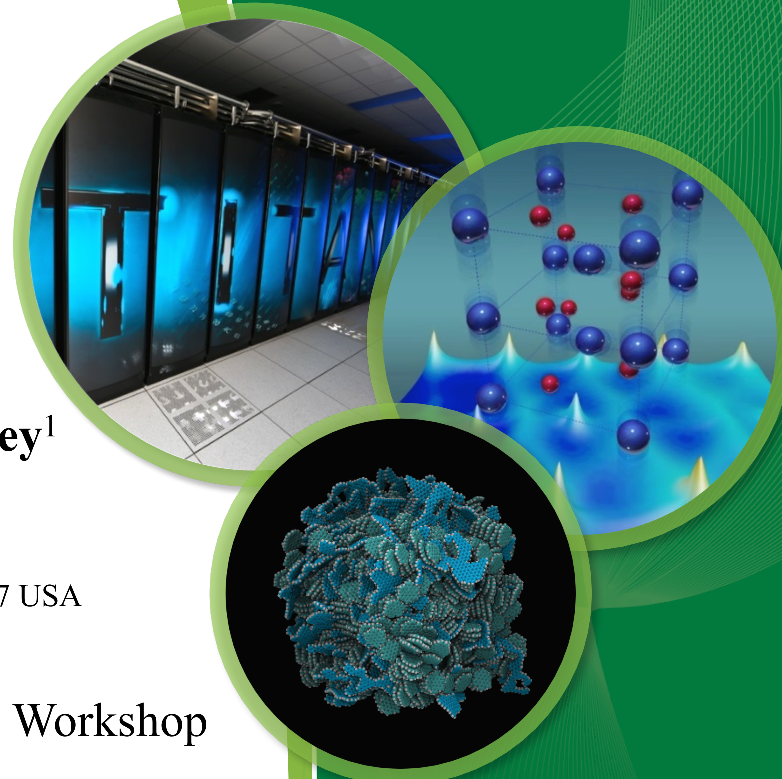
Computational study on biomass fast pyrolysis:

Hydrodynamic effects in a lab-scale fluidized bed pyrolyzer



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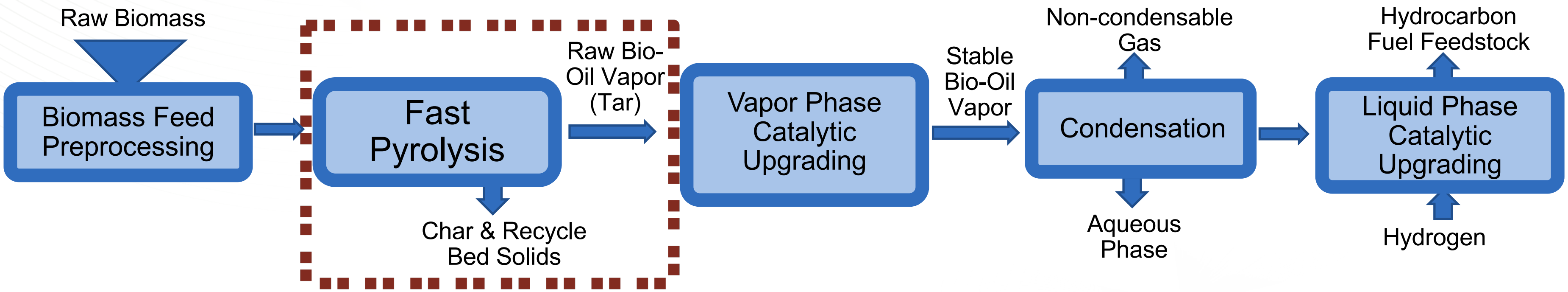
Background and Motivation (1)

Thermochemical conversion of biomass based on fast pyrolysis



- **High yield and composition of raw oil are key.**
- **Process risk and economics depend on accurate prediction of pyrolysis parameters.**
- **Good physics-based models are necessary for interpreting, scaling up lab experiments.**

Background and Motivation (2)

Why model biomass fast pyrolysis in bubbling fluidized beds?

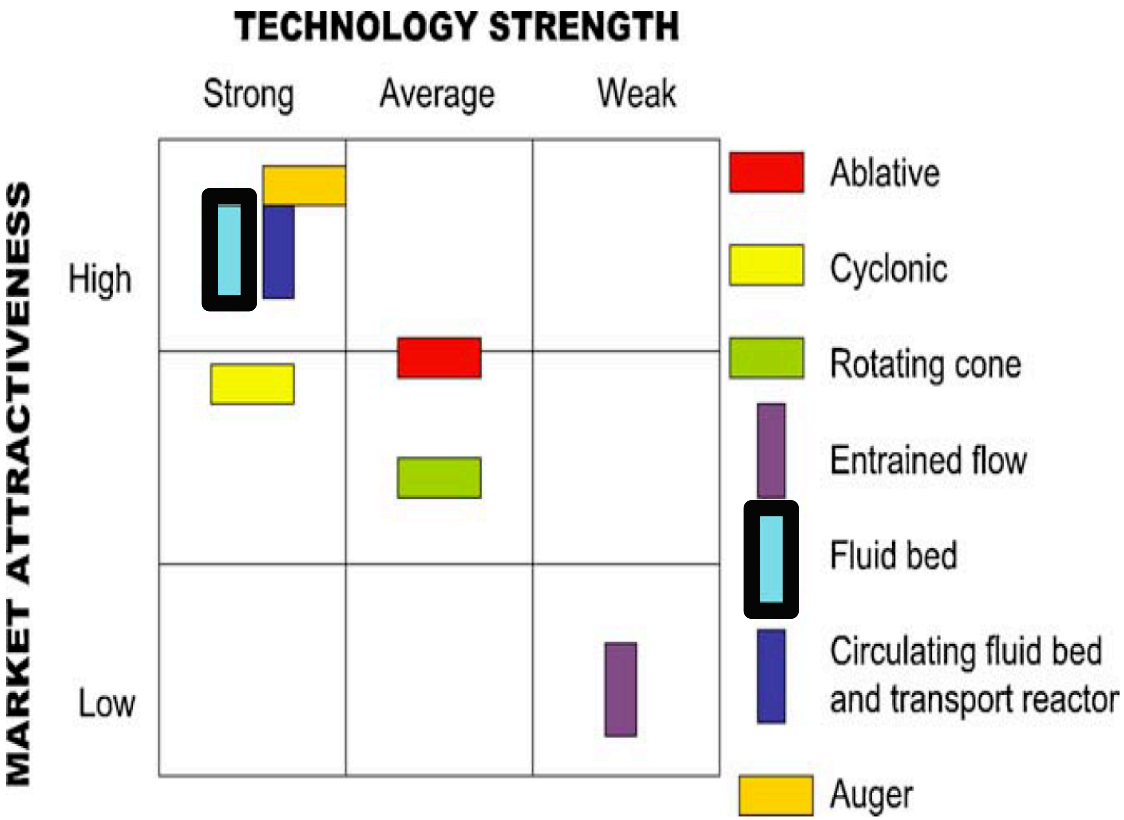


Figure: Brown RC, Holmgren J. Fast pyrolysis and biooil upgrading. National program 207: bioenergy and energy alternatives – distributed biomass to diesel workshop. Richland, WA, USA; 2006. (as cited in E. Butler, G. Devlin, D. Meier, K. McDonnell, A review of recent laboratory research and commercial developments in fast pyrolysis and upgrading, Renewable and Sustainable Energy Reviews 15 (2011) 4171-4186. http:/dx.doi.org/10.1016/j.rser.2011.07.035)

Bubbling beds are widely used in industry for biomass conversion because they provide:

1. Uniform temperatures
2. High heating rates
3. Efficient mass transfer
4. Relatively low particle attrition
5. Low pumping energy requirements

The majority of experimental fast pyrolysis studies in the literature are based on bubbling fluidized bed reactors.

Objective: Assist experimental demonstrations and scale-up studies to predict raw oil production

Account for impact of solids and gas hydrodynamics on raw oil

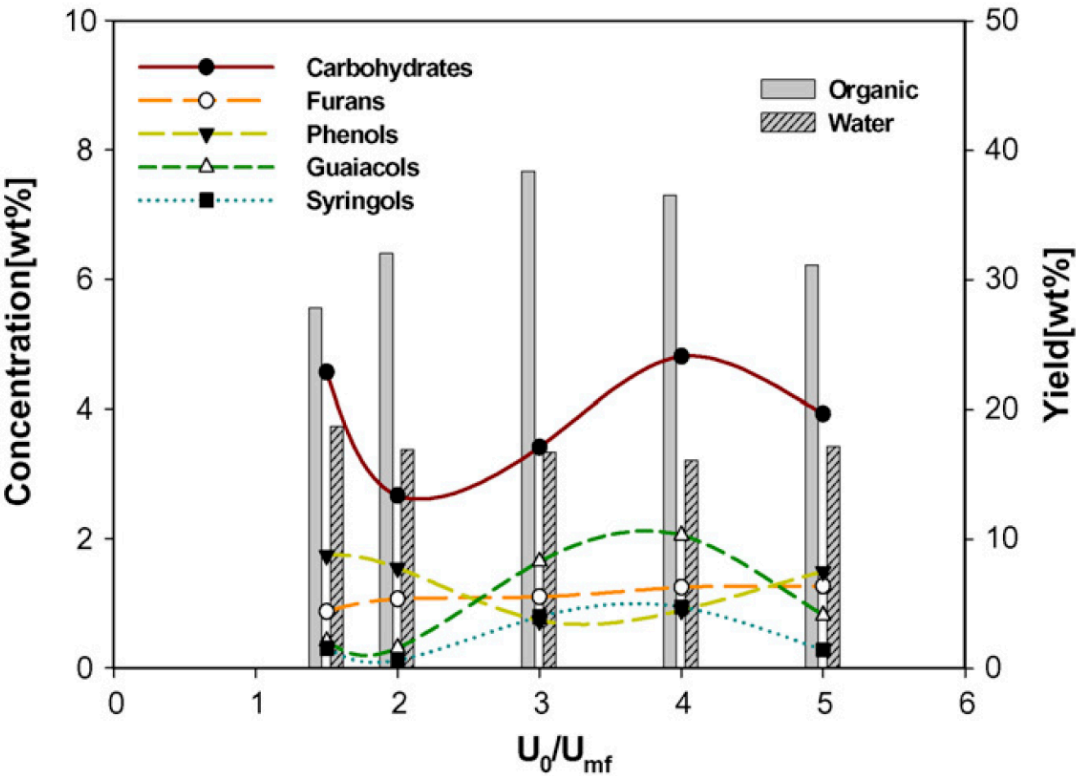


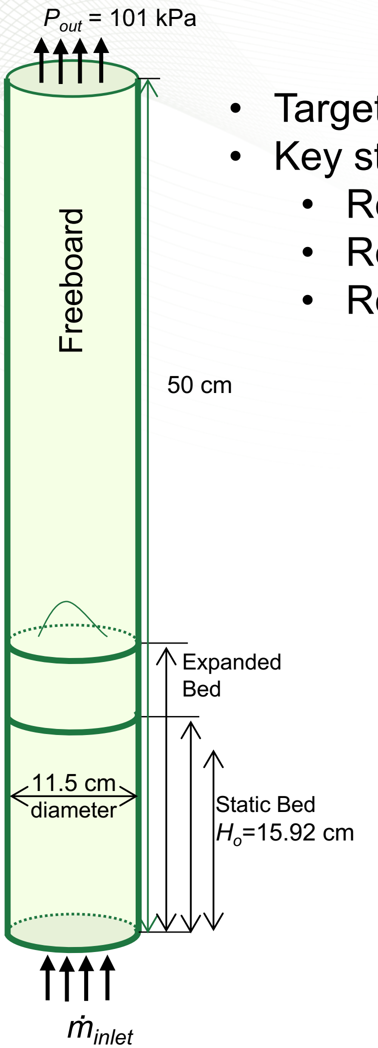
Figure: S.-H. Lee, M.-S. Eom, K.-S. Yoo, N.-C. Kim, J.-K. Jeon, Y.-K. Park, B.-H. Song, S.-H. Lee, The yields and composition of bio-oil produced from *quercus acutissima* in a bubbling fluidized bed pyrolyzer, J. Anal. Appl. Pyrolysis 83 (2008) 110-114. http://dx.doi.org/10.1016/j.jaap.2008.06.006

Hydrodynamics directly impact:

1. Particle residence time
2. Gas residence time
3. Particle heating rate
4. Particle attrition/fragmentation
5. Particle and ash elutriation
6. Particle segregation

All the above significantly impact raw oil yield and composition.

Approach (1): Verify solids mixing trends with literature



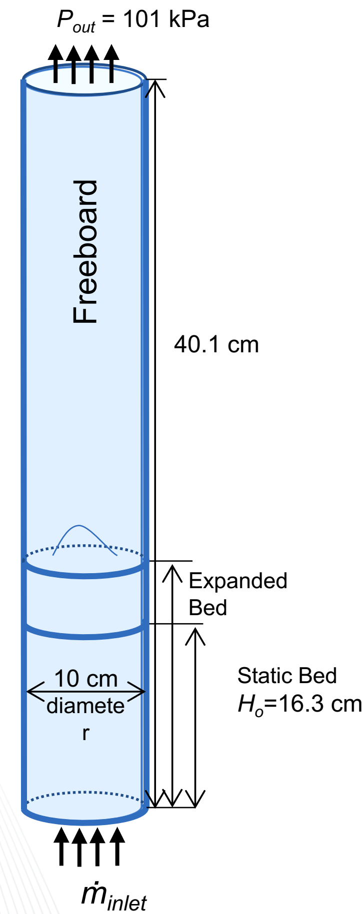
Park and Choi 2013
Mixing biomass char

- Target: Fluidized bed particle studies used to verify model
- Key steps:
  - Reproduce exp. **particle residence time distribution (RTDs)**
  - Relate impact of char elutriation on RTDs
  - Reproduce impact of solids segregation on **mixing**

Property	Units	Mixing Study Park & Choi 2013	RTD Study Berruti 1988
Particle diameter (Sand)	m	387×10^{-6}	710×10^{-6}
Particle density (Sand)	kg/m^3	2383	2470
Particle diameter (Styrofoam/char)	m	957×10^{-6}	450×10^{-6}
Particle density(styrofoam)	kg/m^3	-	82
Particle density(Char)	kg/m^3	391	-
Temperature	K	300	300
Pressure (inlet)	kPa	101	101
Fluidizing N_2 (range)	m/s	0.14 - 0.19	0.554
Minimum fluidization	m/s	0.14	0.30
Coefficient of restitution	-	0.9	0.9
Angle of repose	°	30	30

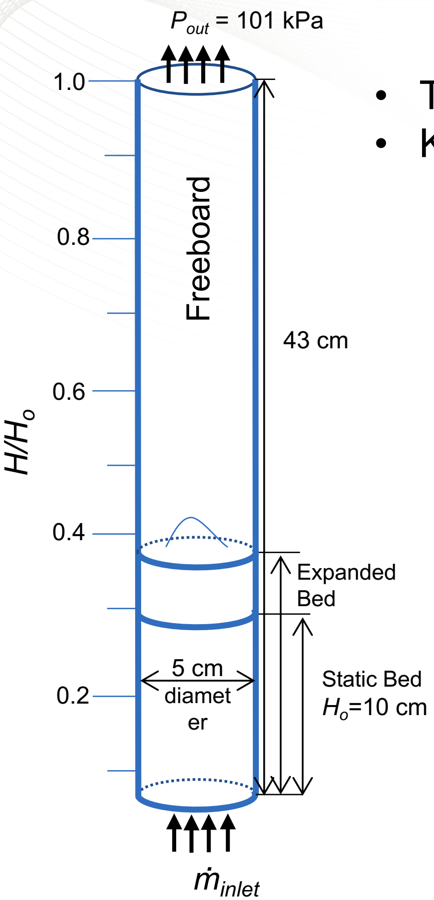
H.C. Park, H.S. Choi, The segregation characteristics of char in a fluidized bed with varying column shapes, Powder Technology 246 (2013) 561-571.

F. Berruti, A.G. Liden, D.S. Scott, Measuring and modelling residence time distribution of low density solids in a fluidized bed reactor of sand particles, Chemical Engineering Science 43 (1988) 739-748.



Berruti 1988
Residence time study

Approach (2): Validation with relevant lab pyrolyzer experiments



- Target: NREL bubbling bed lab pyrolyzer used to study biomass feedstock impact
- Key questions:
  - Can observed bio-oil yield variations be simulated?
  - At what point do we have trust in our model?
  - What criteria must be captured by the model?

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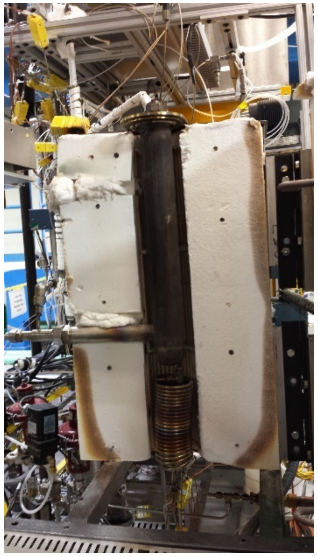


Simulation must capture at least 3 product yields to compare with experiments

1. Tar (or oil) treated as a heavy molecular gas
2. Gas considered light, non-condensable gases
3. Char particle phase properties must be defined such that particle can elutriate

Utilize mixing study and elutriation study to capture flow dynamics

Use elutriation correlations to ensure char will be removed from the reactor

Computational study on biomass fast pyrolysis oil yield: developing a predictive model which includes hydrodynamics of the bubbling-to-slugging transition in a laboratory-scale fluidized bed

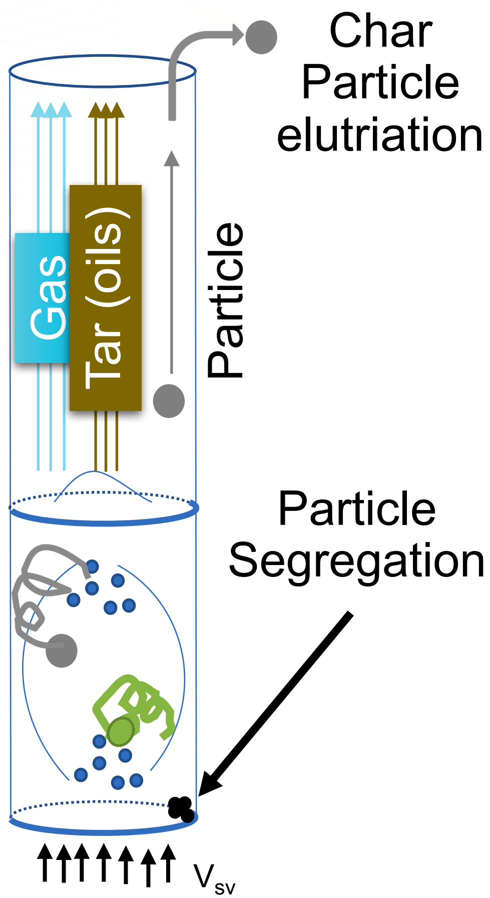
Methods (1): Fast pyrolysis CFD model details

MFiX TFM

– Eulerian-Eulerian (Two-Fluid Model)
– Syamlal-O'Brien drag-model
– Kinetic theory of granular flow
  – Schaeffer frictional stress tensor formulation
  – Hyperbolic tangent stress blending function
– Second order discretization
– 3D cylindrical mesh
– DLSODA ODEPACK chemistry solver

Methods (2): Pyrolysis reaction kinetics- Liden model

- Challenge to implement kinetics coupled with hydrodynamics

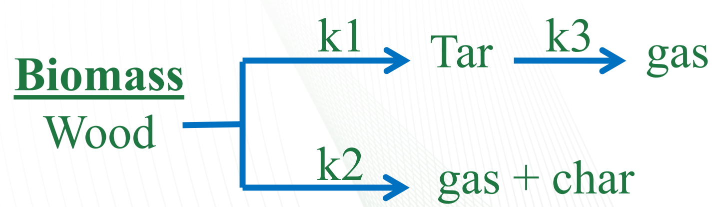


$$\frac{dm_i}{dt} = -mk_i$$

$$k_i = A_i \exp(-E_i / RT)$$

Kinetic scheme

First-order irreversible Arrhenius rate



A.G. Liden, F. Berruti, D.S. Scott, A kinetic model for the production of liquids from the flash pyrolysis of biomass, Chemical Engineering Communications 65 (1988) 207-221.10.1080/00986448808940254

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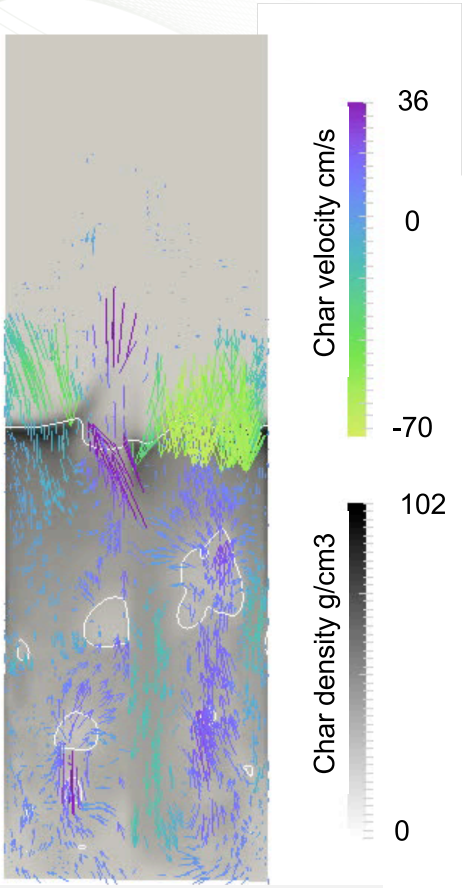
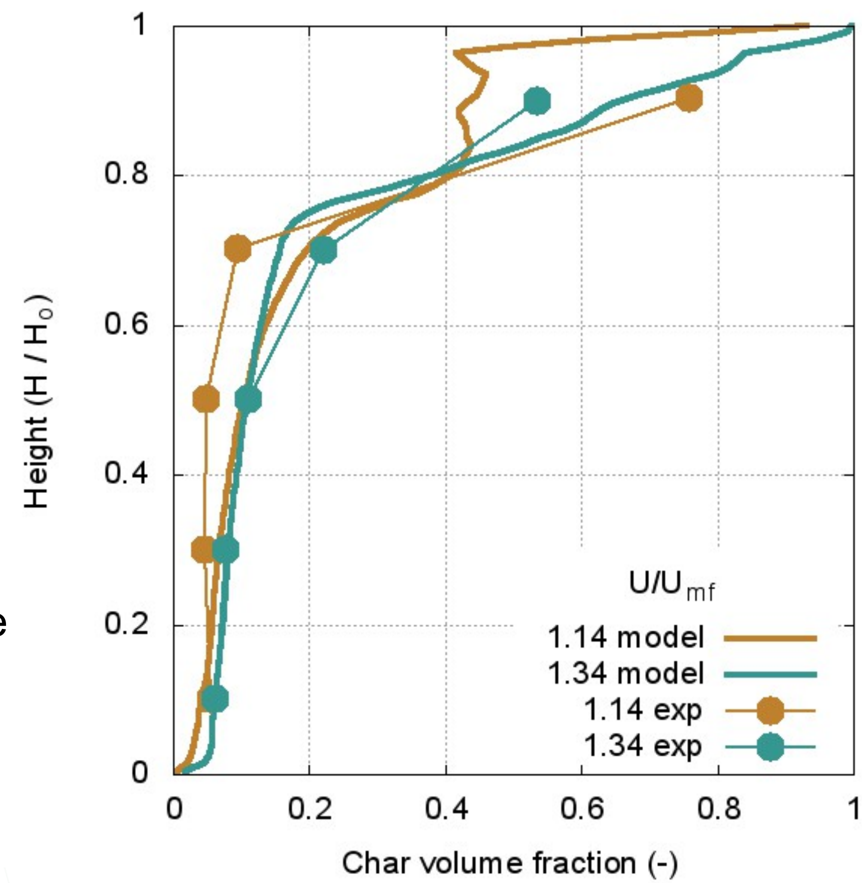
Mixing char/sand in fluidized bed



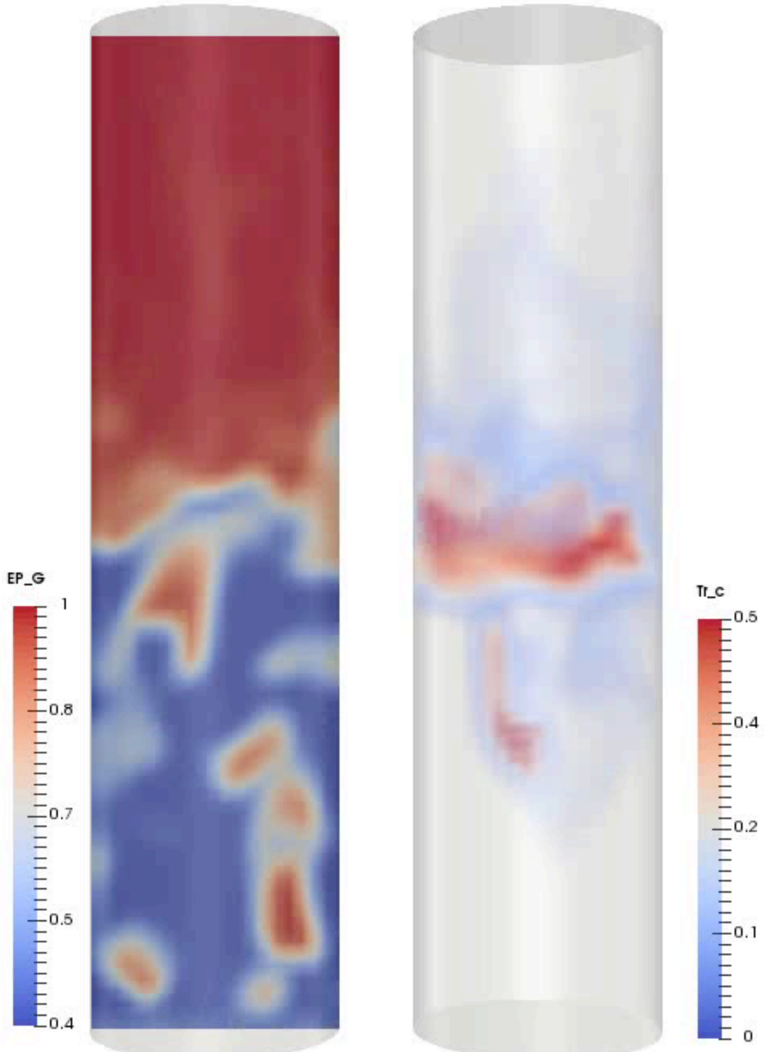
Axial slice of 3D bubbling bed simulation at 1.34 Umf

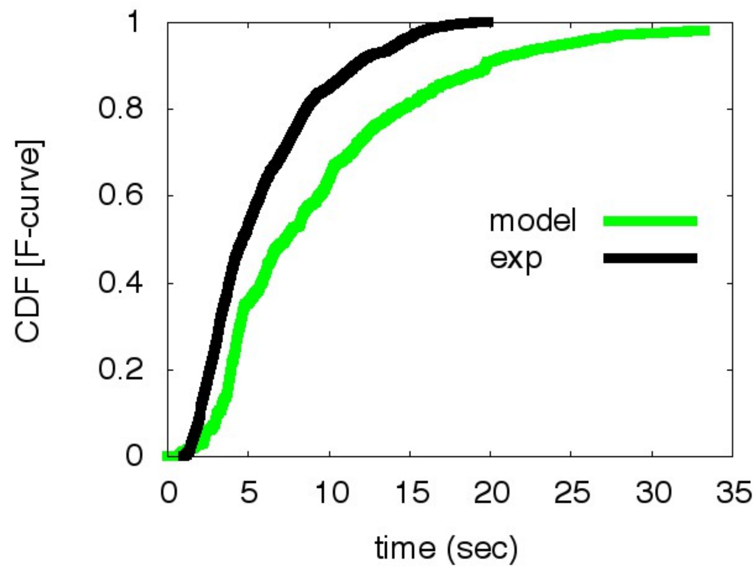
- Char/sand mixing increases with gas flow
- Char layer decreases with gas flow
- Bubbles move char in bed
- Char/gas residence time distribution can be acquired with simulated tracers

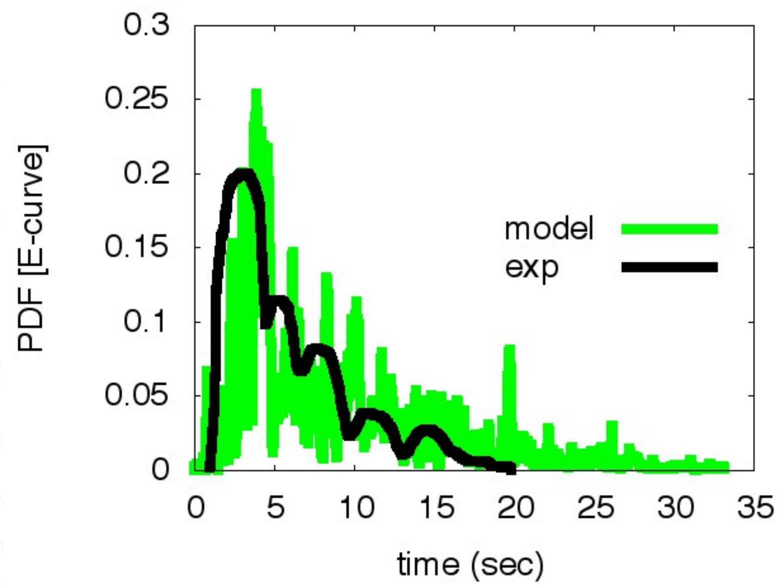


Comparison of simulation and experiment char mixing (Park and Choi 2013)

Initial Results: Char RTD



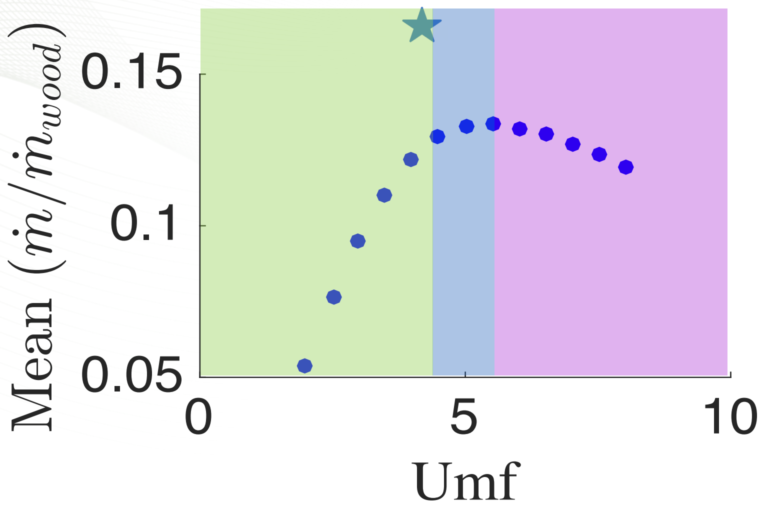




Computational study on biomass fast pyrolysis oil yield:
developing a predictive model which includes hydrodynamics of the bubbling-to-slugging transition in a laboratory-scale fluidized bed

Initial: Pyrolysis chemistry + CFD

Gas



Tar

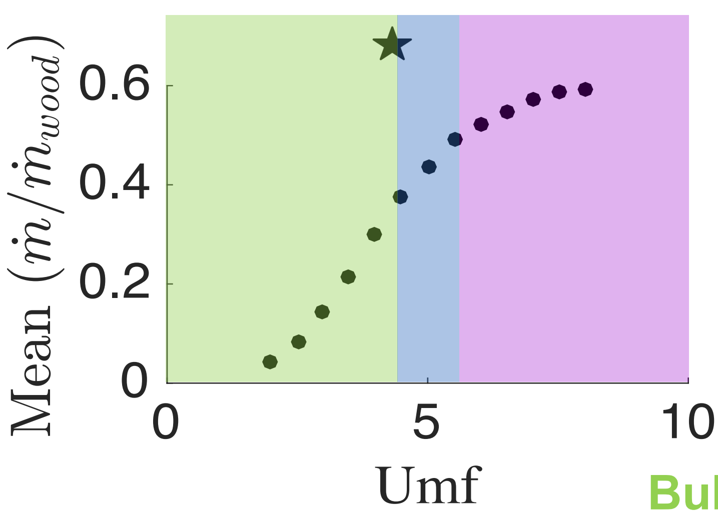


Table: Yield at ~4.4 U_{mf}

	Experiment	Simulation
Tar	0.661	0.377
Gas	0.162	0.129
Char	0.119	0.494

Mean yields did not match experiment

Uncertainty not accounted in results

Hydrodynamics affect kinetic yields in different bubbling regimes

Bubbling = 3.50 U_o/U_{mf}
Transition (BTST) = 5.00 U_o/U_{mf}
Slugging = 7.50 U_o/U_{mf}

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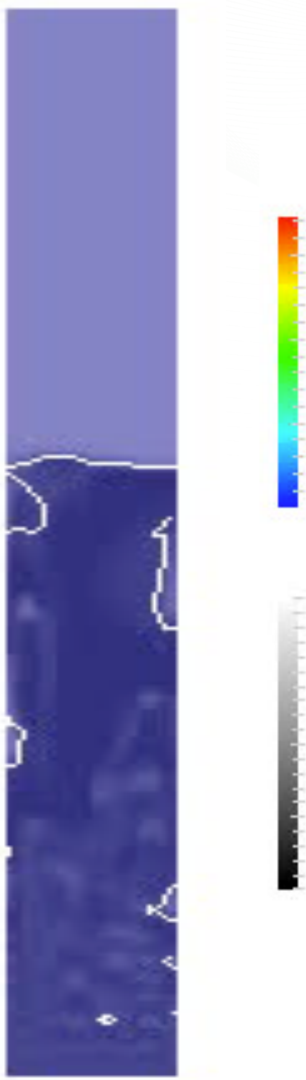
Ongoing: Pyrolysis chemistry + CFD



- Ongoing testing
  1. 2d constant density approach
  2. 2d variable density approach
  3. Comparison with low order models

Computational study on biomass fast pyrolysis oil yield:
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Concluding Remarks

- Results shown were cylindrical coordinate system
- Running equivalent simulations on Cartesian coordinate mesh
  - Mixing
  - Residence time distribution
  - Chemistry
- Next steps
  - Parametric sweep for mixing and residence time studies
  - Continue testing pyrolysis chemistry

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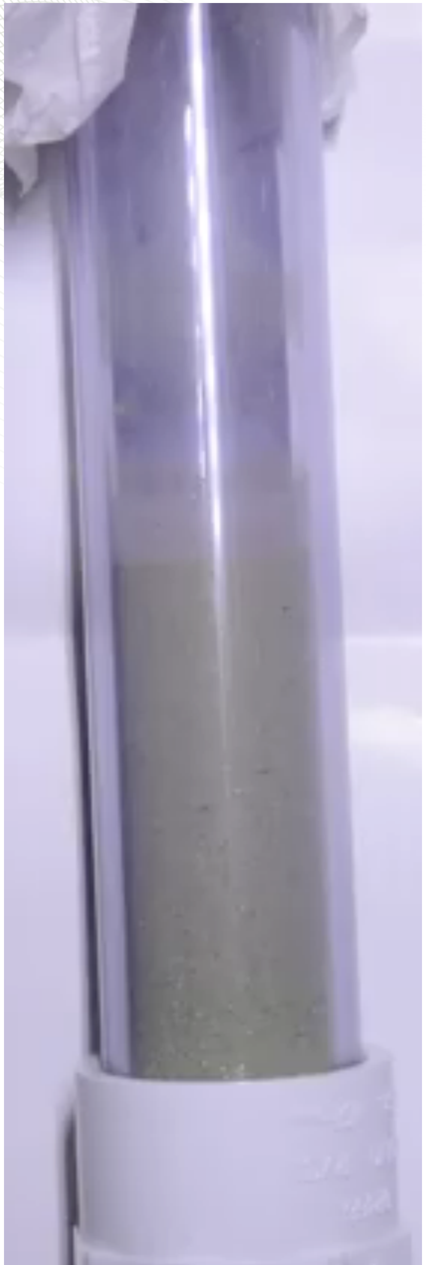

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