Computational study on biomass fast pyrolysis: Hydrodynamic effects on the performance of a laboratory-scale fluidized bed reactor

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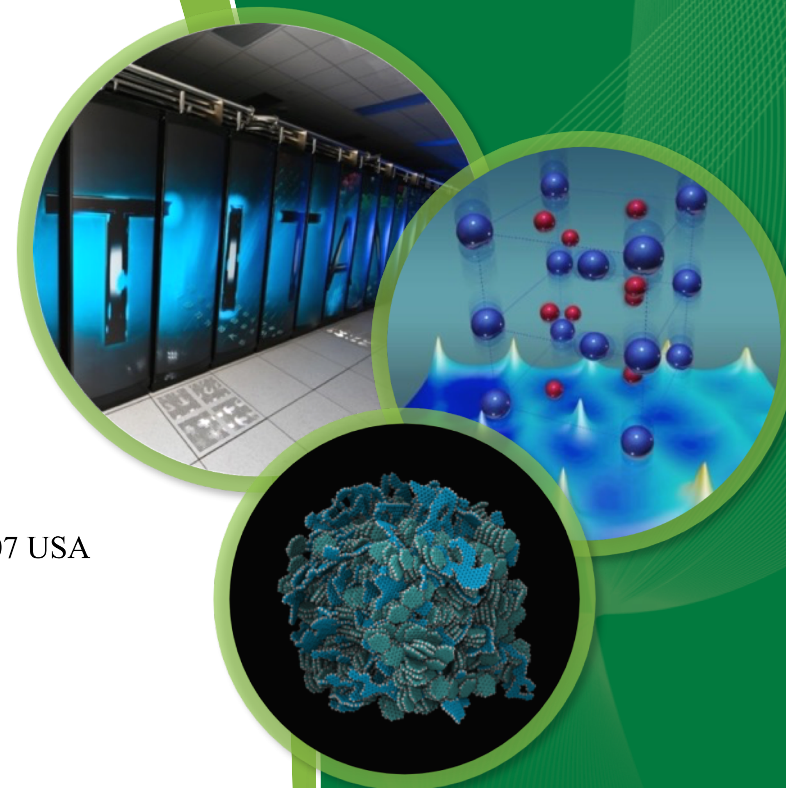

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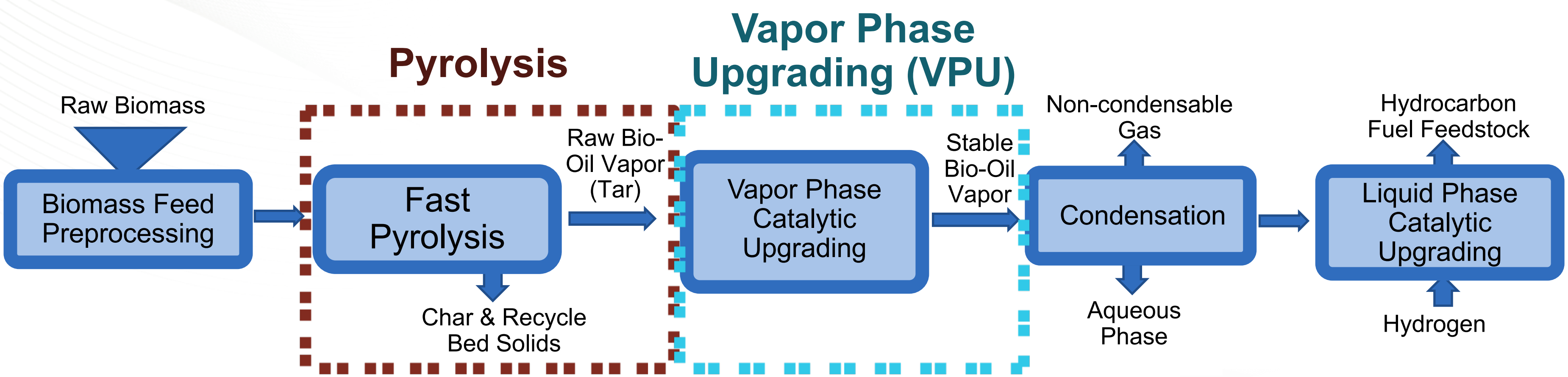
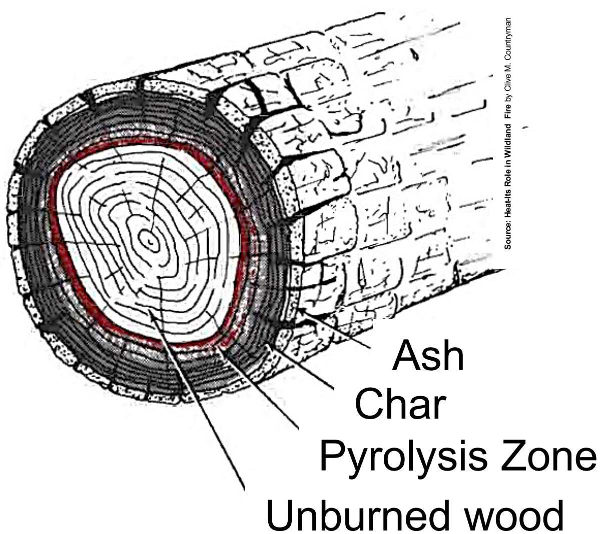
Background and Motivation (1)

Thermochemical conversion of biomass based on fast pyrolysis

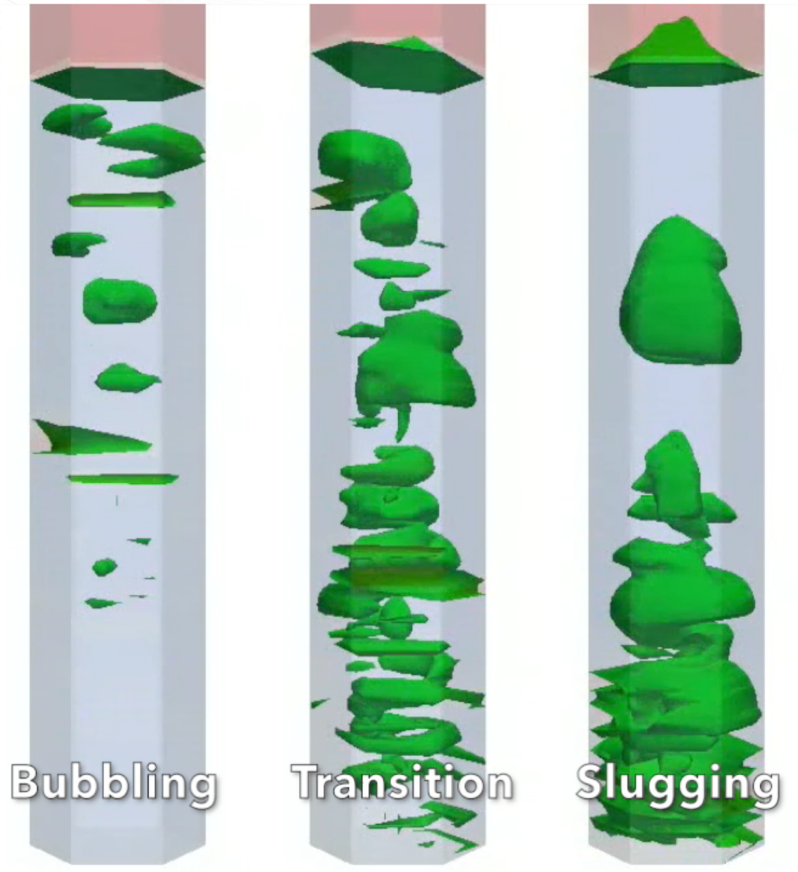




- **High yield and composition of raw oil are key, so commercial risk and economics depend on accurate performance predictions.**
- **Most available basic lab data are from bubbling fluidized bed reactors (FBRs).**
- **Good physics-based models are necessary for interpreting, scaling up lab experiments.**

Background and Motivation (2)

How should lab FBR data be interpreted/analyzed?



FB 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

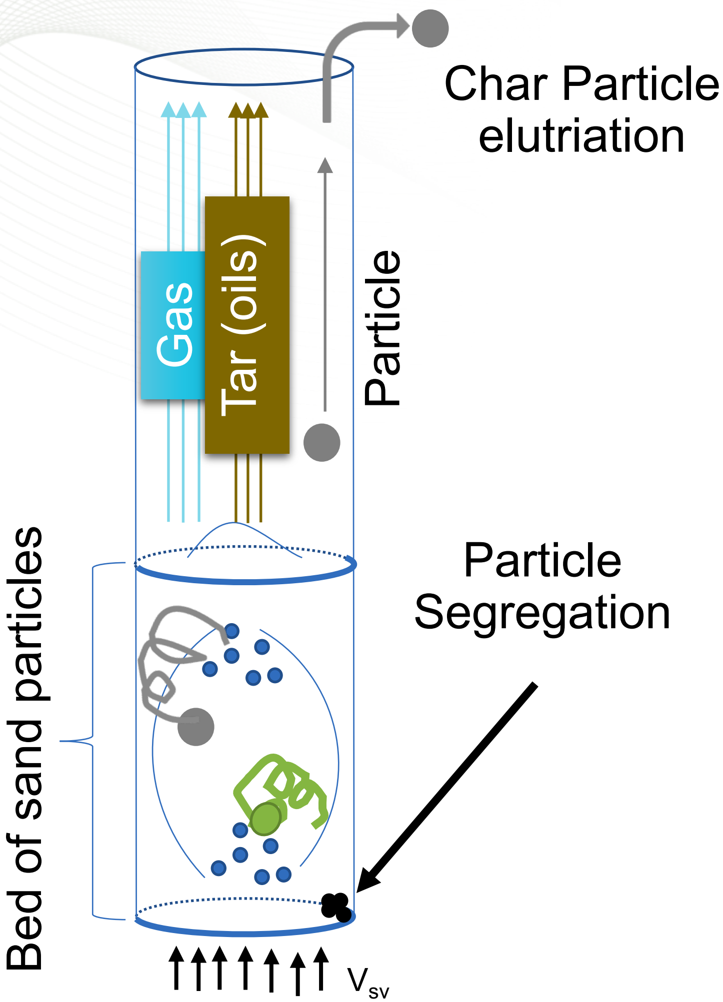
All the above significantly impact raw oil yield and composition.

Note: Bubble boundary depicted where void fraction > 0.65

E. Ramirez, C.E.A. Finney, S. Pannala, C.S. Daw, J. Halow, Q. Xiong, Computational study of the bubbling-to-slugging transition in a laboratory-scale fluidized bed, Chemical Engineering Journal 308 (2017) 544-556. http://dx.doi.org/10.1016/j.cej.2016.08.113

Approach (1): MFIX simulations of FBR pyrolysis

Pyrolysis reactor physics

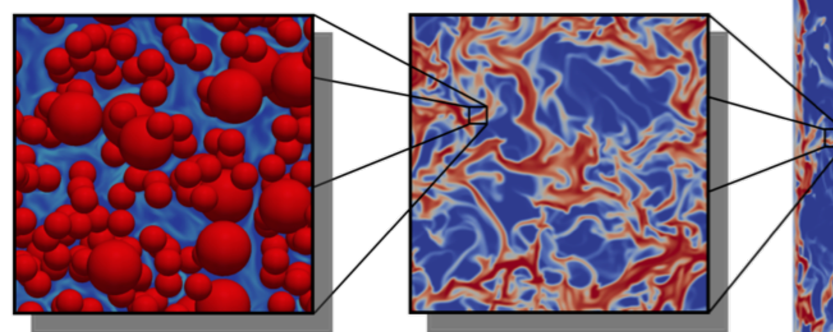


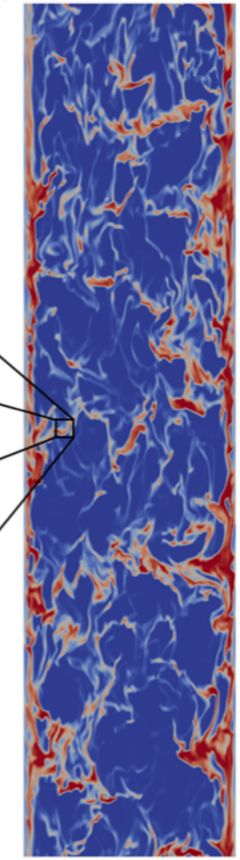
Two-Fluid CFD Model

CADES

ParaView Parallel Visualization Application

MFiX DEM MFiX TFM





- Eulerian-Eulerian
- Kinetic theory of granular flow
- 3D cylindrical mesh
- DLSODA ODEPACK chemistry solver
  - First order irreversible Arrhenius rates
  - Liden 1988 biomass pyrolysis kinetics

$$\text{wood} \xrightarrow{k1} \text{Tar} \xrightarrow{k3} \text{gas}$$

$$\text{wood} \xrightarrow{k2} \text{gas} + \text{char}$$

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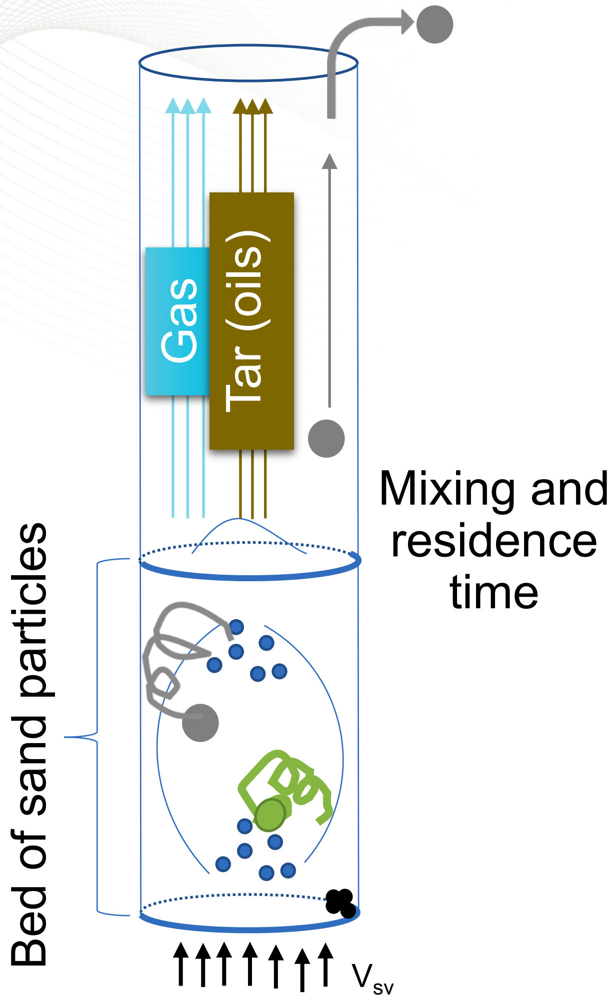
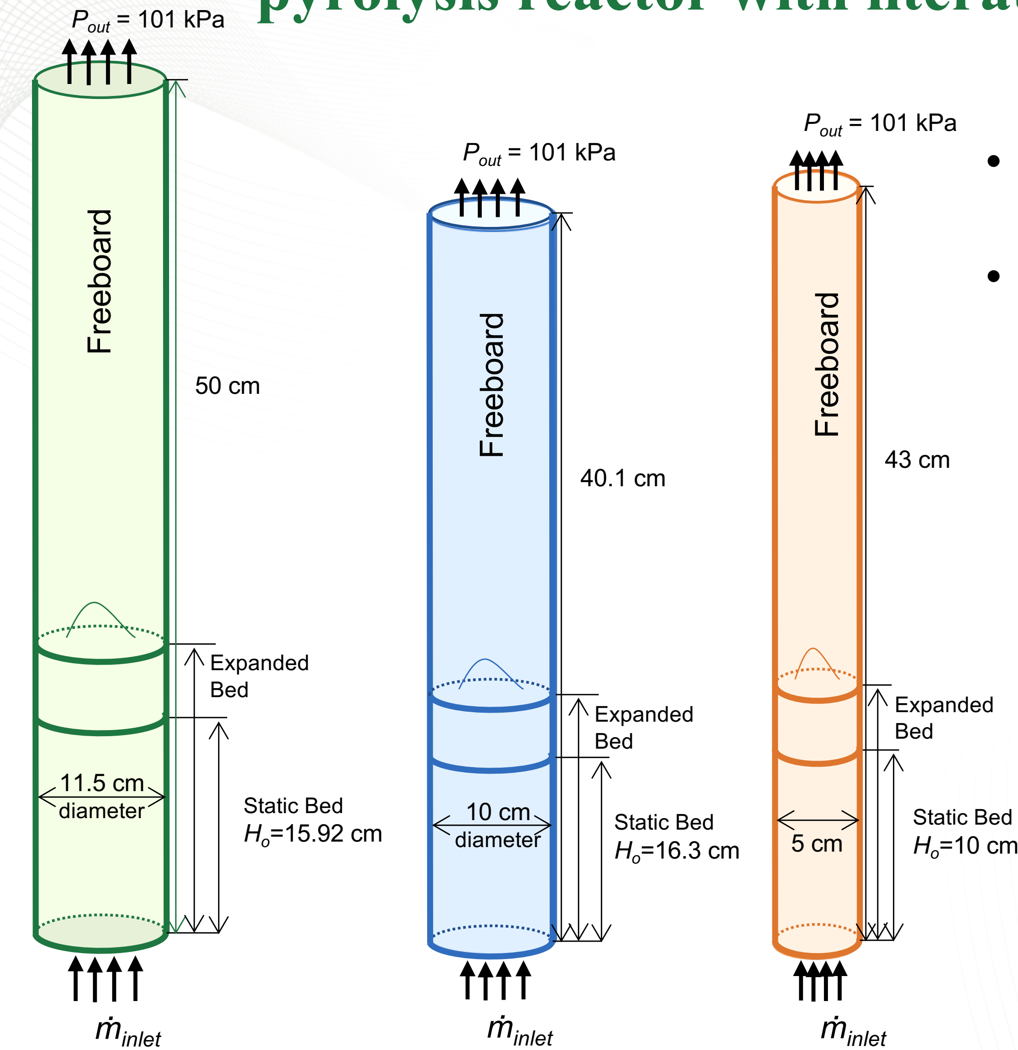
Approach (2):Interpret MFIX Results with Low-Order Models



Use simplified reactor models to 'compress' essential hydrodynamic information from MFIX and combine it with pyrolysis chemistry

- Quantify impact of bubbles and bed solids circulation on biomass solids and py vapor RTDs
- Identify major reaction/mixing zones needed to understand/approximate performance trends
- Relate solids and gas RTDs to predict trends for how biomass particle properties and reaction chemistry impact overall yields
- Utilize low-order models for rapid studies of operating/design parameter sweeps

Approach (3): Compare MFIX predictions for lab-scale FB pyrolysis reactor with literature and experiments



Mixing biomass char
Park and Choi 2013

RTD study
Berruti 1988

NREL Pyrolysis Experiment

- Target: Select NREL lab-scale pyrolysis experiment as typical lab-scale example
- Key steps:
  - Simulate expected particle and gas RTDs with MFIX including segregation and elutriation
  - Are MFIX mixing patterns consistent with the literature?
  - Can existing FB correlations capture MFIX predicted RTD trends?
  - When chemistry is added, do predicted bio-oil yields agree with experiments?
  - Are MFIX improvements needed?

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.

Approach (4): NREL lab pyrolyzer details

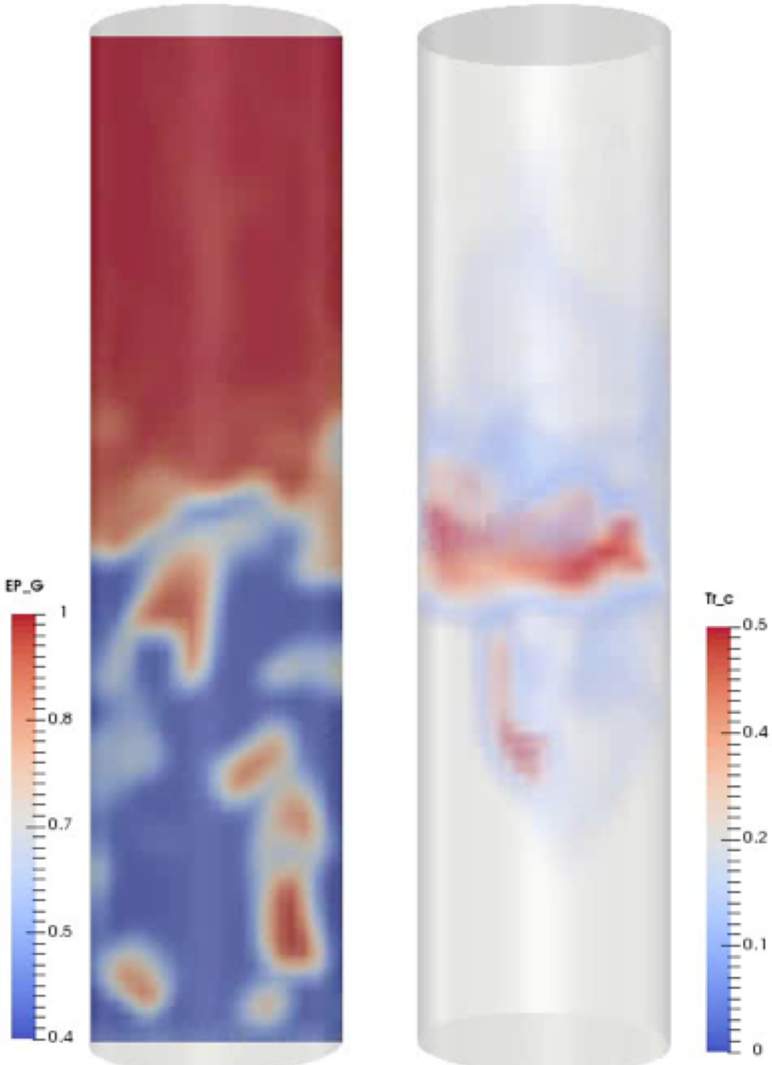
- Target: Fluidized bed particle studies used to verify model
- Key steps:
  - Reproduce exp. **particle residence time distribution (RTDs)**
  - Relate impact of char elutriation and mixing on RTDs
  - Reproduce impact of solids segregation on **mixing**

Property	Units	Mixing Study Park & Choi 2013	RTD Study Berruti 1988	NREL Exper.
Particle diameter (Sand)	m	387×10^{-6}	710×10^{-6}	500 × 10-6
Particle density (Sand)	kg/m^3	2383	2470	2500
Particle diameter (Styrofoam/char)	m	957×10^{-6}	450×10^{-6}	278×10^{-6}
Particle density(styrofoam)	kg/m^3	-	82	-
Particle density(Char)	kg/m^3	391	-	80
Temperature	K	300	300	773
Pressure (inlet)	kPa	101	101	133
Fluidizing N_2 (range)	m/s	0.14 - 0.19	0.554	0.13 - 0.47
Minimum fluidization	m/s	0.14	0.30	0.0565
Coefficient of restitution	-	0.9	0.9	0.9
Angle of repose	°	30	30	30
Friction coefficient	-	0.1	0.1	0.1

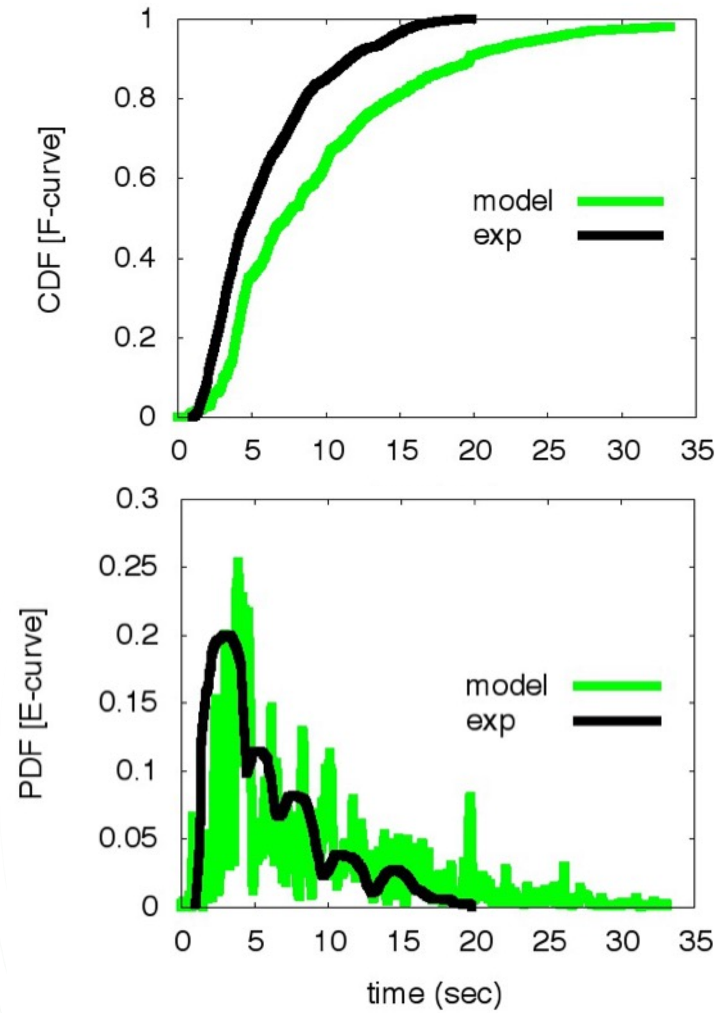
H.C. Park, H.S. Choi, The segregation characteristics of char in a fluidized bed with varying column shapes, Powder Technology 246 (2013) 561-571.

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.

Preliminary MFIX Results(1): Biomass Particle RTD

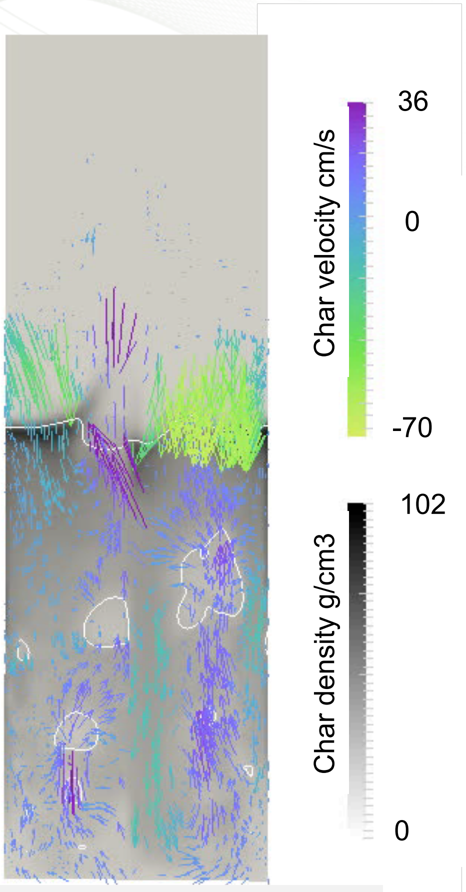


Axial slice of 3D bubbling bed simulation
Residence time distribution (RTD) study



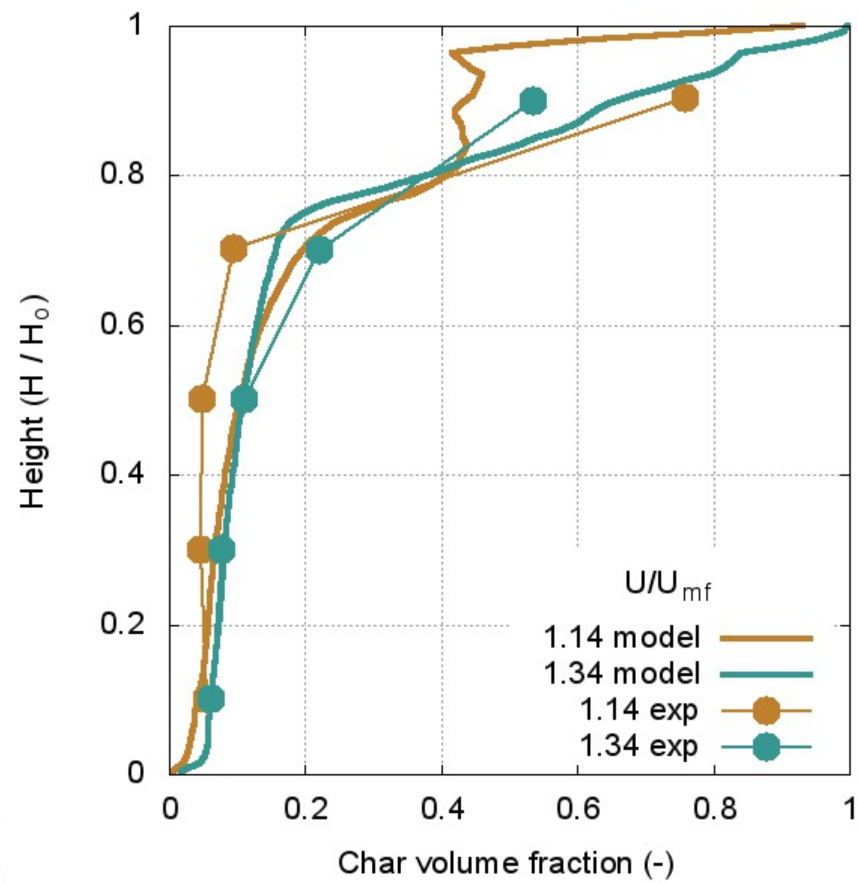
Comparison of simulation and experiment RTD (Berruti 1988)

Preliminary MFIX Results(2): Biomass Particle Segregation



Axial slice of 3D bubbling bed simulation at 1.34 U_{mf}

- Bubbles are the main mixing mechanism
- More bubbles, more char/sand mixing
- Char layer decreases with gas flow
- Simulated tracers track char/gas mixing and RTD's

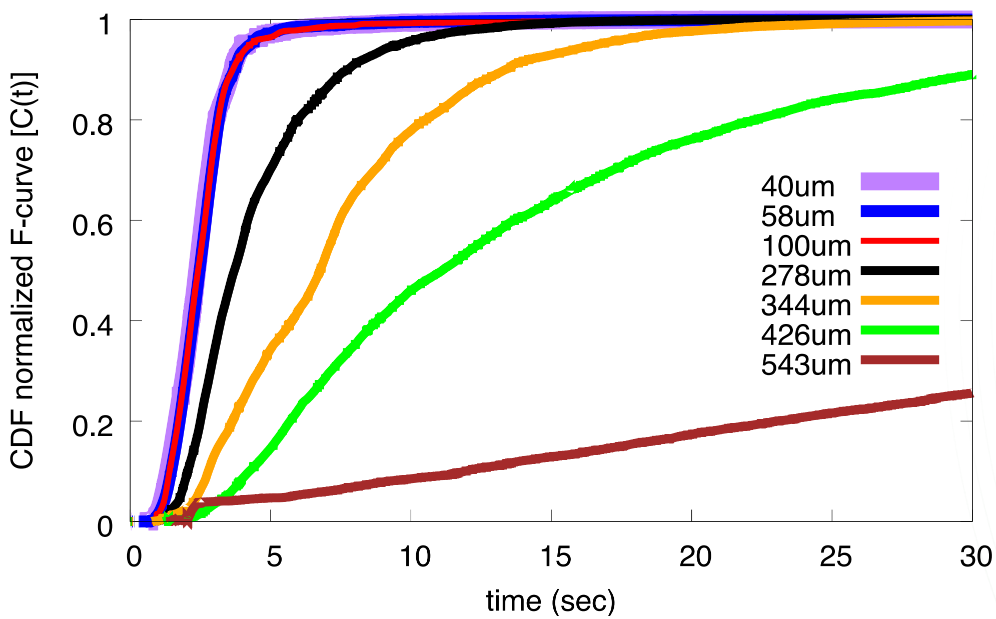


Comparison of simulation and experiment char mixing (Park and Choi 2013)

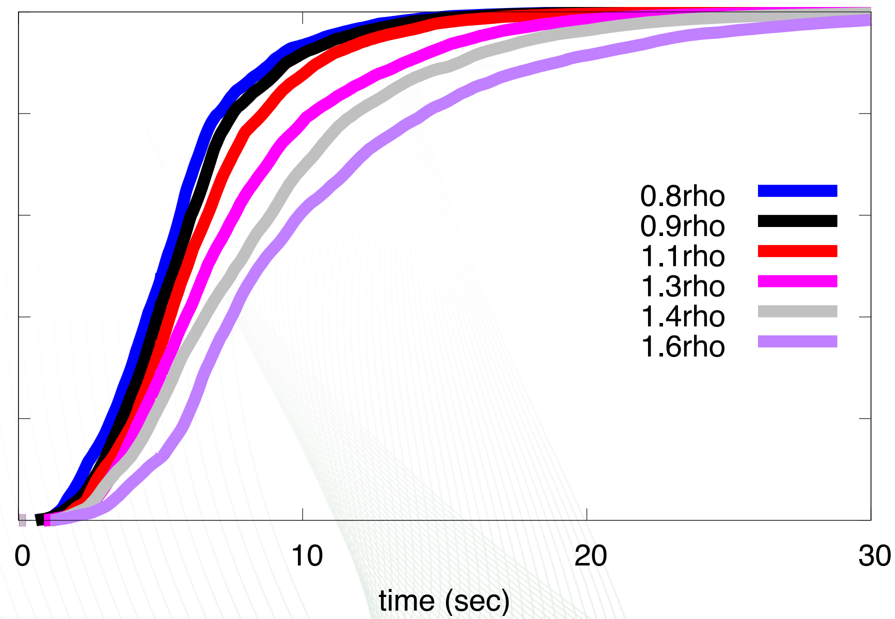
Preliminary MFIX Results (3): Biomass Particle Elutriation

Particle size and density must be selected carefully such that elutriation will occur

Biomass particle size



Biomass particle density



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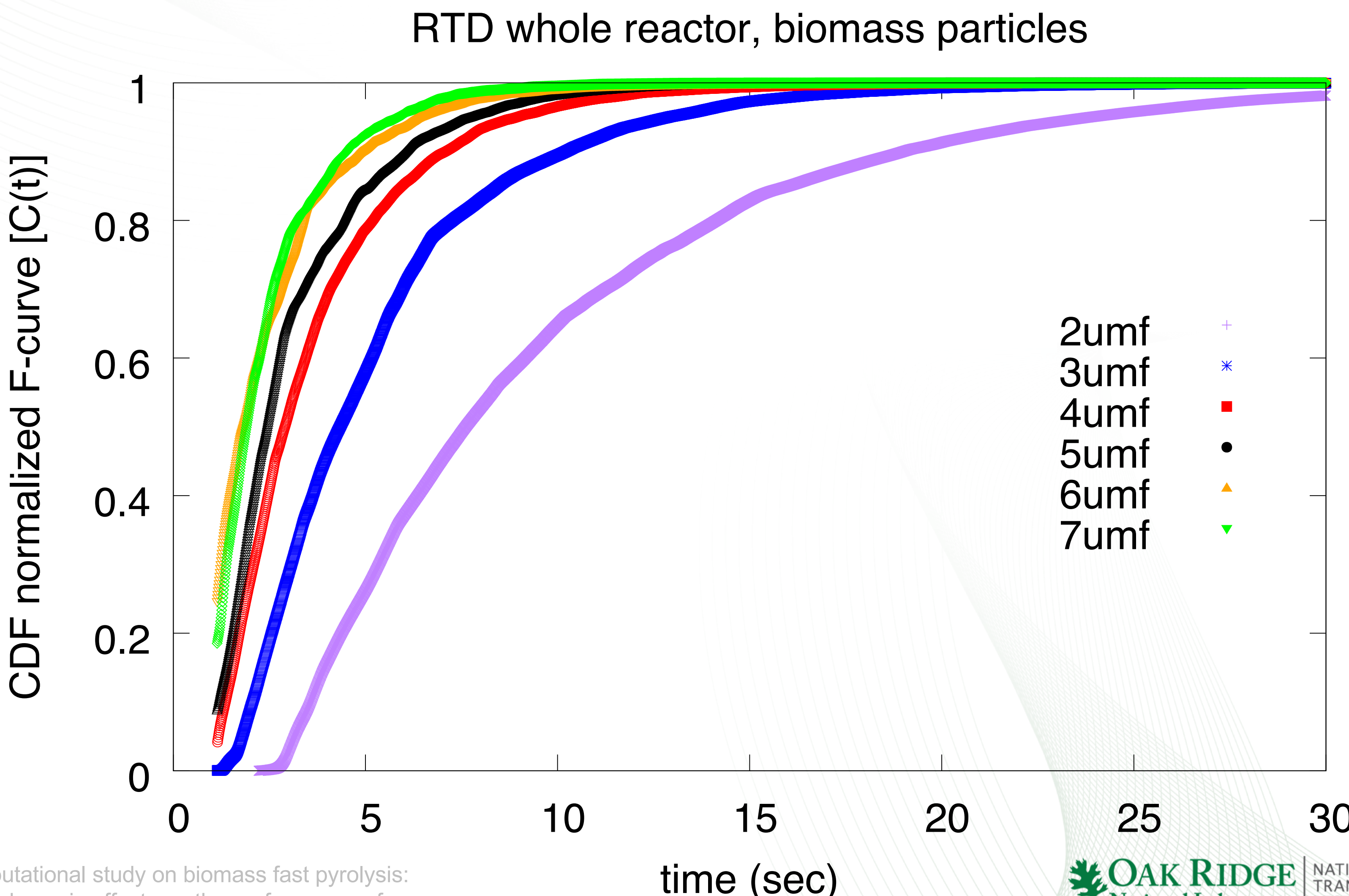
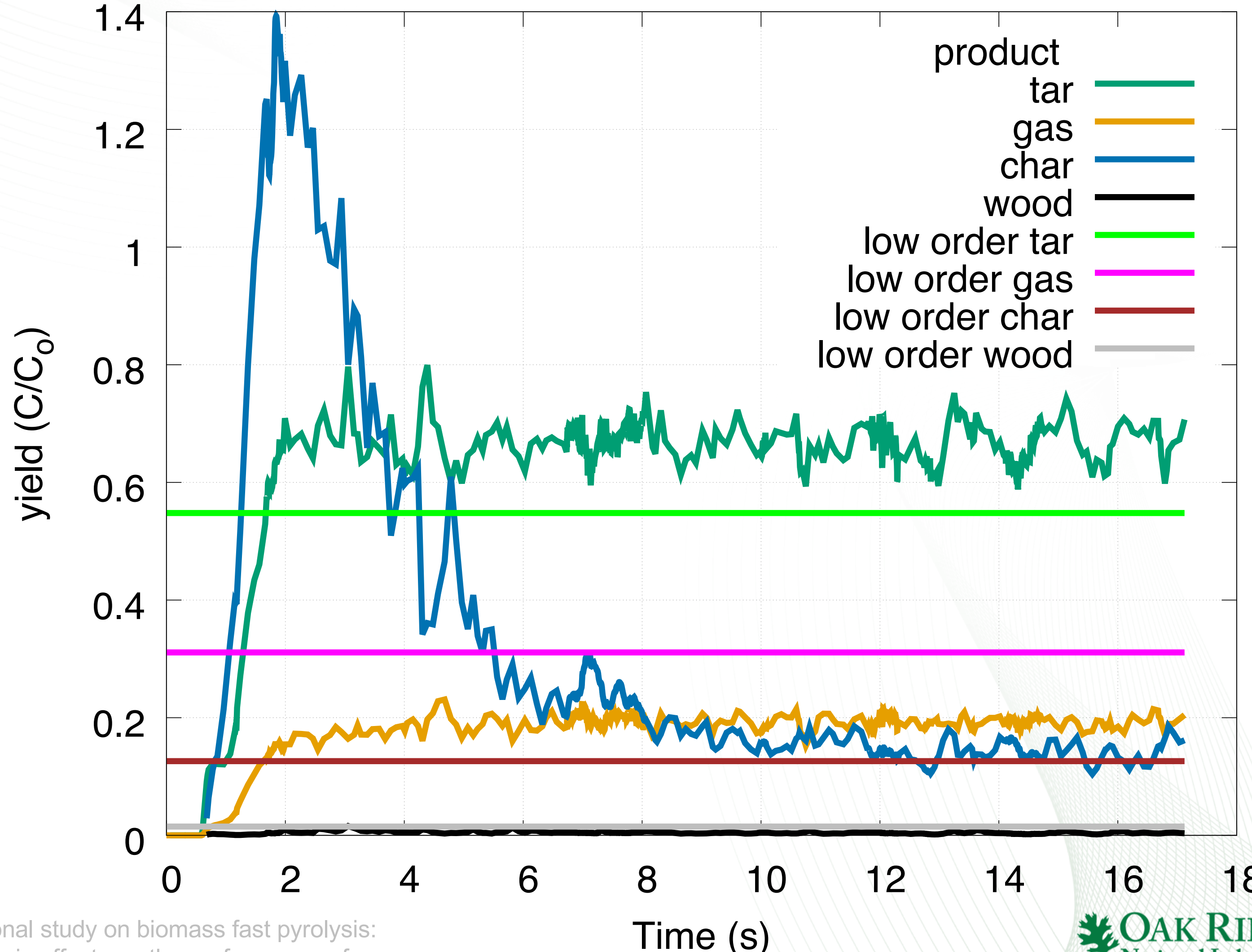
Preliminary MFIX Results (4): Biomass Particle Elutriation

As inlet gas flow increases, biomass particle RTD converges to a limit



Preliminary MFIX Results (5): Yield Convergence with Chemistry

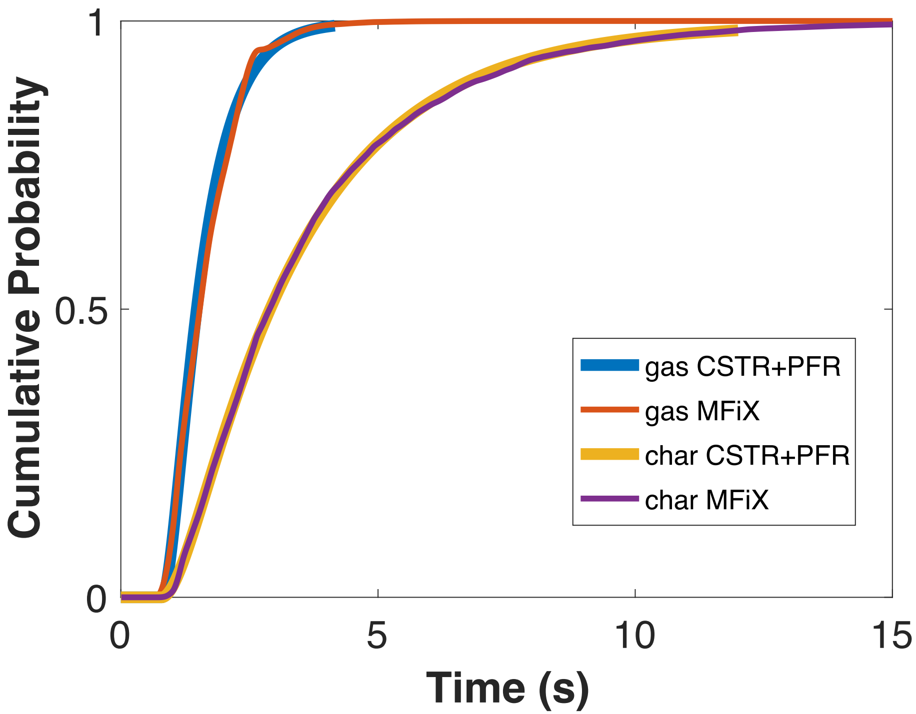
Liden lumped kinetics in MFiX reactor and low order reactor model predict tar experiment yields

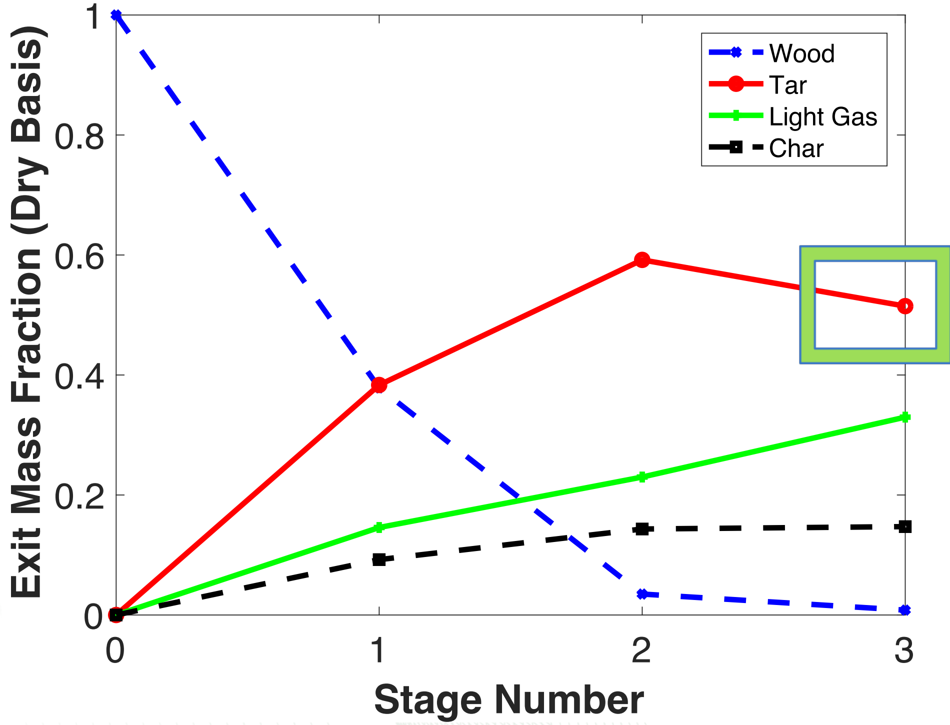


Preliminary Low-Order Results: Chemistry + MFiX Hydrodynamics (Possible 'Hybrid' Modeling Approach)

1. Use MFiX gas and biomass RTDs to create zone reactor model approximation

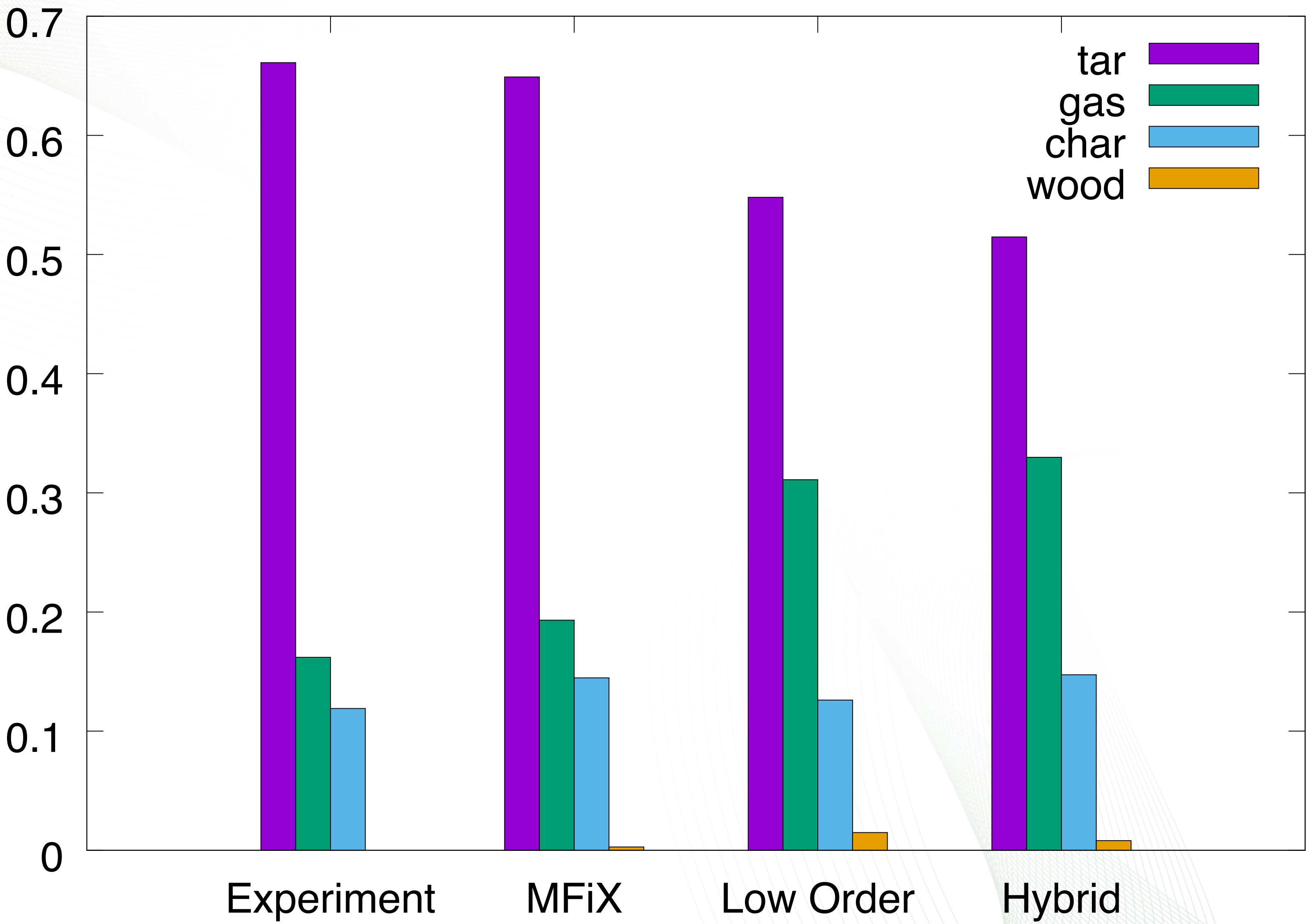
2. Use zone model + Liden kinetics to predict yields





E. Ramirez, Tingwen Li, Mehrdad Shahnam, C. Stuart Daw, Computational study on biomass fast pyrolysis: Hydrodynamic effects on the performance of a laboratory-scale fluidized bed reactor, **Manuscript in preparation**.

How do the models compare with experimental data?



Concluding remarks

- Quantifying the combined effects of hydrodynamics and chemistry is essential in utilizing lab-scale biomass pyrolysis reactor data for scale up
- Biomass particle properties and fluidization intensity have major impacts on product yields
- A key question remains: Is there a single combination of biomass feed particle size and fluidization intensity where tar yield is maximized?
- Two-fluid codes like MFIX can yield useful details about pyrolyzer hydrodynamics and gas and solid RTDs but improvements to the physics are still needed
- Combining MFIX hydrodynamics with low-order chemistry models appears to offer potential benefits

Acknowledgements

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