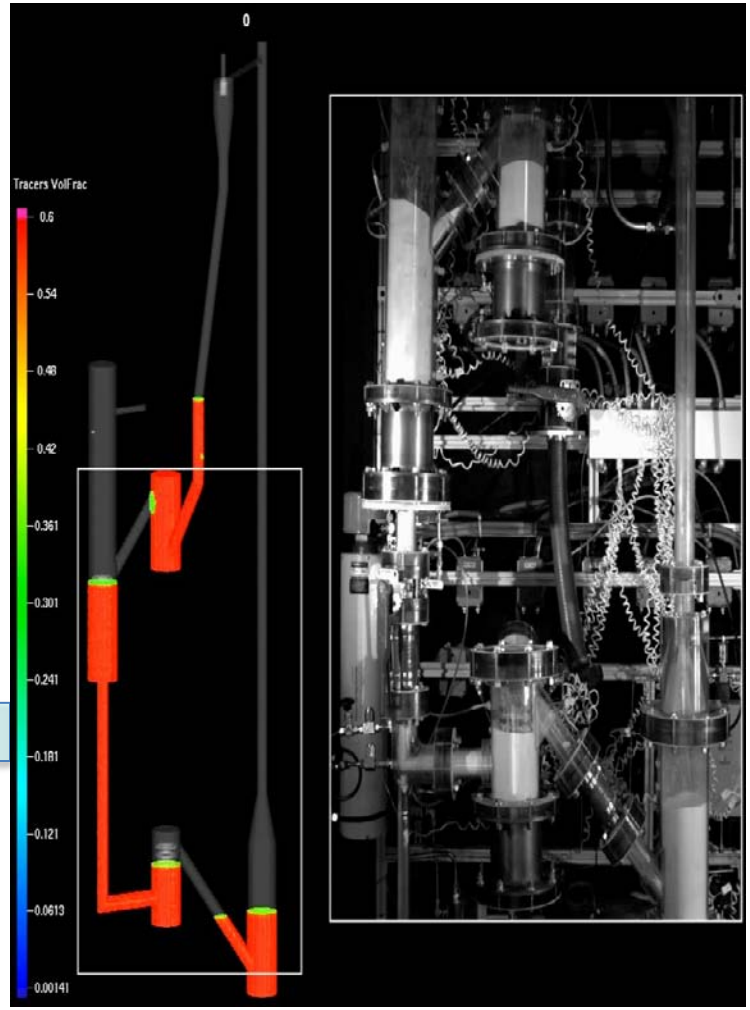




C2U – Generating data for validating carbon capture device-scale models

- Carbon Capture Unit (C2U) System rebuilt and shake down tests completed
- Batch tests conducted on sorbent capacity, heats of reaction, and heat transfer coefficient.
- Elutriation tests defined solids circulation rate operating map
- Diffusion controlled nucleation and growth rate kinetics developed and confirmed in C2U batch tests[1].





$$\frac{dX}{dt} = 0.42e^{\frac{662}{T}} y_{CO_2}^{0.693}(1-X)\sqrt{-\ln(1-X)}$$

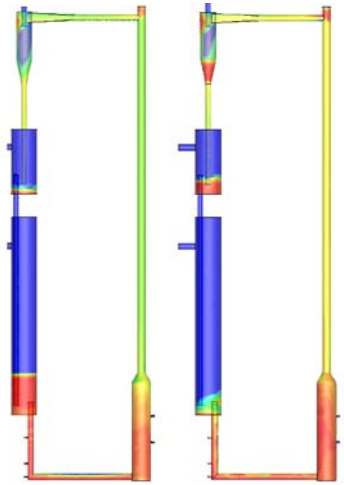
1.Monazam, et al. (2012)…Absorption Kinetics…by Solid Supported Amine Sorbent, AIChE Journal.

Chemical Looping Reactor Simulations

NETL's CLR being installed

Air reactor bubble caps

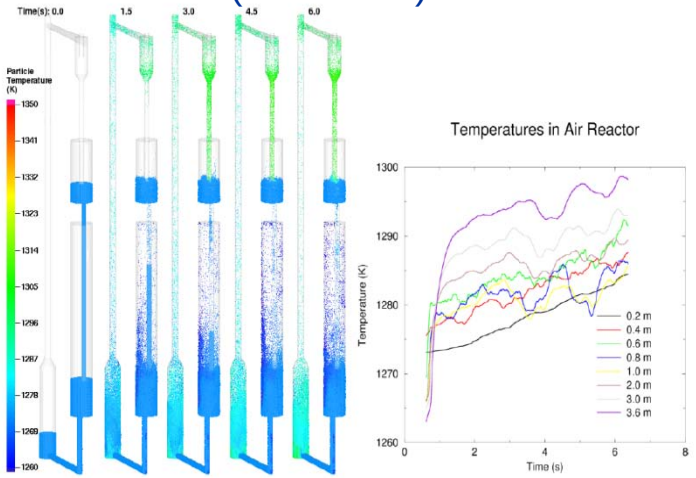
Non-reacting Simulation (FLUENT)



Investigated the effect of L-valve flow on circulation rate

Liu, Huckaby, Gallagher, Carpenter, "3D CFD Simulation of Interconnected Air and Fuel Reactors for Chemical Looping Combustion", 2012 AIChE and PCC

Chemical Looping Combustion of Coal (Barracuda)



- The fuel reactor is fluidized with N_2, H_2O and CO_2
- Kinetics of illmenite carrier based on Zaragoza group
- Coal kinetics are from C3M

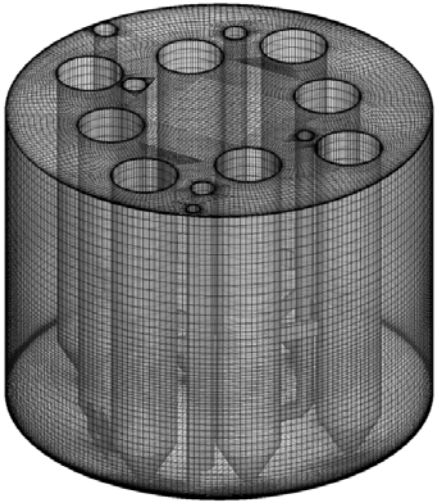
J. Parker, "Computer Simulation of a full Chemical Looping Combustion System", 2012 AIChE

Hanford Site Nuclear Waste Cleanup

- $12.2 billion project to process and stabilize (vitrify) 56 million gallons of cold-war era nuclear waste from 177 existing underground tanks to prevent sub-surface contamination
- Current design calls for using conventional **Pulse Jet Mixers (PJM)** to keep nuclear waste well mixed during pre treatment before virtrification
- Bechtel National, Inc (BNI) uses CFD for confirmation calculations of the PJM
- Modeling challenges: complex gas-liquid-solids system with wide size and density distribution, scale-up, material properties, strict mixing requirements, …

NETL wins Secretary's Achievement Award

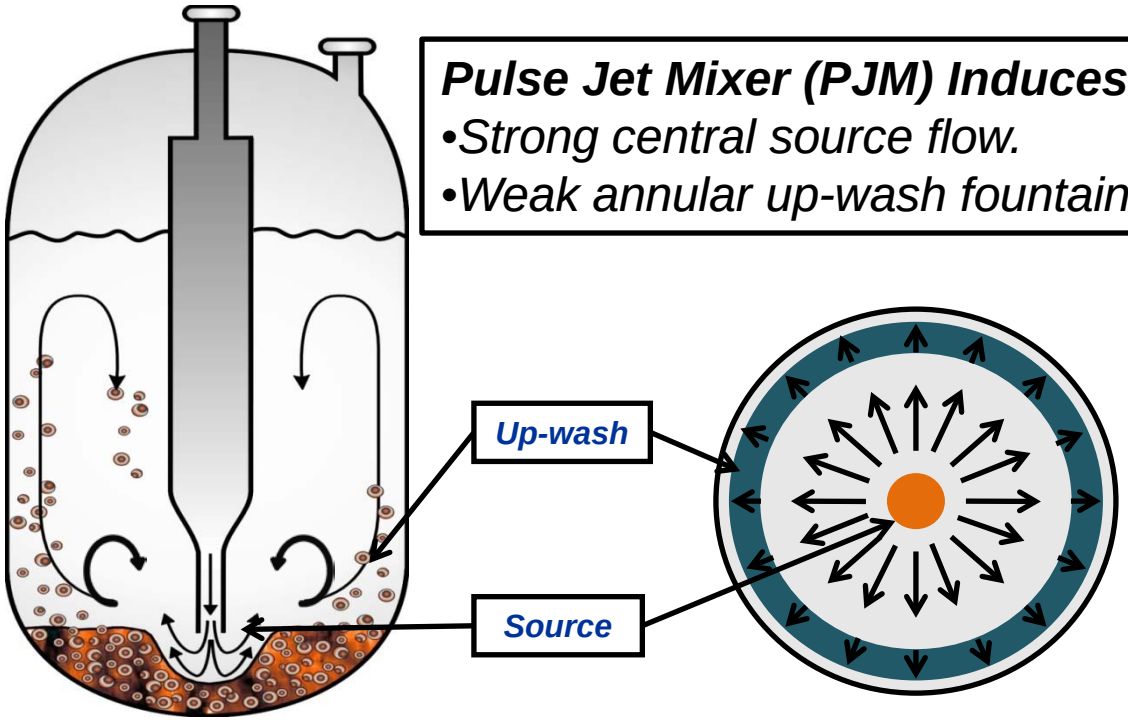
Design tool



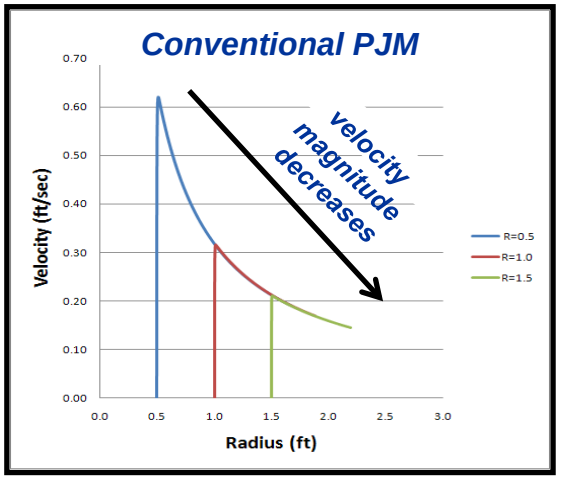
NETL review team responsibility:

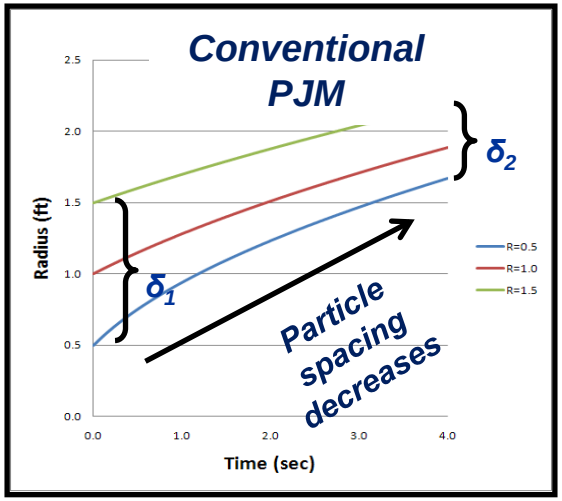
- ✓ Review BNI's reactive multiphase flow CFD model as a design tool for Pulse Jet Mixing vessels.
- ✓ Identify data gaps in the proposed and past experiments
- ✓ Provide recommendations on the CFD model and/or propose further experimental testing.

NETL Introduces Improvements over Conventional PJM Vessels



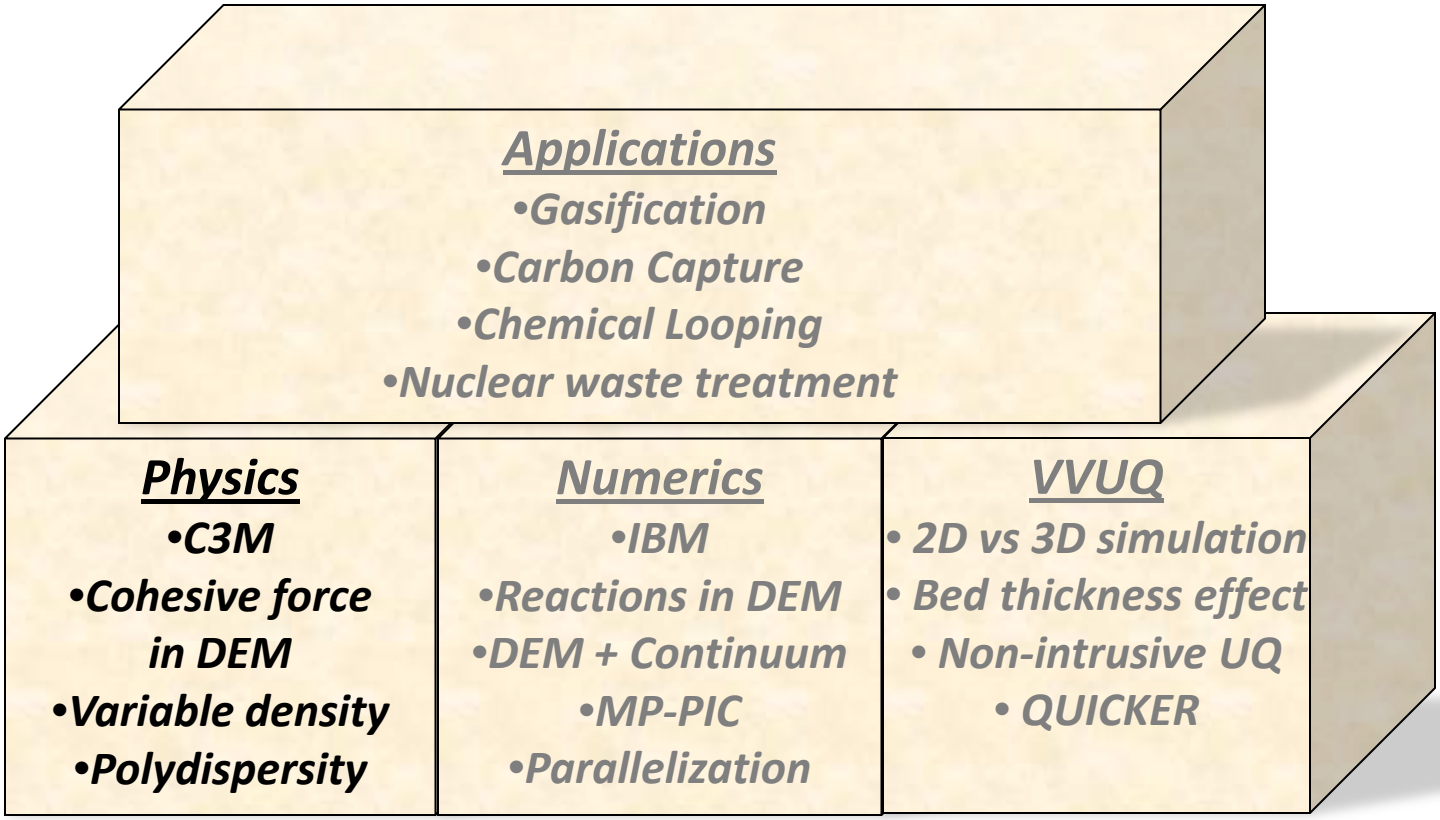
Pulse Jet Mixer (PJM) Induces:
- *Strong central source flow.*
- *Weak annular up-wash fountain.*



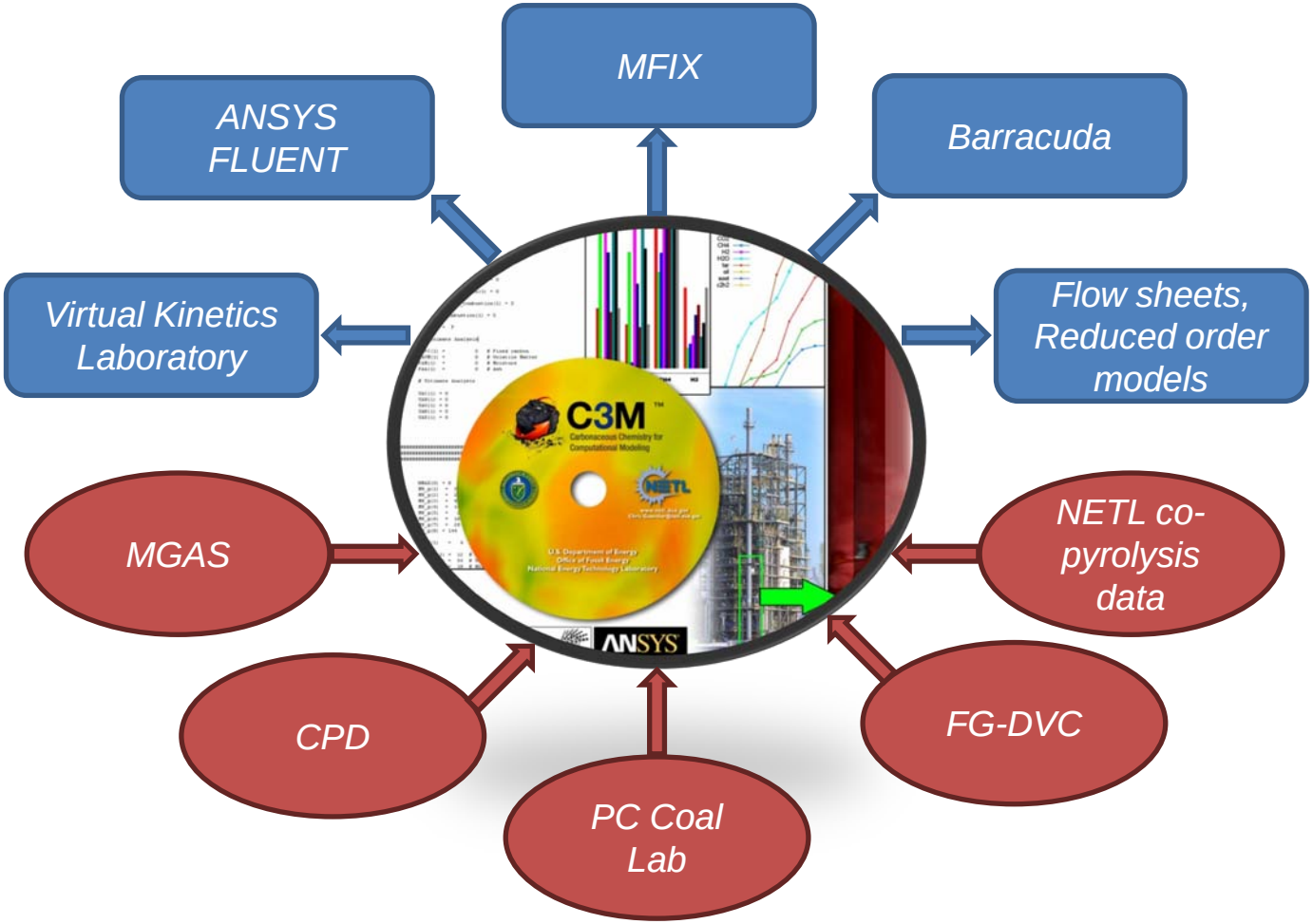


- Conventional PJM creates a crater and pile of particles away from the crater, reducing the mixing
- NETL has proposed an alternative design: *J. VanOsdol, "Radial Flow Pulse Jet Mixer," patent applied for*

Advancing multiphase flow science in support of energy applications

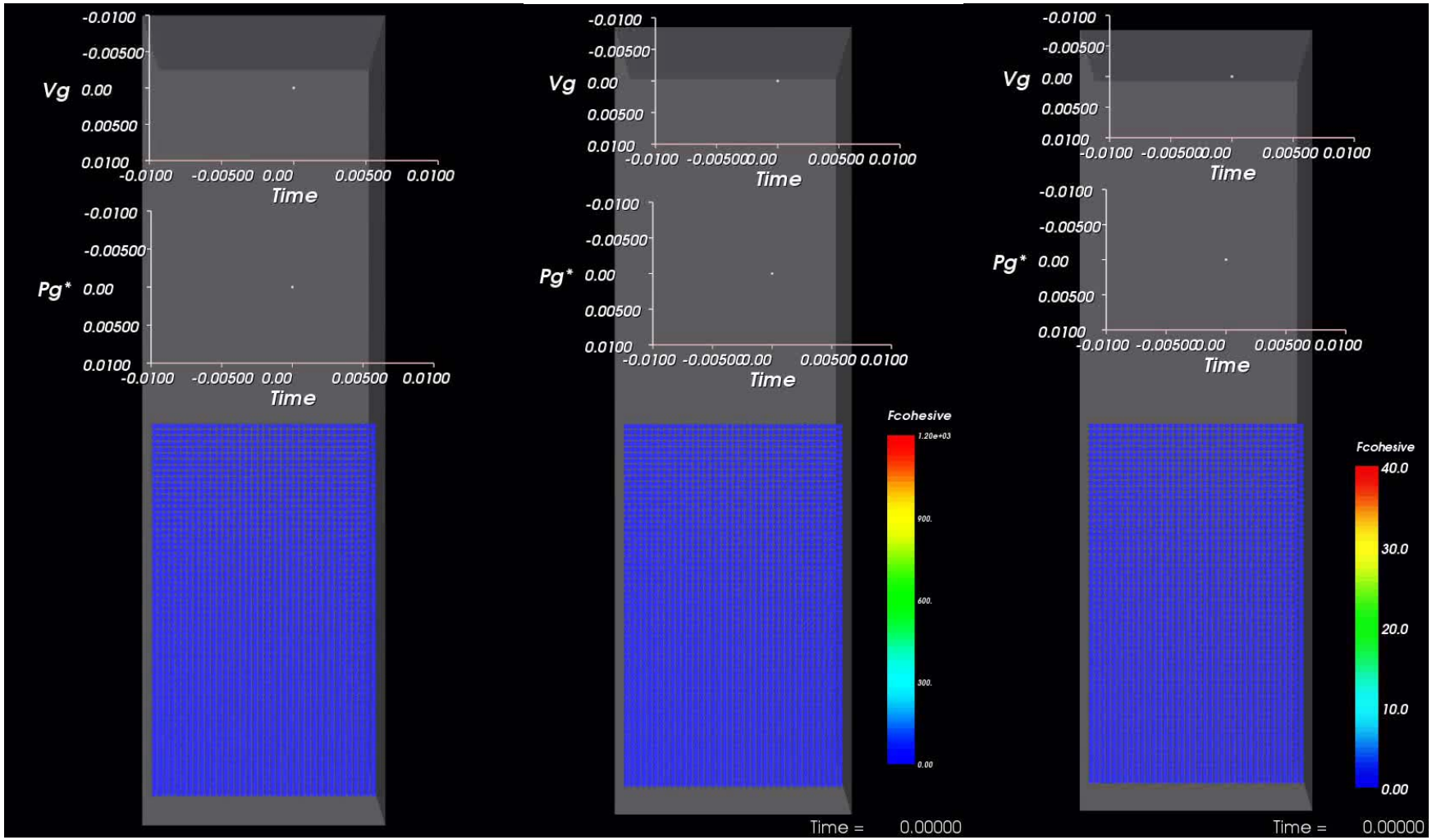


C3M: Unified interface to diverse carbonaceous chemical kinetics



Predictions provided with quantified uncertainty

Cohesive force implemented in MFIX



Non Cohesion

Hamaker vdW

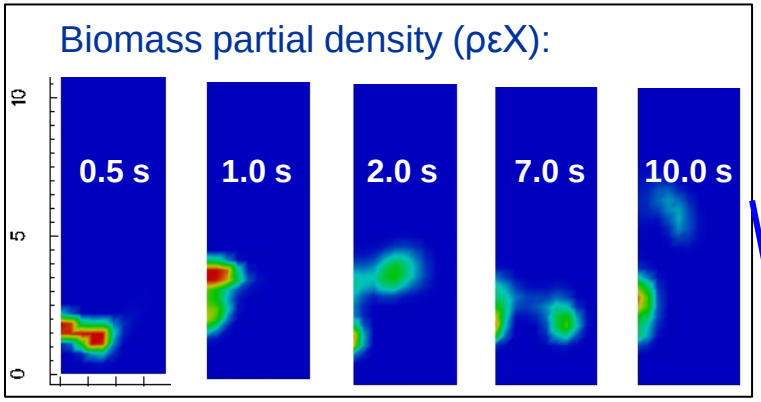
$$F_{vdW} = \frac{AR}{12H_0^2}$$

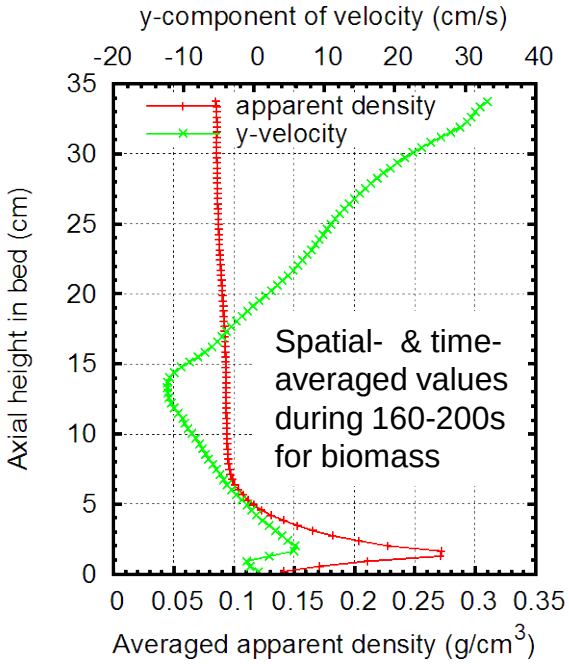
Rumpf vdW

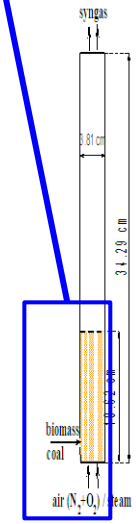
$$F_{vdW} = \frac{AR}{12H_0^2}\left\{\frac{r}{r+R} + \frac{1}{(1+r/H_0)^2}\right\}$$

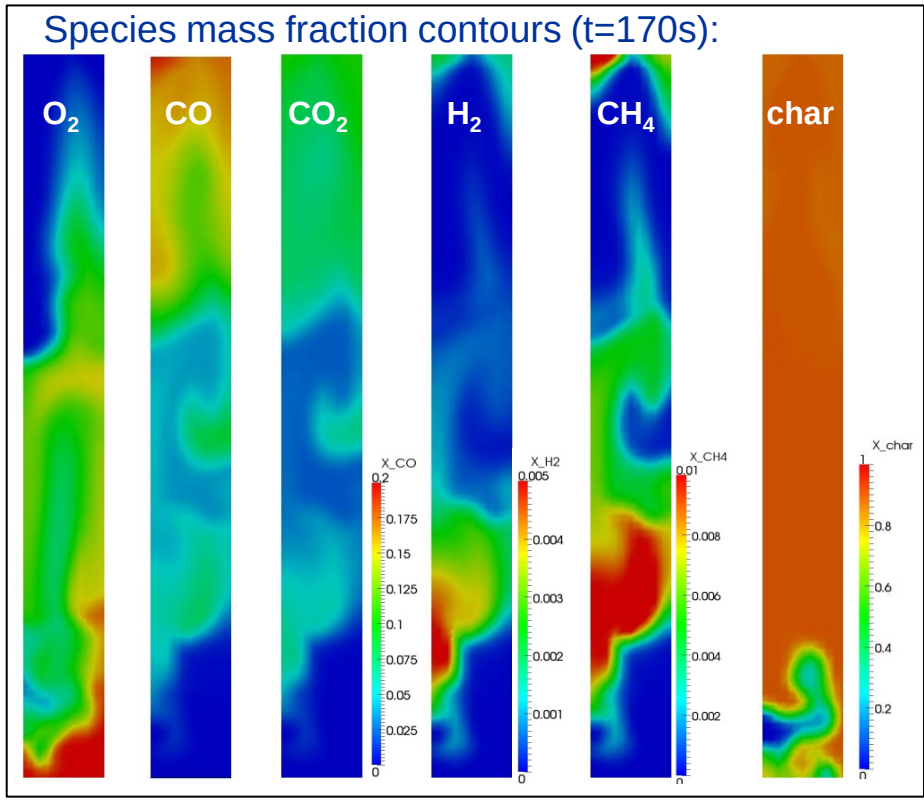
Only a slice of 3-particle diameter is shown.

Biomass gasification with variable-particle-density added to MFIX-Continuum







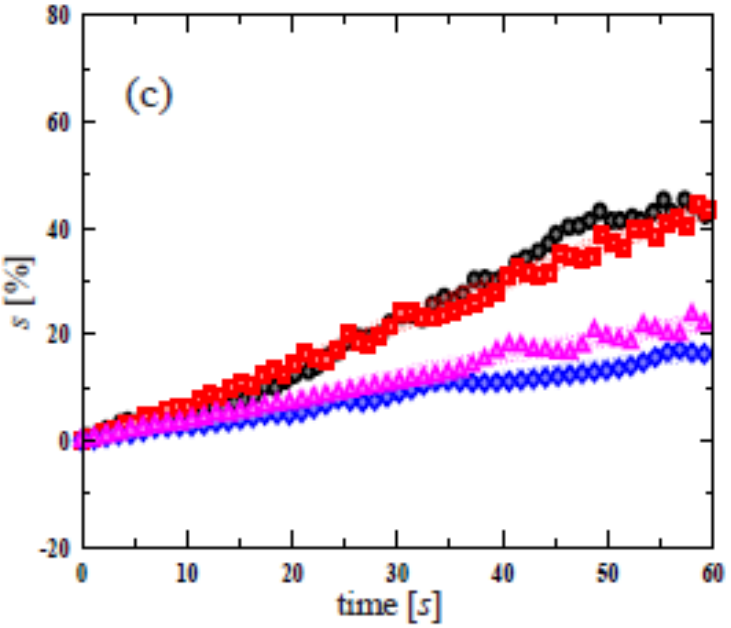


- **Biomass/char particles' physical process is modeled via variable particle porosity.**

Xue, Q., Heindel, T.J. and Fox, R.O., "A CFD model for biomass fast pyrolysis in fluidized-bed reactors", Chemical Engineering Science (2011) 66: 2440-2452.

Simonin-Toulouse theory and two drag models implemented in MFIX and tested

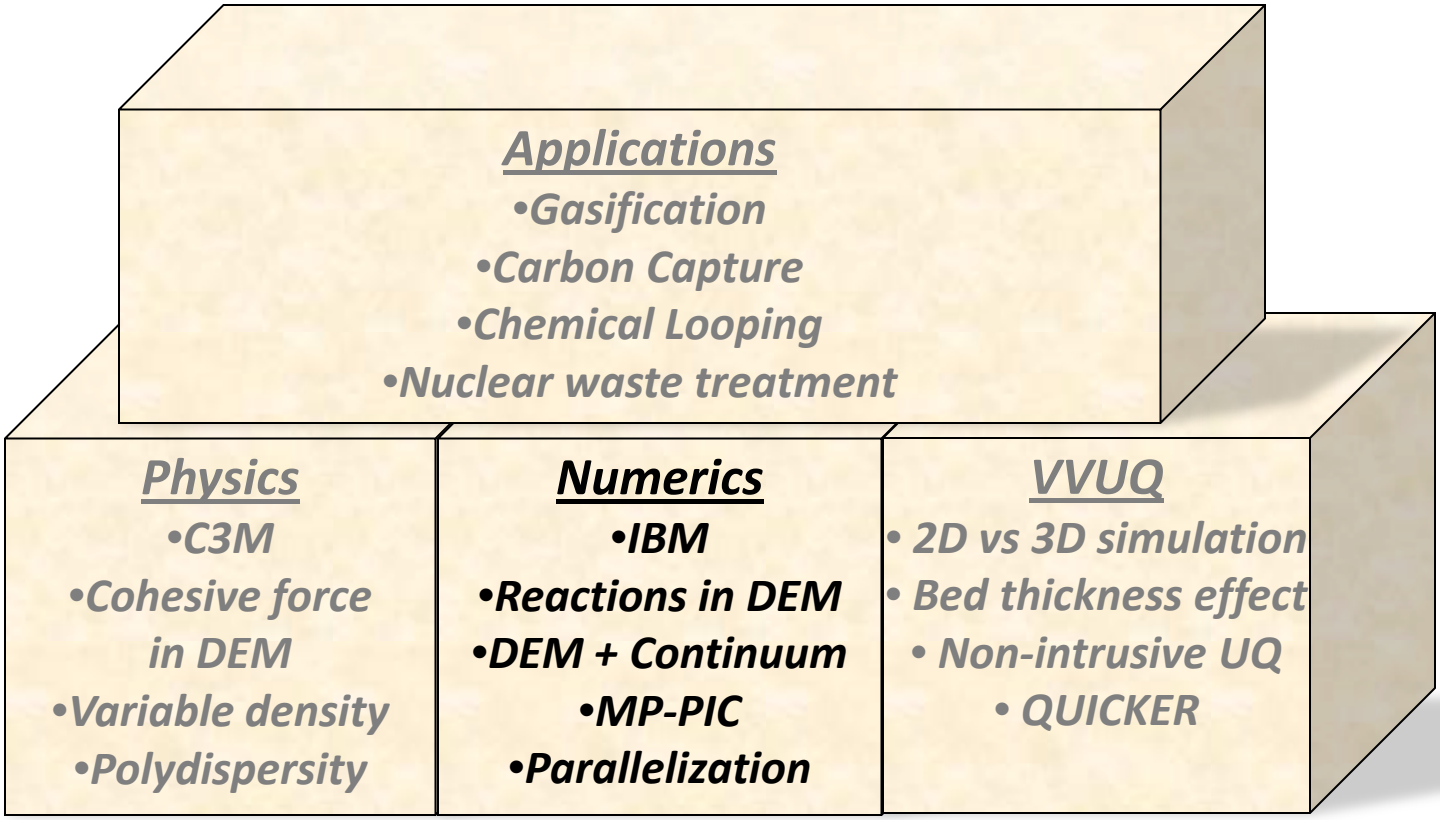
- **Implemented Simonin-Toulouse polydisperse kinetic theory of granular flow**
- **Implemented two drag models**
  - Gobin et. al. – mono-disperse drag model
  - Cello et. al. – poly-disperse drag model
- **Simulated "Goldschmidt" Binary Segregation experiment**
  - Carrier-Bed separation
  - Better predictions with mono-disperse drag



Black – experiment
Red – Gobin/Tolouse, mono-disperse drag
Blue – Cello, poly-disperse drag
Pink – Beestra, poly-disperse drag

Konan, Huckaby and O'Brien, "CFD modeling and analysis of segregated binary mixture fluidized bed", 2011 Aiche Conference

Advancing multiphase flow science in support of energy applications

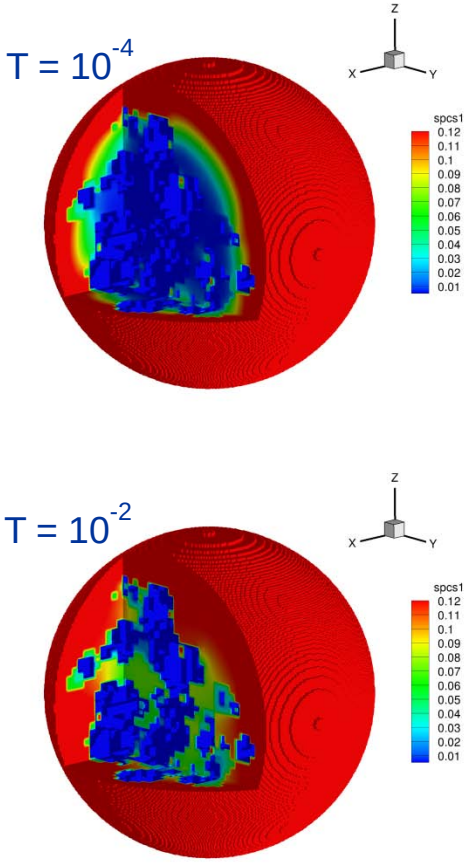


Modeling the details of CO_2 capture process in porous sorbent particles

D. Tafti & N. Krishnamurthy (Virginia Tech.)

- **Objectives**
  - Enable accurate characterization of the effect of porous microstructure on CO_2 capture by solid sorbents
  - Develop accurate particle-scale reduced-order models

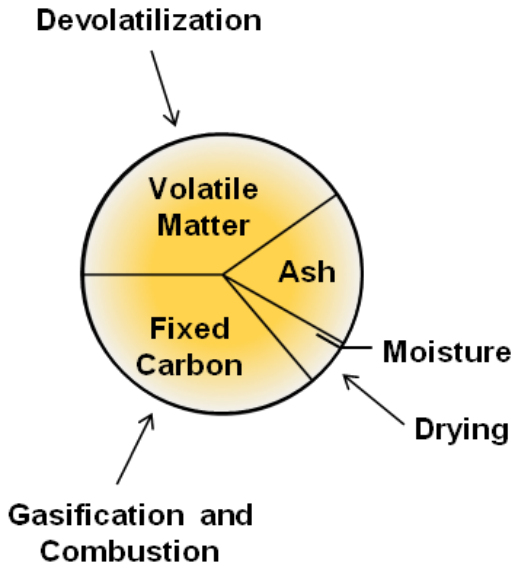
- **Project highlights**
  - Parallelized IBM flow solver to simulate flow, (conjugate) heat transfer and species transport
  - Used stochastic reconstruction to create realistic sorbent particles
  - Computed diffusion rates of CO_2 through reconstructed porous spherical particles

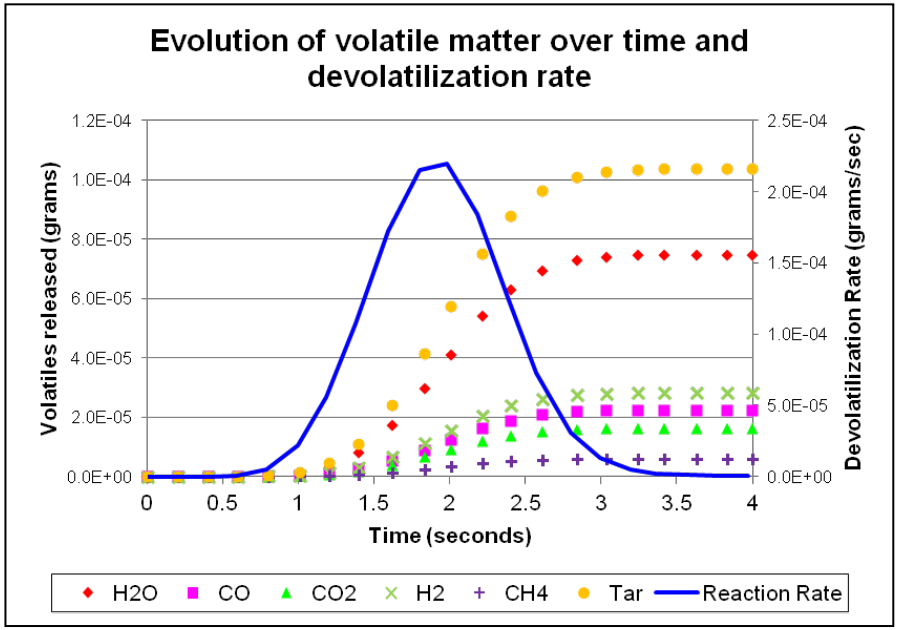


CO2 levels obtained from a 3D simulation of diffusion through a porous particle (ε = 0.40)

Capability for modeling chemical reactions added to MFIX-DEM

- Flexible framework supports user-defined gas-solids reactions
- Testing to ensure interphase mass conservation
- Incorporating C3M gasification reactions is underway





$$\text{Volatile Matter} \rightarrow \alpha_d \text{Tar} + \beta_d^{\text{CO}}\text{CO} + \beta_d^{\text{CO}_2}\text{CO}_2 + \beta_d^{\text{CH}_4}\text{CH}_4 + \beta_d^{\text{H}_2}\text{H}_2 + \beta_d^{\text{H}_2\text{O}}\text{H}_2\text{O}$$

Musser, J., "Modeling of heat transfer and reactive chemistry for particles in gas-solid flow utilizing continuum-discrete methodology (CDM)," West Virginia University, PhD Thesis 2011.

Hybrid discrete-element/continuum model under development

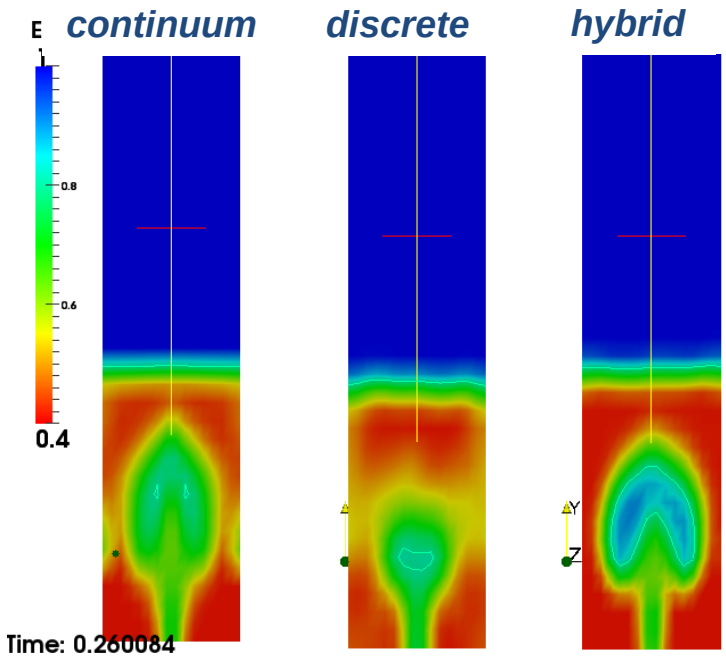
Motivation: coal gasification

- Continuum model not as accurate
- Discrete model computationally prohibitive

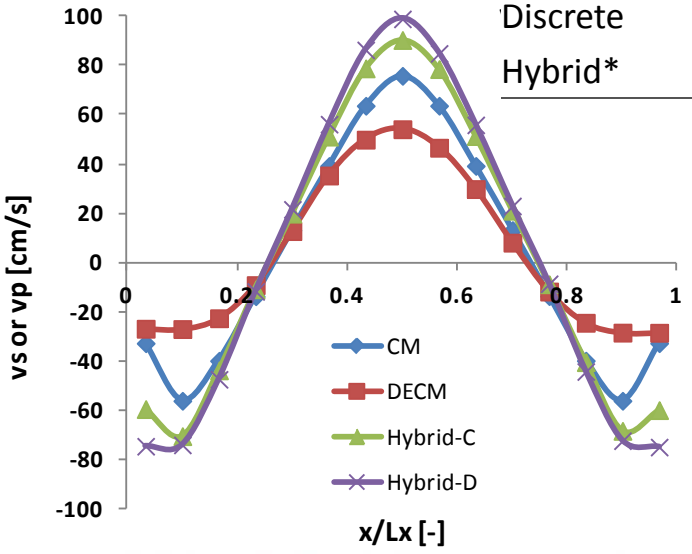
→ *Reduce cost & provide more details*

Objective: develop Hybrid DECM

- *User selects* DEM or CM for a particular solids phase (based on physics of problem)
- *Coal gasification:* DEM for sparse solids phase and CM for the dense solids phase

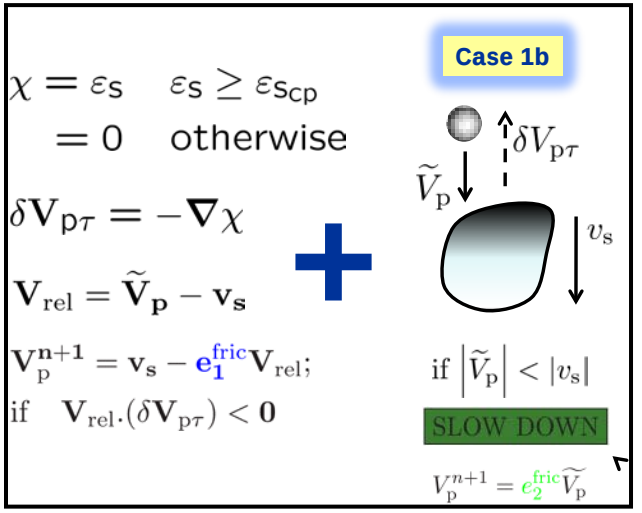


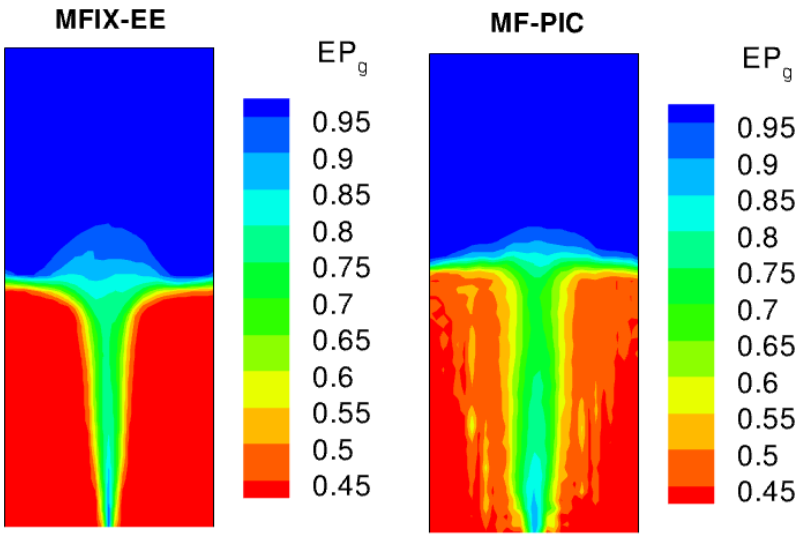
Run Times for 20s	
Continuum	1.57
Discrete	4.18
Hybrid*	3.57



MP-PIC model implemented in MFIX

- Solids represented by notional particles/parcels
- Exact collisions not resolved
- Developed and implemented a novel two parameter MP-PIC model for frictional stresses
- The MP-PIC model was found to be unconditionally stable and yields quick turn around CFD simulations of dense gas-solids flows
- The method has been extended to Cartesian grid for complex geometries





CPU time: 400 min

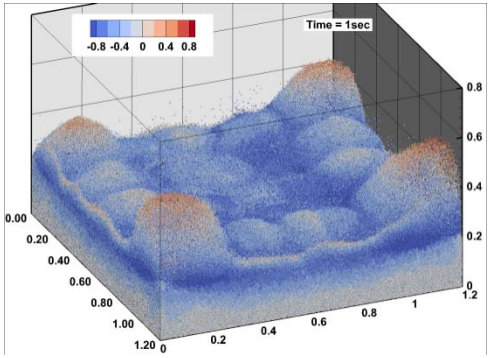
80 min

R. Garg "A novel open-source MP-PIC model for dense gas-solids flows" AIChE meeting 2012

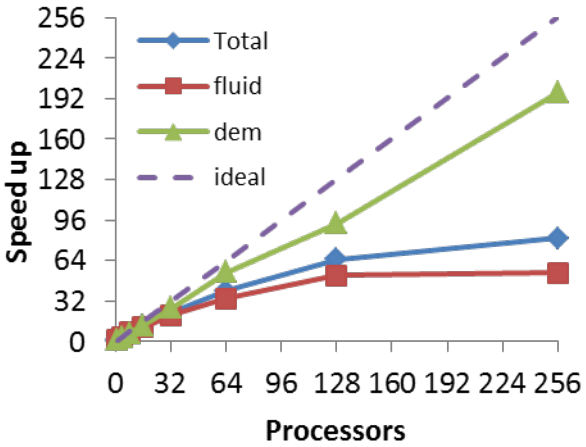
Accelerating MFIX on distributed/shared memory and heterogeneous systems

D. Tafti, P. Gopalakrishnan & H. Liu (Virginia Tech.)

- **Objective**
  - Accelerate performance of MFIX using parallel computing paradigms on emerging architectures
- **Project highlights**
  - Distributed memory systems: Incorporated MPI-parallelism in MFIX-DEM → factor of 80 speed up on 256 cores
  - Shared memory systems: Investigate OpenMP parallelism for MFIX-DEM
  - Heterogeneous CPU/GPU systems: Investigate OpenACC for co-processing



Bubbling fluidized bed with 5 million particles



Strong scaling of MFIX-DES with 2.56 million particles using MPI

Gopalakrishnan, P. and Tafti, D. K., Development of parallel DEM for the open source code MFIX, submitted to Powder Tech. Dec. 2011

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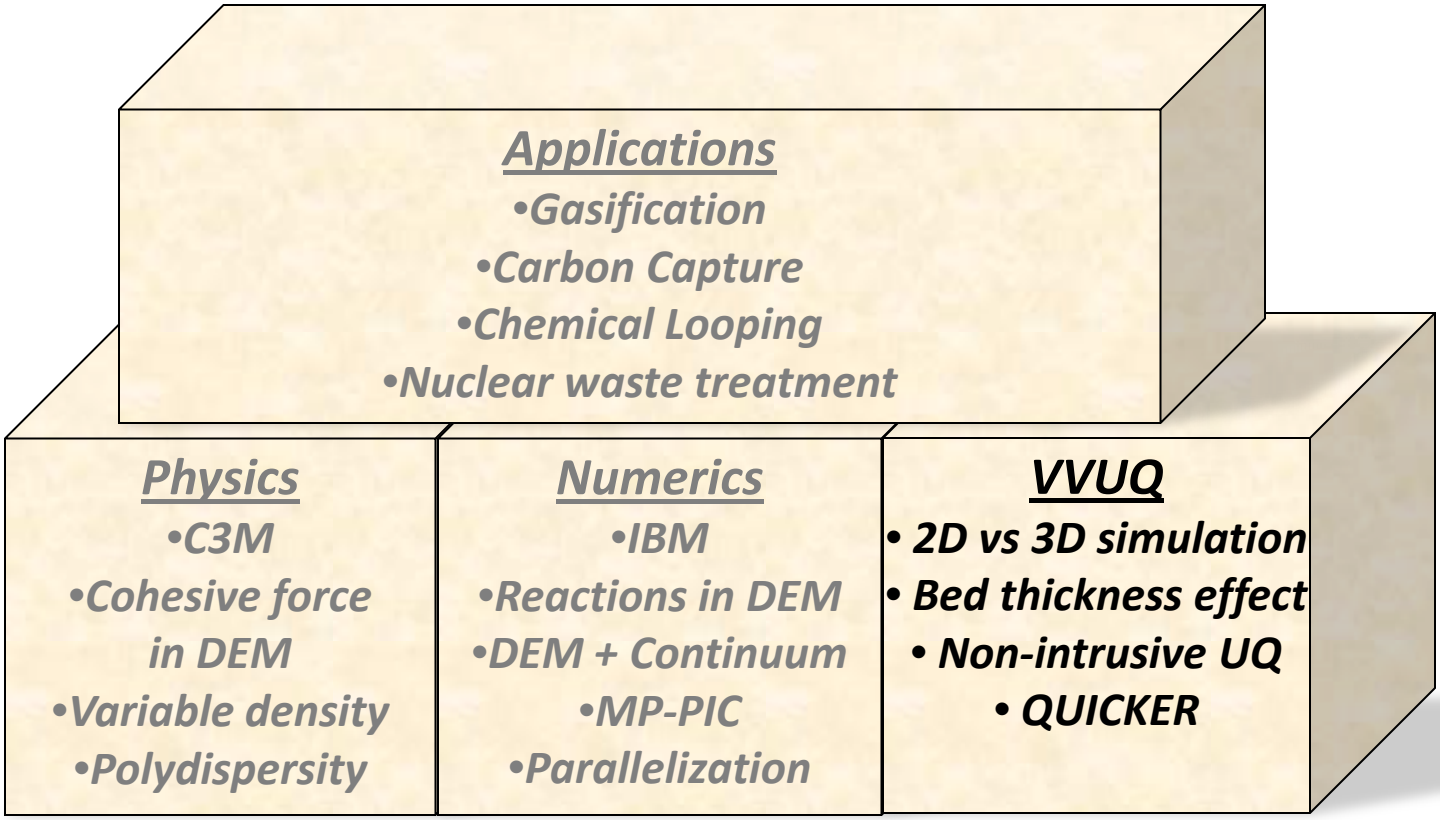
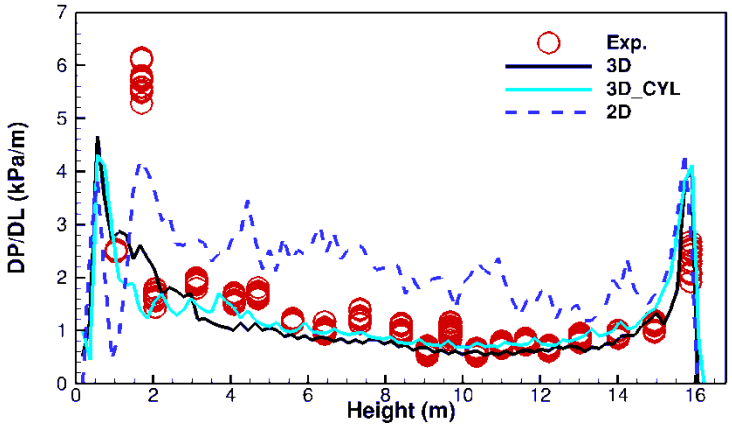
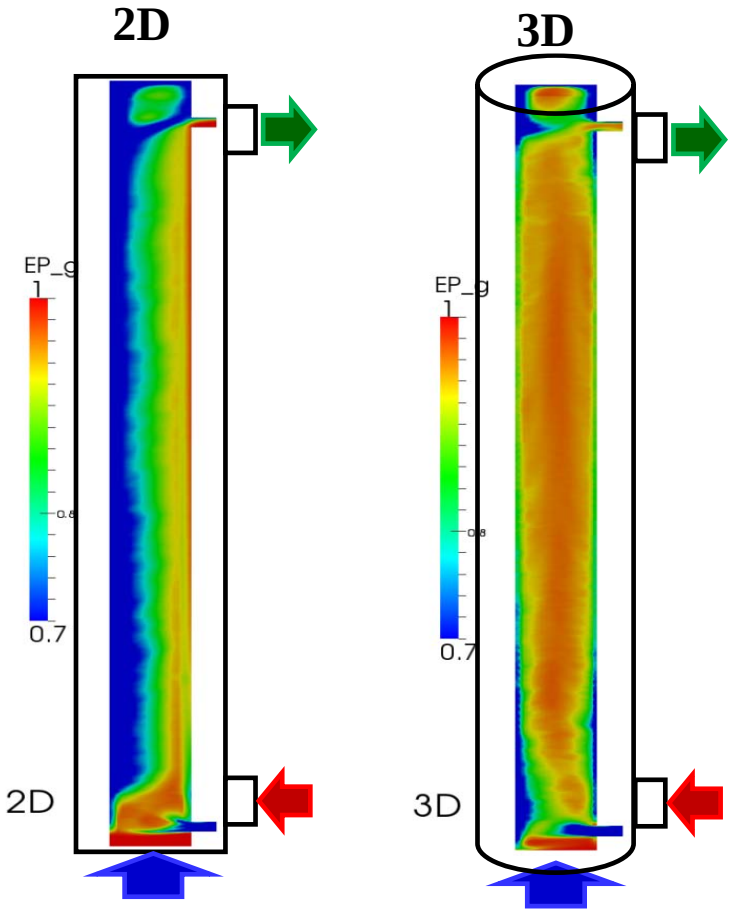


Evaluated differences between 2D and 3D simulations of CFB risers

- Three different circulating fluidized bed risers are simulated with CFD
- Differences between 2D and 3D simulations of CFB riser are investigated
- 2D simulation is only recommended for qualitative study of CFB riser



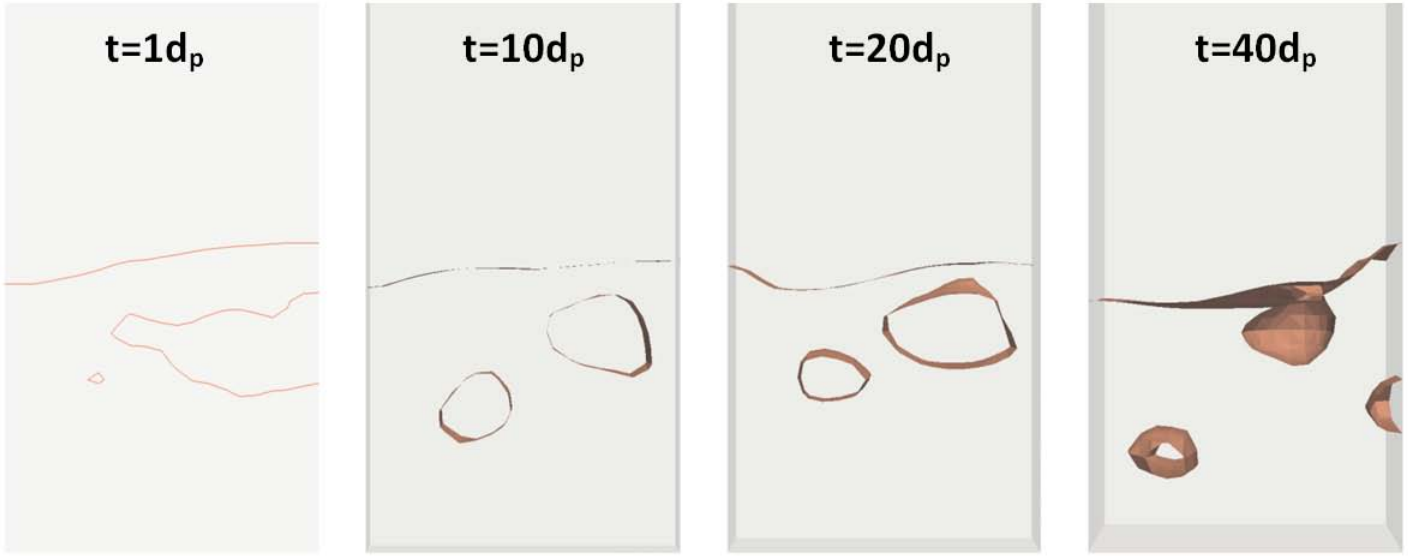


2D vs. 3D simulation of NETL B22 riser

T. Li, S. Pannala, and M. Shahnam, 2D versus 3D CFD simulations of circulating fluidized bed risers, 2012 Multiphase Flow Science Workshop, May 22-24, 2012, Morgantown

Effect of bed thickness on fluidized bed simulations ascertained

- **DEM simulations show that transition from 2D flow to 3D flow occurs within the range of 20 to 40d_p**
- **Therefore, wall effect cannot be neglected in continuum simulations of pseudo-2D beds.**



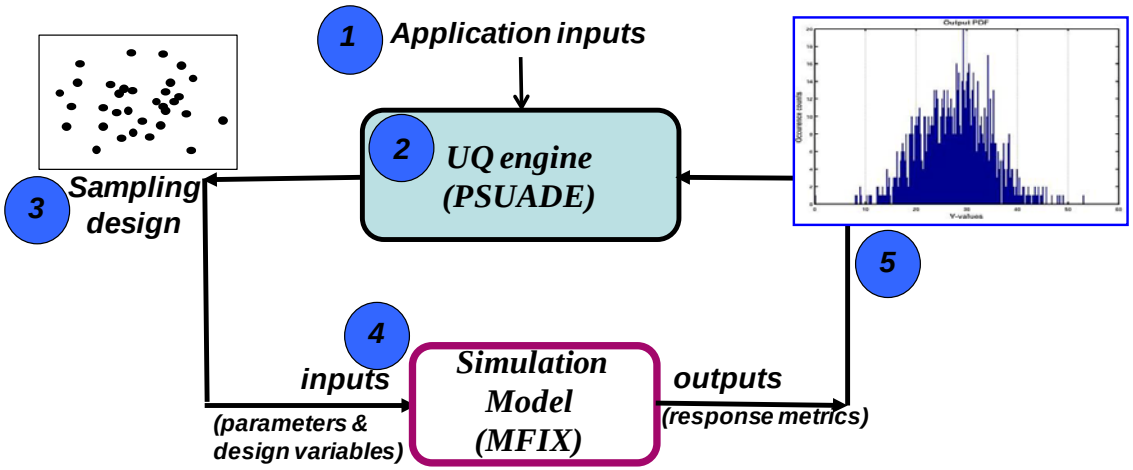
Snapshots of bubble behavior for different bed thicknesses

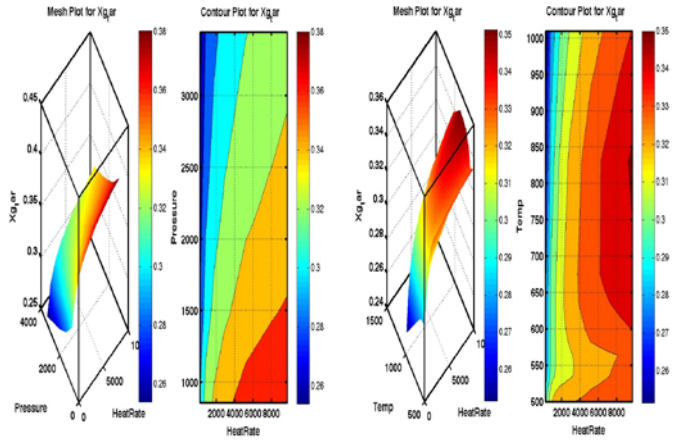
T. Li, P. Gopalakrishnan, R. Garg, and M. Shahnam, CFD-DEM study of effect of bed thickness for bubbling fluidized beds, Particuology, 10.1016/j.partic.2012.02.006.

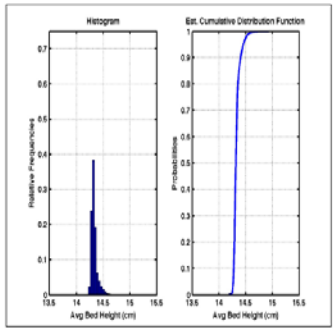
Non-intrusive propagation of input uncertainties demonstrated

- **Linked open source codes MFIX and PSUADE**
- **Developed a surrogate model**
- **Performed sensitivity study for the input uncertainties**

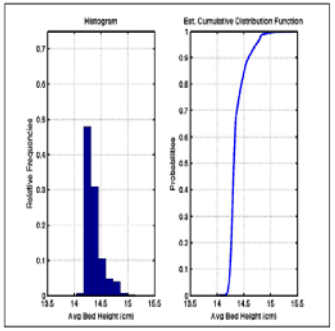
Surrogate models such as data fitted response surface models employed for propagating input parameter uncertainty and sensitivity analysis







(a) Normal distribution(μ= 0.8, σ= 0.05) assigned for particle to particle restitution coefficient, $e_{p,n}$



(b) Normal distribution(μ= 0.8, σ= 0.05) assigned for particle to wall restitution coefficient, $e_{w,n}$

Gel et al., "Uncertainty quantification in reactive multiphase CFD," presented at The 6th Sino-US Joint Conference of Chemical Engineering, Nov. 7-10, 2011, Beijing, China

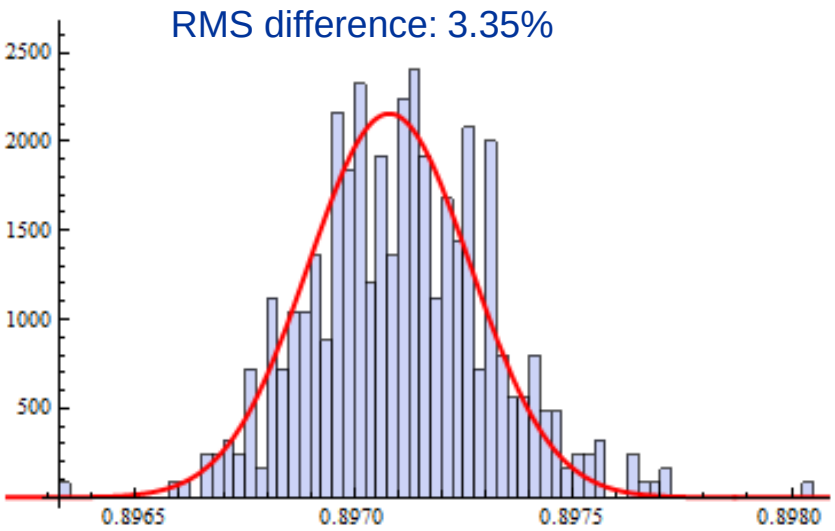
QUICKER: A novel tool for speeding up uncertainty quantification

A. Donato and Professor R. Pitchumani (Virginia Tech)

- A novel methodology, Quantifying Uncertainty In Computational Knowledge Engineering (QUICKER), has been developed
- When compared against Latin Hypercube Sampling (LHS), ***typical time-savings are approximately 95%, with RMS differences typically less than 7%***
- The methodology has been validated for a variety of MFIX scenarios, and several "blind" C3M scenarios where the QUICKER developers had no prior knowledge of the scenario

Computational time (h)

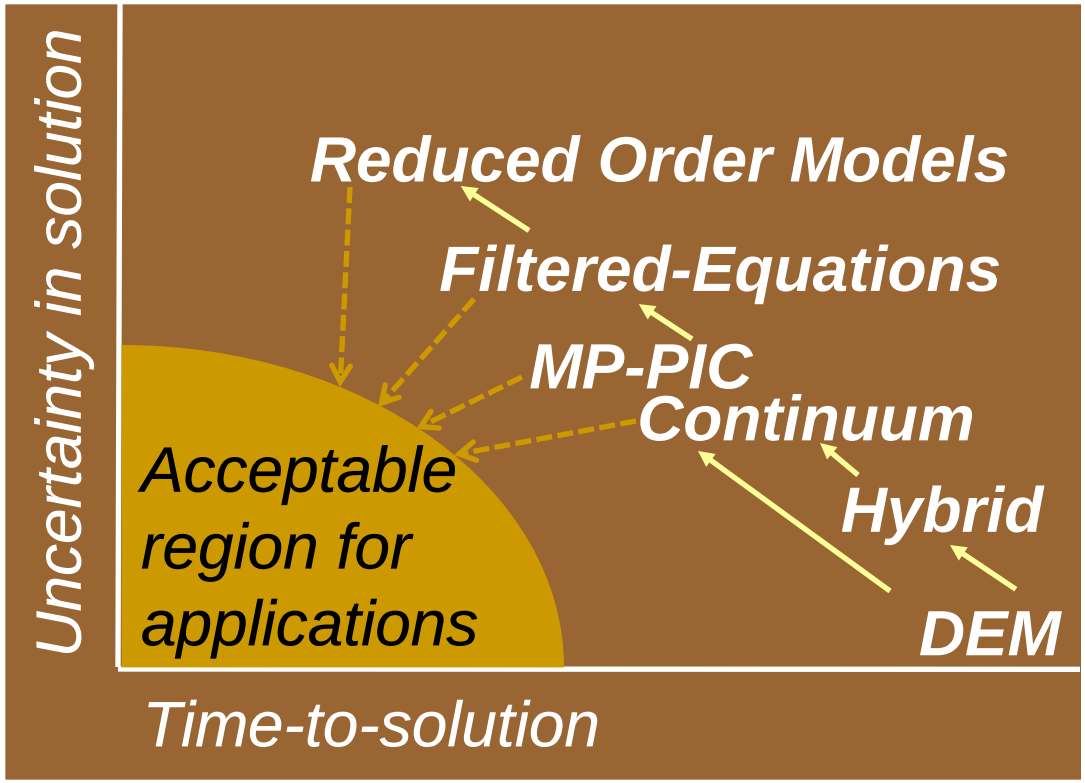
LHS	QUICKER
126	5



Comparison of LHS results (histogram) with QUICKER results (red line) for the 3dCfb MFIX tutorial

Reduce uncertainty and time-to-solution in multiphase-CFD for energy applications

- **Develop the open-source MFIX suite: DEM, Hybrid, MP-PIC, Continuum, Filtered-continuum, ROM**
- **Develop constitutive models for chemistry and hydrodynamics**
- **Generate accurate validation data from physical & numerical experiments**



- **Validate CFD models of *reacting gas-solids* flows and quantify the uncertainty in the predictions**

“Fret no more, … conference attendees. Scientists have learned how to avoid … spilled coffee.”

The Fluid Mechanics Of Walking With Coffee

Fret no more, overburdened conference attendees. Scientists have learned how to avoid a common research pitfall: spilled coffee.

Rouslan Krechetnikov, a mechanical engineer at the University of California, Santa Barbara, and graduate student Hans Mayer studied the problem, which involves the mechanics of walking as well as liquid sloshing, an interplay of accelerations, torques, and forces. They asked a person, filled mug in hand, to walk at different speeds, either focusing on the mug or looking straight ahead. A camera recorded the person’s motion and the mug’s trajectory while a tiny sensor on the mug recorded the instant of spillage.

In their paper published last month in *Physical Review E*, Krechetnikov and Mayer show that everyday mug sizes produce natural frequencies that happen to match those of a person’s leg movements during walking. So walking alone is tuned to drive coffee to oscillate in a mug. But small irregularities in walking can amplify oscillations, or sloshing.

So how to avoid a spill? Walk more slowly, the researchers say, and leave a gap between the top of the coffee and the mug’s rim. And watch what you’re doing—so long as your mug isn’t filled too high, a watched mug almost guarantees a clean run.

http://scim.ag/spilledcoffee

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