Tracking of Simulated Biomass Particles in Bubbling Fluidized Beds

Stuart Daw, Jack Halow, Sreekanth Pannala, Gavin Wiggins, and Emilio Ramirez

2013 AICHE National Meeting

52: Fluidization and Fluid-Particle Systems for Energy and Environmental Applications I

San Francisco, November 4, 2013

This presentation does not contain any proprietary, confidential, or otherwise restricted information

U.S. DEPARTMENT OF ENERGY

SEPARATION DESIGN GROUP
Technology for a sustainable energy future

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE U.S. DEPARTMENT OF ENERGY

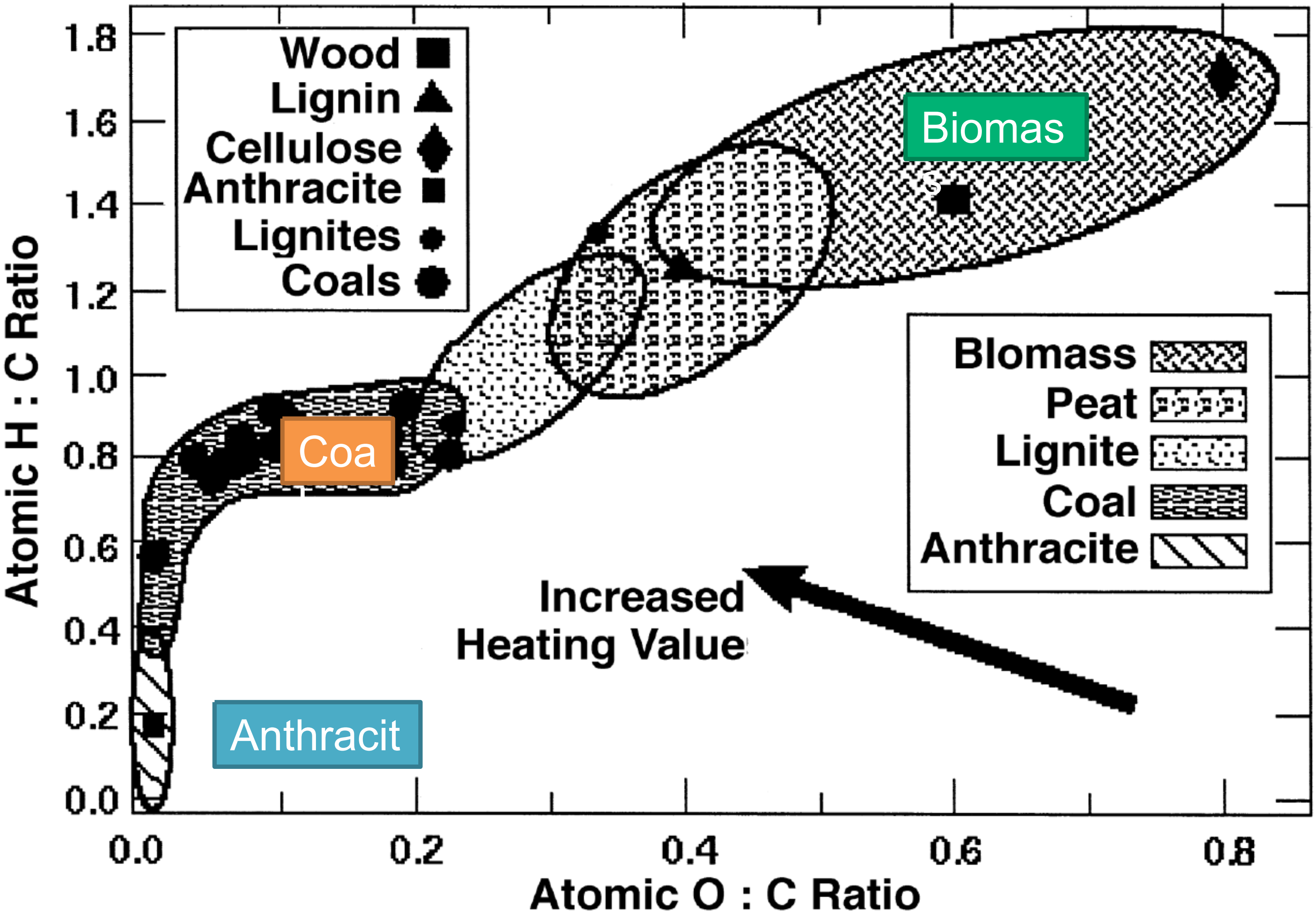
Outline

- Objectives
- Background and Motivation
- Experimental Setup and Example Observations
- Modeling Approach and Preliminary Results
- Summary and Status

Objectives

- **Utilize magnetic particle tracking to measure dynamic behavior of simulated biomass particles in bubbling fluidized beds**
- **Develop a simple model that mimics observed particle behavior and apply it to simulate bubbling bed pyrolysis**

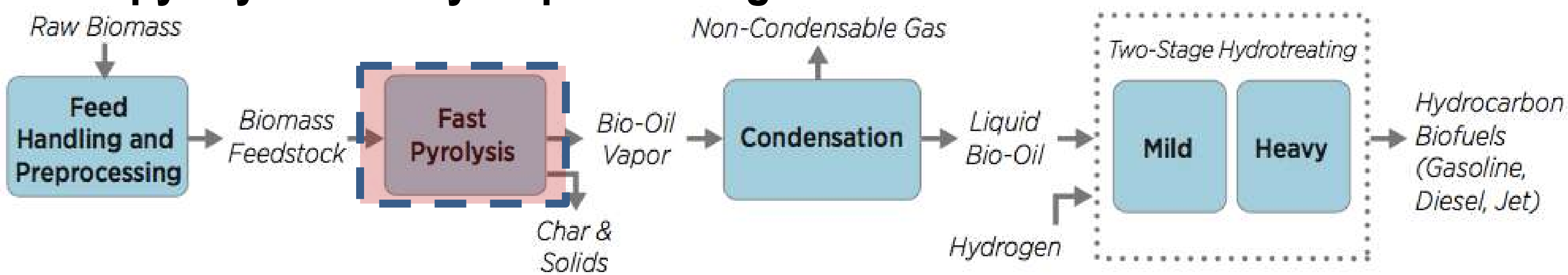
Background: Biomass conversion to liquid fuels



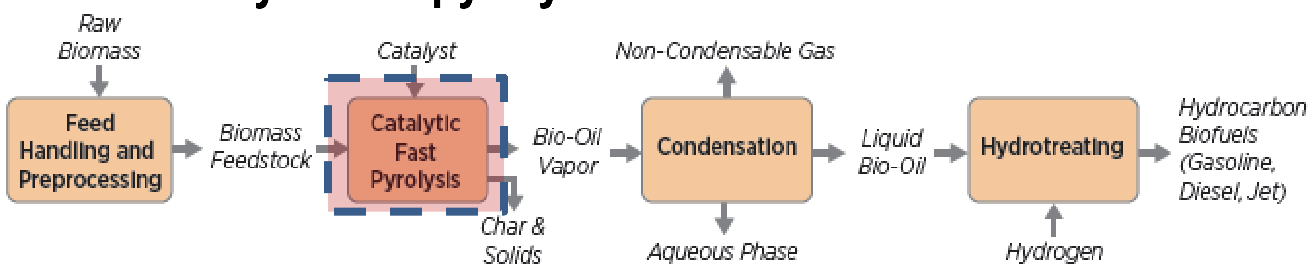
Source: B.M. Jenkins, et al., Fuel Processing Technology, 54 (1998), 17-46

Background: Fast pyrolysis is a critical step in 3 biomass-to fuel processes

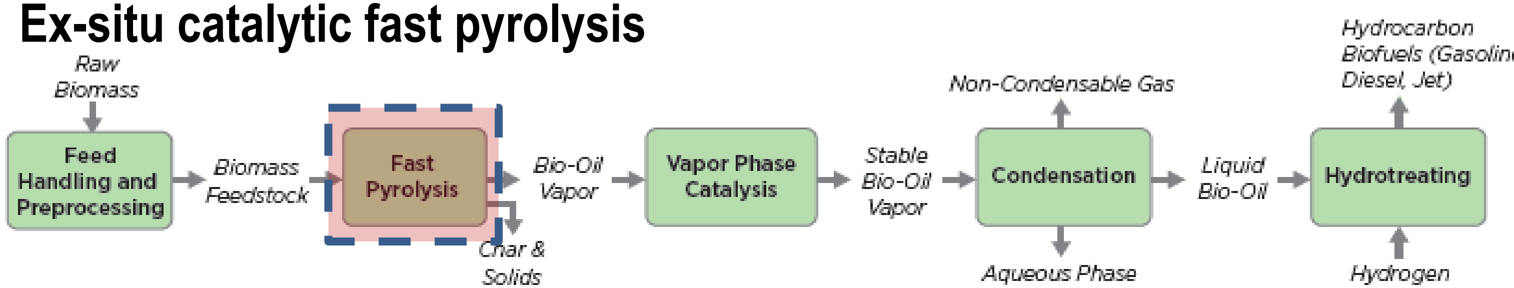
Fast pyrolysis and hydroprocessing



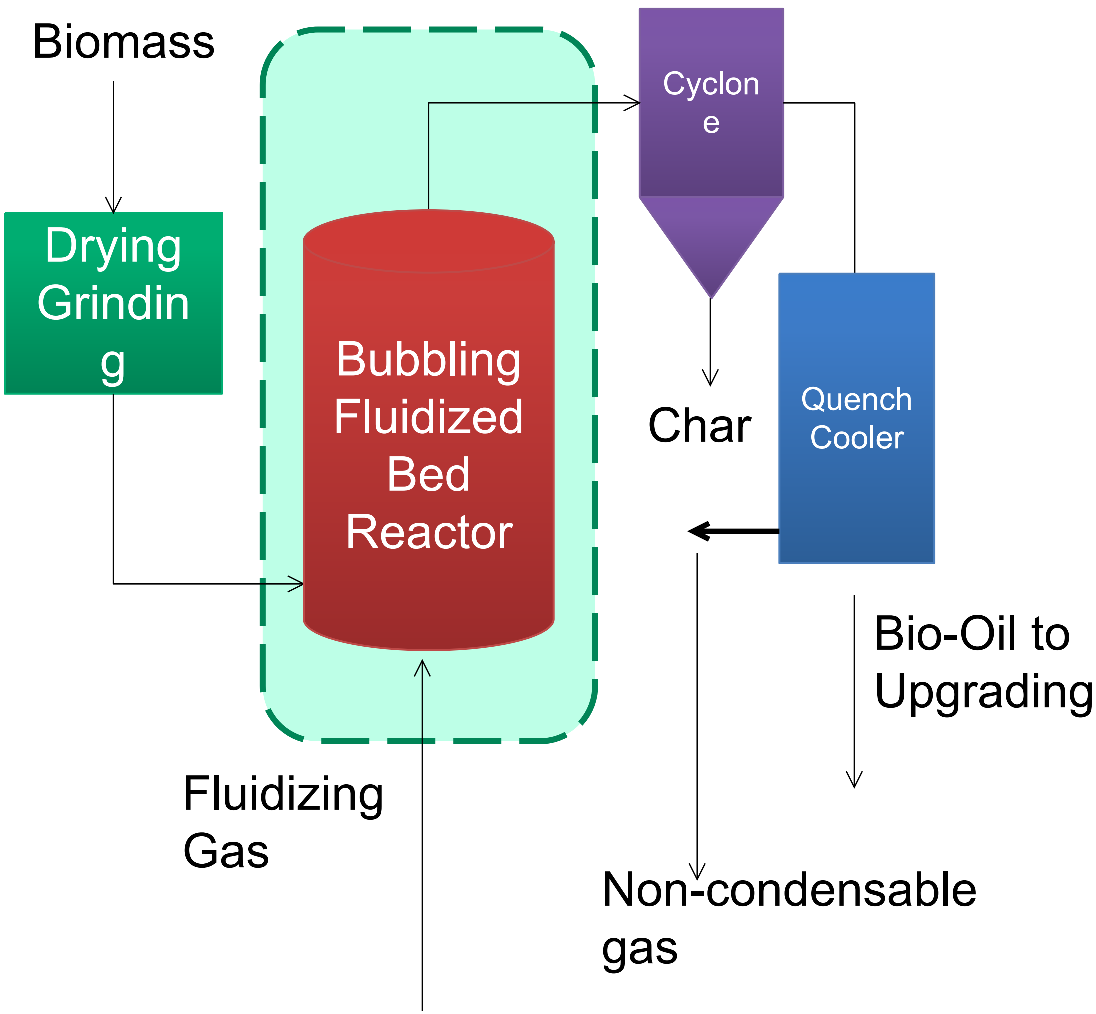
In-situ catalytic fast pyrolysis



Ex-situ catalytic fast pyrolysis



Background: One widely used approach for fast pyrolysis utilizes bubbling beds



- **Group B bed solids (e.g., sand) with or without catalyst**
- **Bed fluidized under no-oxygen conditions (mostly N_2, CO_2, H_2O)**
- **Raw biomass injected as particles and removed as char**
- **Biomass typically <1% of bed mass**
- **Bed temperature 400-600°C**
- **Very rapid heat up (up to 1000°C/s)**
- **Mixing and particle RTD very important to product composition and conversion**

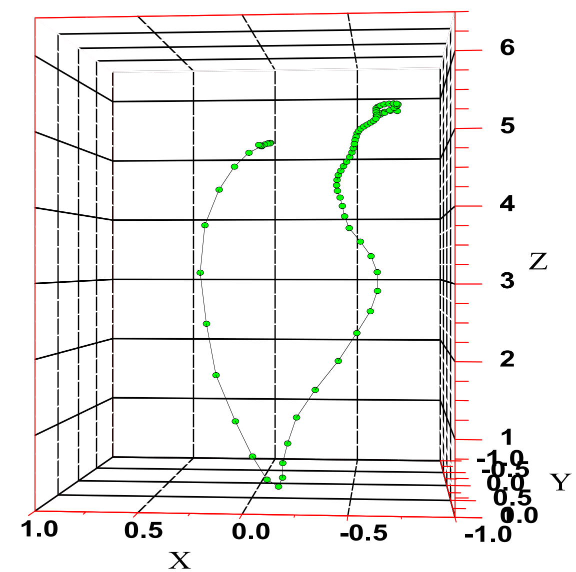
Motivation: Accurate pyrolysis reactor modeling is needed to assess options

- Complex heat, mass, and momentum transport
  - Within biomass particles
  - Between biomass and bed particles
  - Particle mixing and residence time in bed
  - Released pyrolysis products (char, tar, light gases)
- Complex chemistry
  - Intra-particle (decomposition, cracking, polymerization)
  - Catalysis of released gases
- Variable feedstock properties and conditions
  - Chemical composition (C, H, O, moisture)
  - Particle size and shape
  - Fluidization state, reactor size, temperature, pressure

Experimental Approach: Magnetic particle tracking to simulate biomass mixing*

- **Simulated biomass (tracer) particles are constructed by inserting tiny neodymium magnets into balsa wood cylinders (typically >1 mm diameter, 0.4-1 g/cc)**
- **Bed particles (e.g., 207 micron glass, 2.5 g/cc) are fluidized with ambient air (1.0 <= U/Umf <=5.0)**

090701T03vector.pdw
2.0 mm glass beads
6.5 cm deep bed
85 LPM



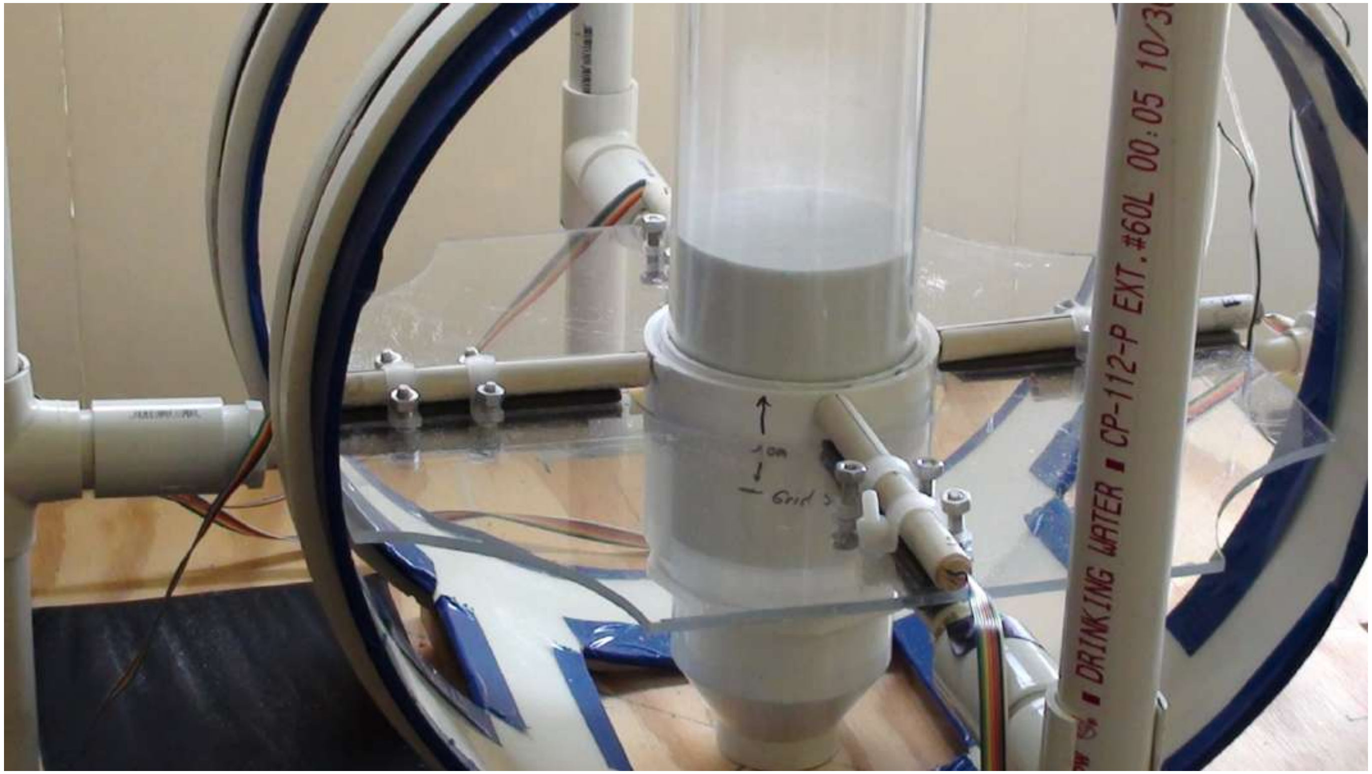
- **Single tracer particles are injected in bed at specific fluidization conditions and tracked**
- **Special algorithms de-convolute signals to give 3D particle trajectory**
- **Experimental facility at Separation Design Group Lab**

***See IECR* 2010, *49,* 5037–5043 and 2012, *51*, 14566–14576**

SEPARATION DESIGN GROUP
Technology for a sustainable energy future

Experimental Approach: 5.5 cm bed

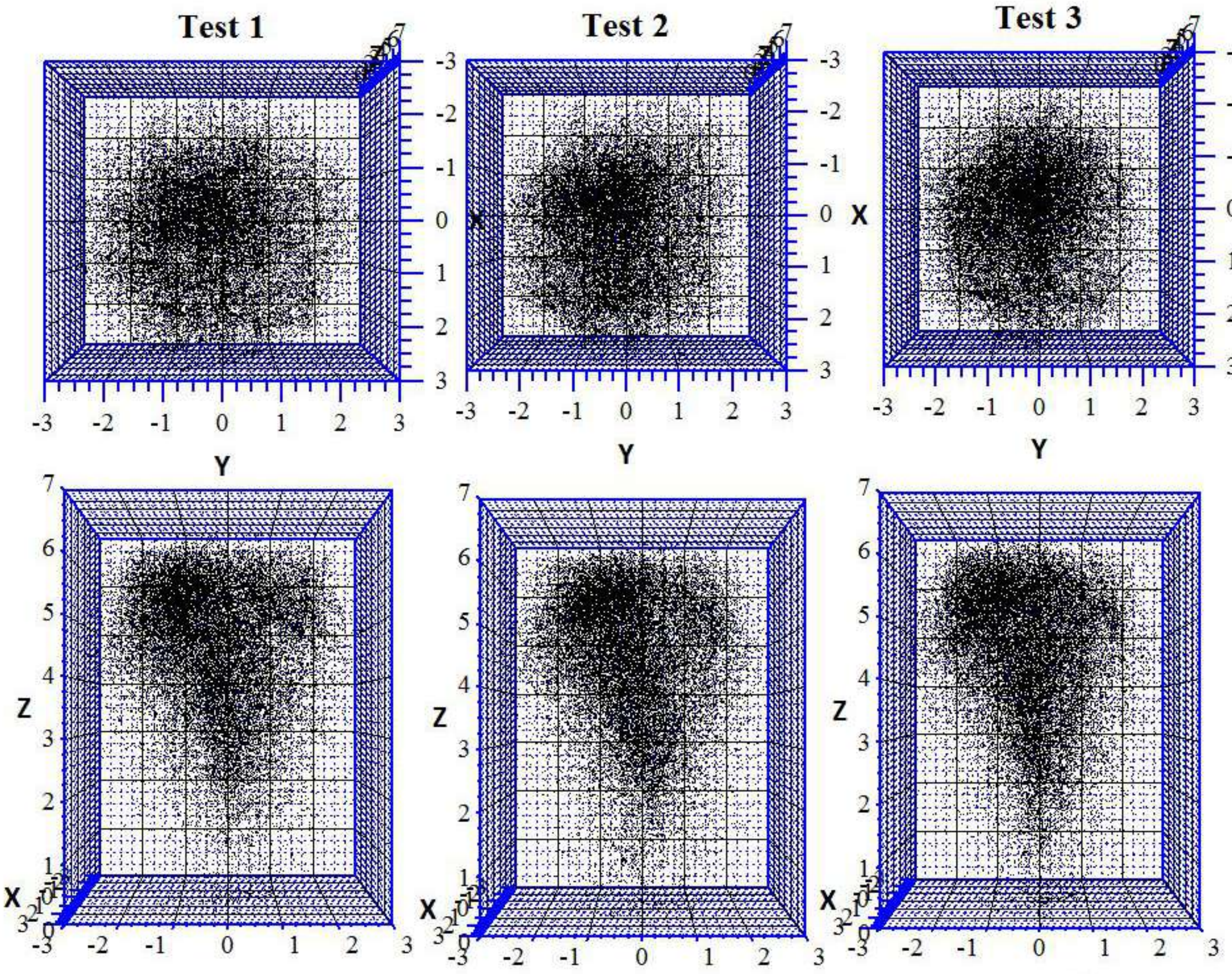
- Probes aligned North, South, East, West
- Helmholtz coils modify earth's magnetic field in bed
- Non-metallic bed and supports
- 100 Hz sampling rate
- 5 min runs (30,000 points)
- Porous plate distributor



Experimental Results: Trajectories map 3D time-average mixing

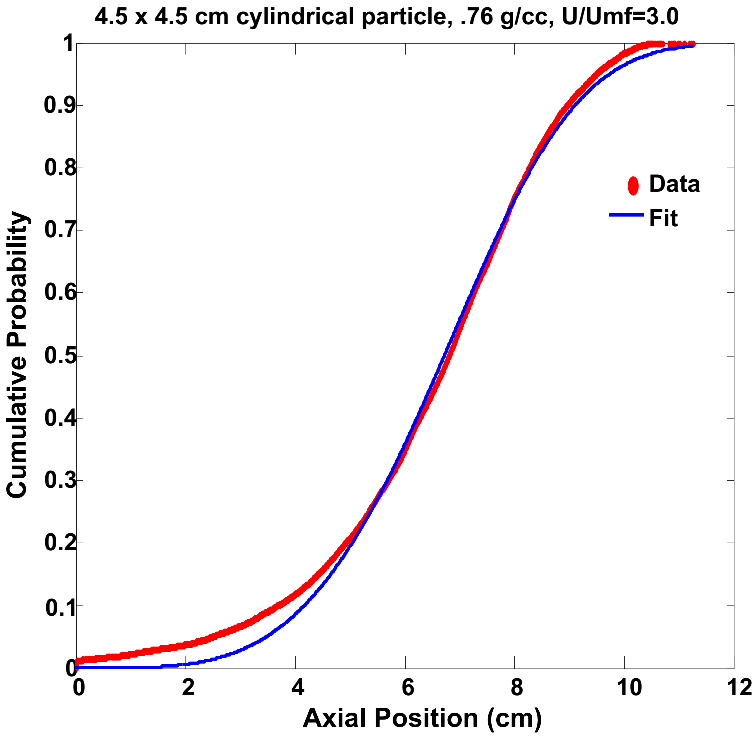
Top View

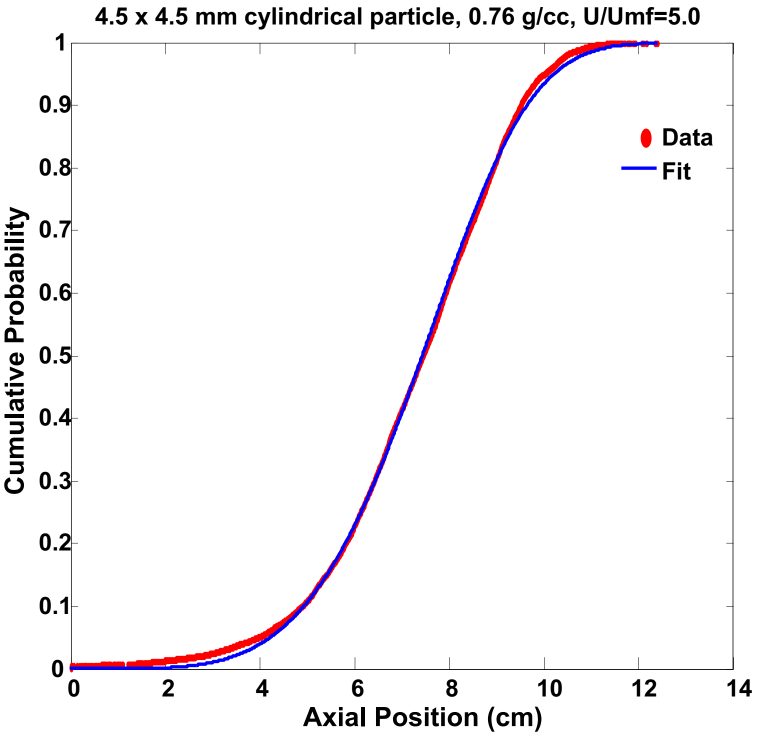
Side View



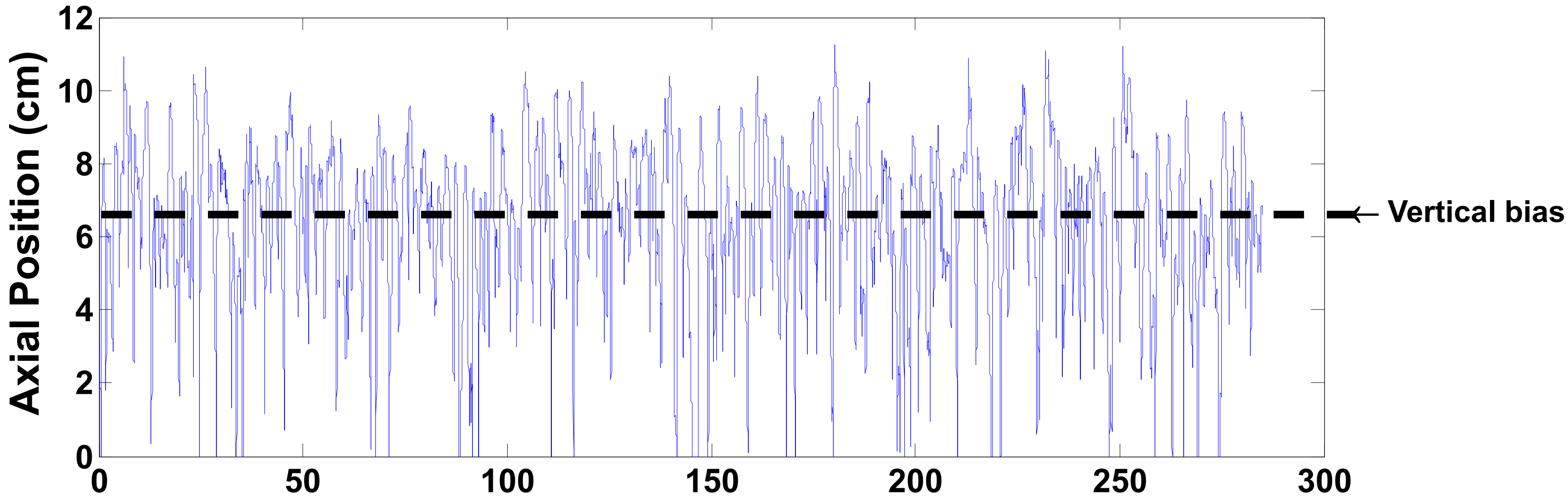
Experimental Results: Vertical mixing profiles follow Weibull statistics

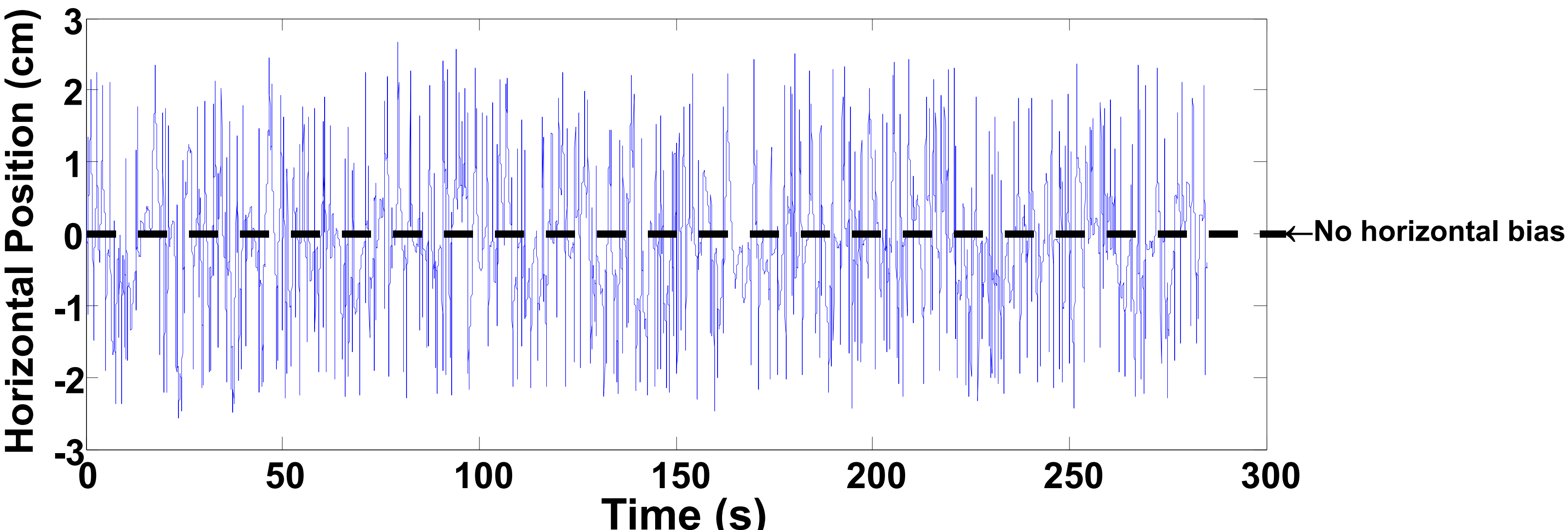
$$f(z) = \frac{k}{\lambda}\left(\frac{z}{\lambda}\right)^{k-1} e^{-(z/\lambda)^k}; C(z) = 1 - e^{-(z/\lambda)^k}$$





Experimental Results: Time series data reveal dynamics of particle motion





Modeling Approach: Low-order dynamic biomass pyrolysis reactor model

- Develop dynamic particle model that yields correct mixing statistics (multiple particles and different particle histories)
- Account for changes in biomass particle properties as pyrolysis occurs (translate tracking data to dynamic context)
- Key assumptions:
  - Initial focus on steady state
  - Released pyrolysis gases do not alter the fluidization state
  - Bed temperature is uniform
  - Biomass is represented by a single equivalent particle size
  - Each biomass particle follows a similar heat-up and devolatilization trajectory (from separate model)

Modeling Approach: Langevin model

Paul Langevin
(1872-1946)

$$\frac{\quad}{\quad} = - \; \frac{\quad}{\quad} + \; (\;)$$

x= position; t = time; m = particle mass; λ= friction coefficient
η(t) = stochastic perturbations

- **Originally proposed by Paul Langevin (*C. R. Acad. Sci. (Paris)* 146: 530–533, 1908) to describe Brownian motion**

We propose a modified version of this model for biomass particles in bubbling beds. In the vertical direction:

$$\frac{\quad}{\quad} = - \; \frac{\quad}{\quad} + \quad + \quad + \; (\;)$$

f_d = time average gas drag; f_g = gravitational force; ( )= vertical perturbations

- **A similar force balance can be written for horizontal particle position except that we assume no time-average drag or gravitational forces:**

$$\frac{\quad}{\quad} = - \; \frac{\quad}{\quad} + \; (\;)$$

$\eta_h(t)$ = horizontal perturbations

Modeling Approach: A discrete Langevin approximation

- Approximating derivatives over discrete time intervals and combining and rearranging terms for vertical motion results in:

$$(\quad + \quad) = \quad \cdot \; (\;) - \quad \cdot \; (\quad - \quad) + \quad + \quad ' \; (\;)$$

  z(t) = axial position at time t
  a, b, and c = empirical parameters that reflect time average forces
  $\eta'_v(t)$ = vertical stochastic particle shifts

- a, b, and c can be estimated with experimental particle position time series
- Stochastic inputs, $\eta'(t)$, can be estimated from stepwise prediction errors

- For horizontal motion, the result is:

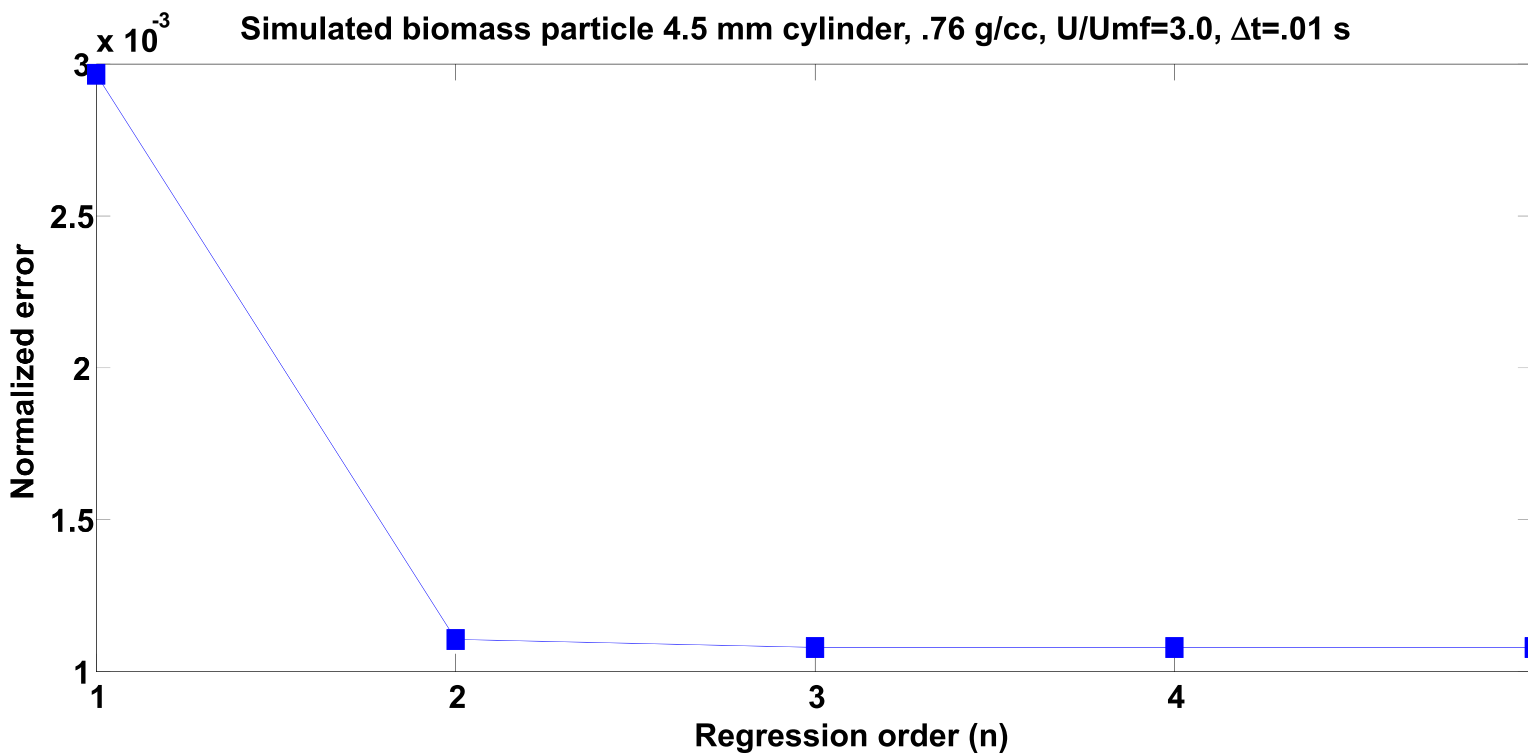
$$(\quad + \quad) = \quad \cdot \; (\;) - \quad \cdot \; (\quad - \quad) + \quad ' \; (\;)$$

  z(t) = axial position at time t
  a and b = empirical parameters that reflect time average forces
  $\eta'_h(t)$ = horizontal stochastic particle shifts

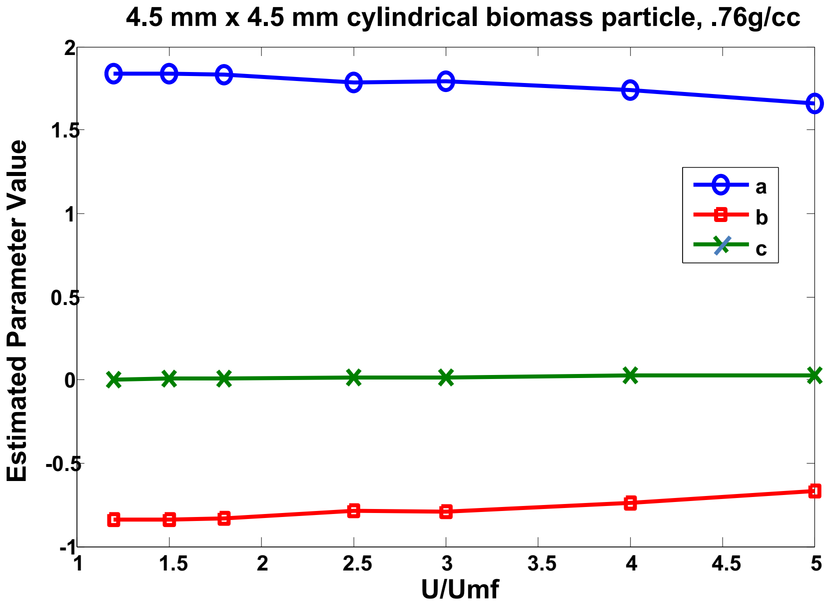
Modeling Results: 2nd-order regression is sufficient for magnetic particle motion

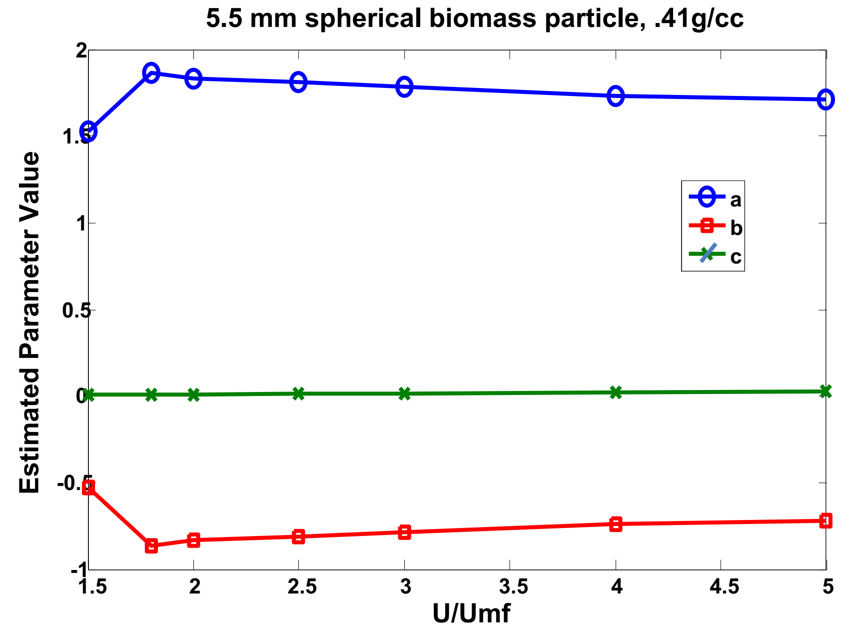
$$(\;+\;) = \sum_{=} (\,)\cdot(\;+\;-\;) + \;+\; {}'(\;)$$

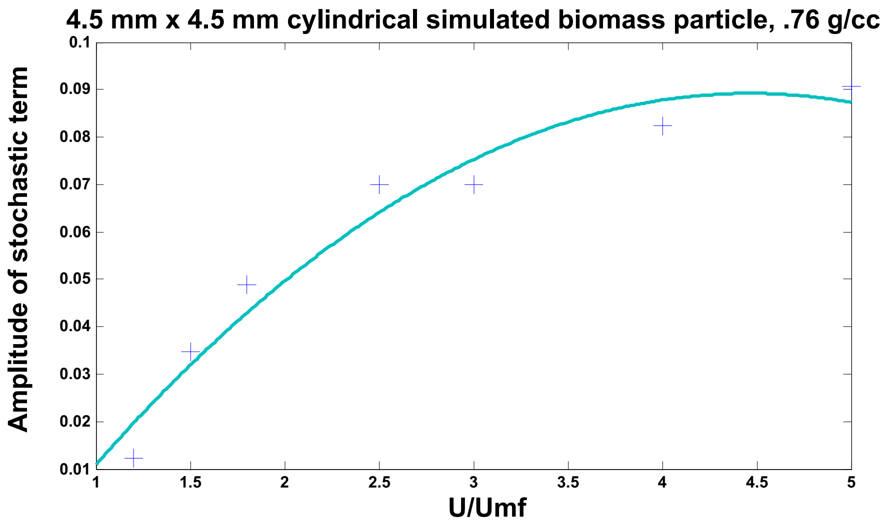
- Evaluate change in error (prediction) with increasing order
- Stop increasing order when error converges

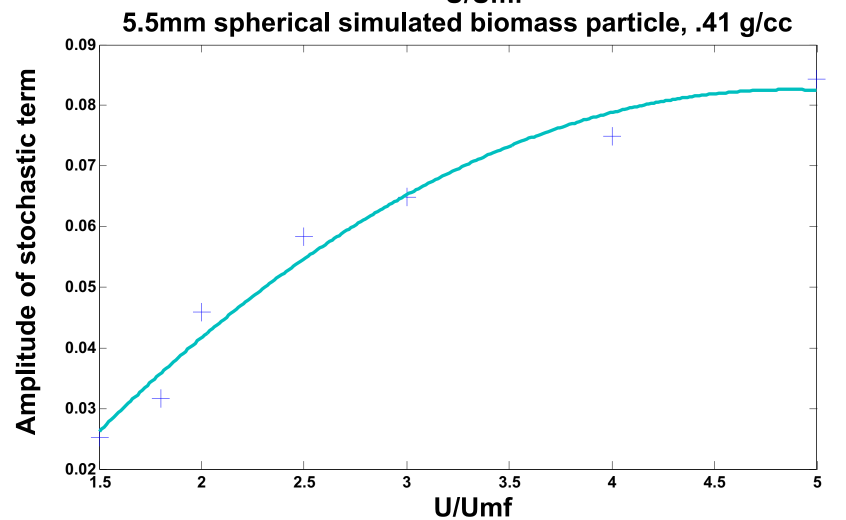


Preliminary Results: Parameter values follow simple trends

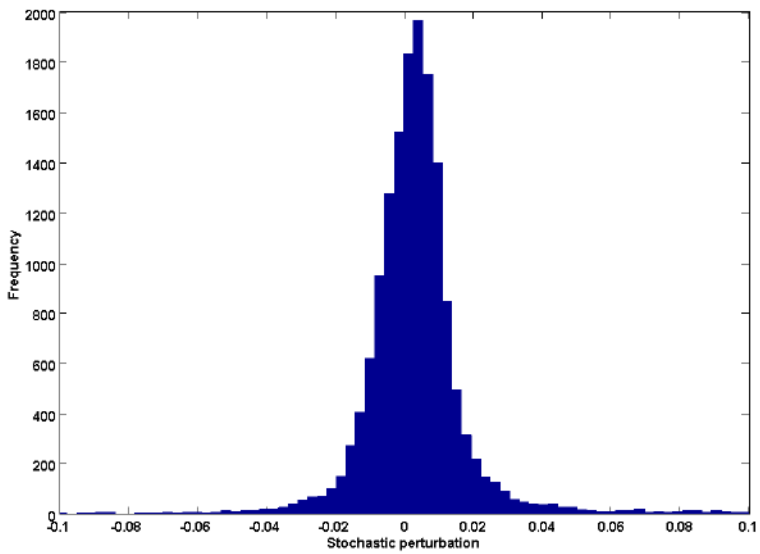




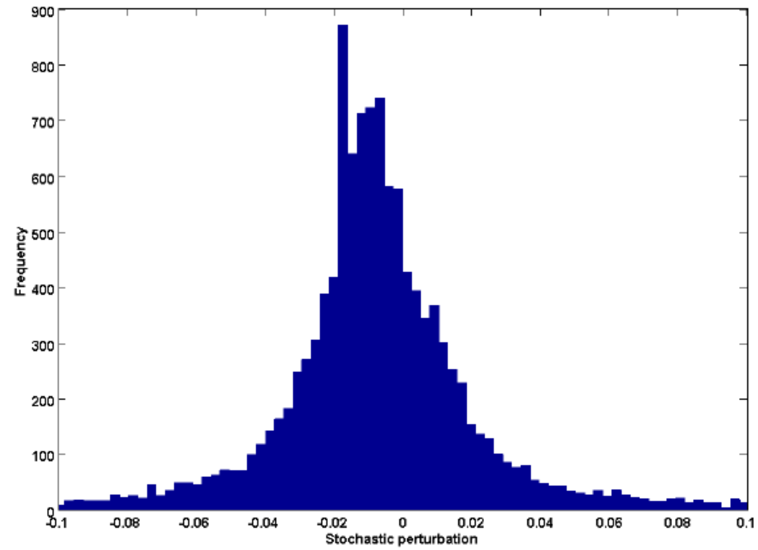




Preliminary Results: Stochastic effects vary spatially over the bed



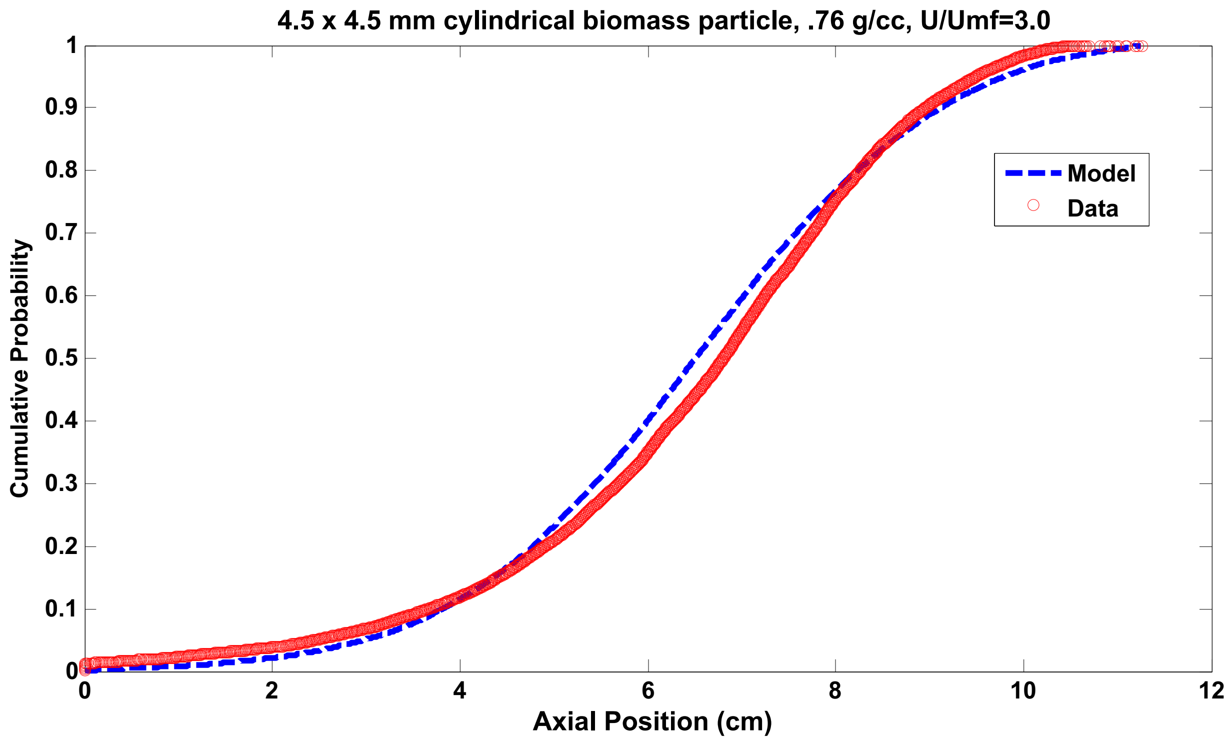
Vertical stochastic fluctuations in upper bed



Stochastic fluctuations in lower part of bed

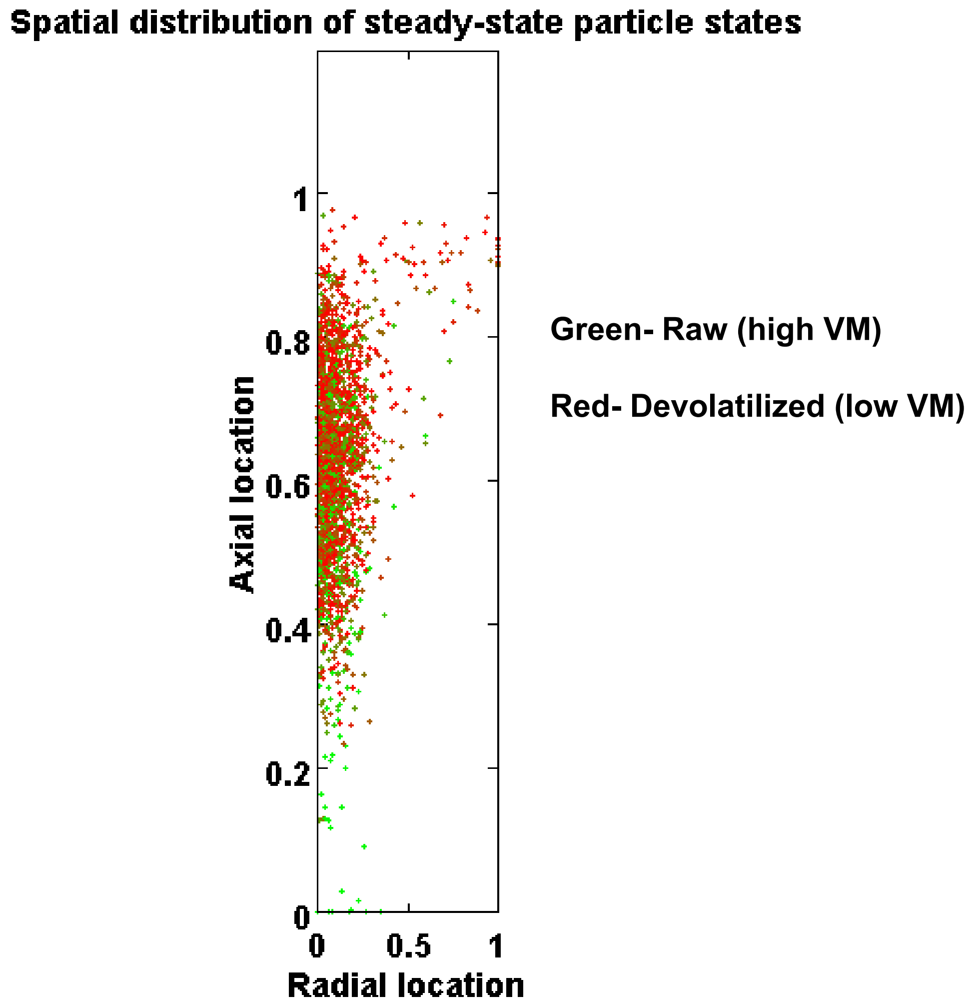
- Need to understand more details about these variations
- CFD may be a useful tool

Preliminary Results: Simplified model can closely approximate particle statistics



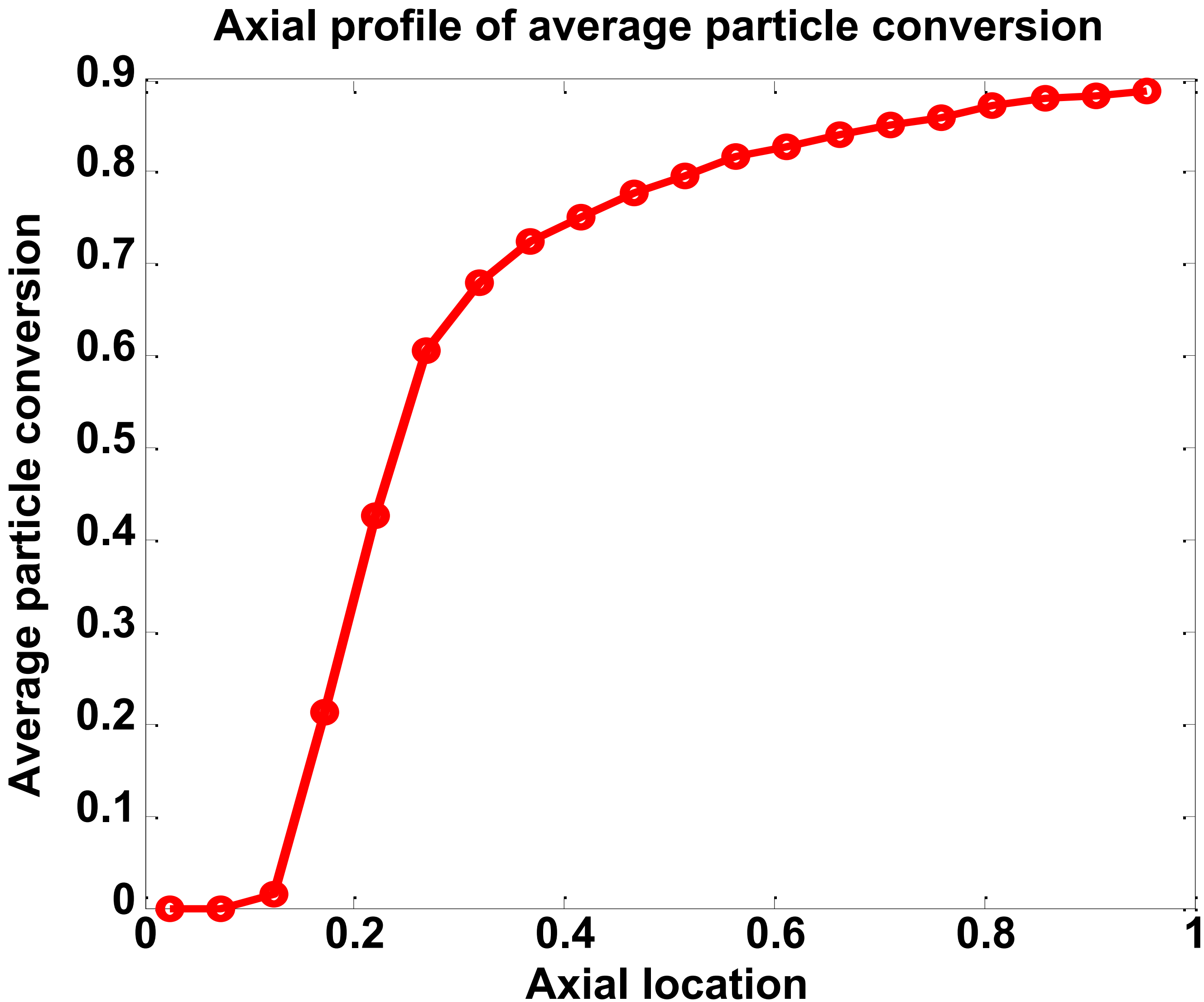
Observed particle statistics are closely approximated by the model already, but simulation of spatial variations in stochastic fluctuations can be improved

Preliminary Results: Particle distribution in integral reactor

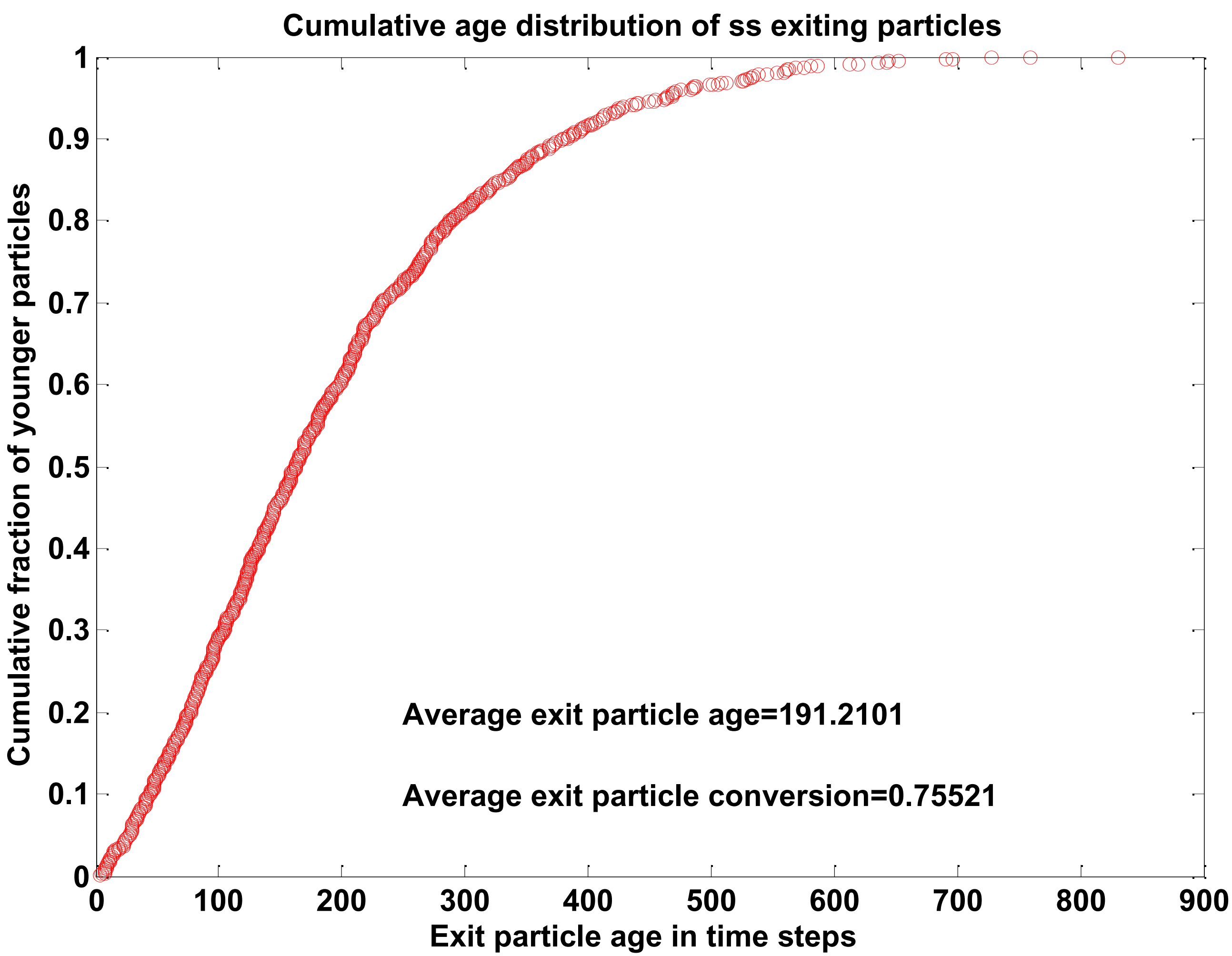


- Track 100s-1000s of particles in steady-state reactor
  - Specify biomass injection location and steady-state bed inventory
  - Specify condition for char particles to exit the bed (e.g., location, density)
  - Inject new particle each time one exits (maintain steady state)
  - Increment position of each particle by Langevin rules
  - Particles devolatilize according to heat up and reaction models

Preliminary Results: Integral model yields ss pyrolysis rates, conversions



Preliminary Results: Integral model yields ss pyrolysis rates, conversions



Summary and Status

- Magnetic particle tracking yields unprecedented details about single particle motion in bubbling beds
- A discrete Langevin model replicates the observed particle mixing statistics and time correlations
- Langevin parameters can be correlated with changes in particle properties and fluidization state
- Monte Carlo reactor simulations yield spatio-temporal distributions of ss particle residence time, age, and state of devolatilization
- The above can predict pyrolysis performance trends with changes in feed properties and reactor conditions
- Additional studies are underway to understand/improve the stochastic Langevin terms (CFD/DEM opportunities)

Acknowledgements

- Melissa Klembara: U.S. Department of Energy, Bioenergy Technologies Office
- Tim Theiss, Charles Finney : Oak Ridge National Lab
- Separation Design Group, Waynesburg, PA
- Computational Pyrolysis Project Partners
  - Mark Nimlos, David Robichaud: National Renewable Energy Lab
  - Robert Weber: Pacific Northwest National Lab
  - Larry Curtiss: Argonne National Lab
  - Tyler Westover: Idaho National Lab