CFD Modeling of KiOR's Proprietary CFP Reactors Using Barracuda™

NETL Multiphase Workshop 2019
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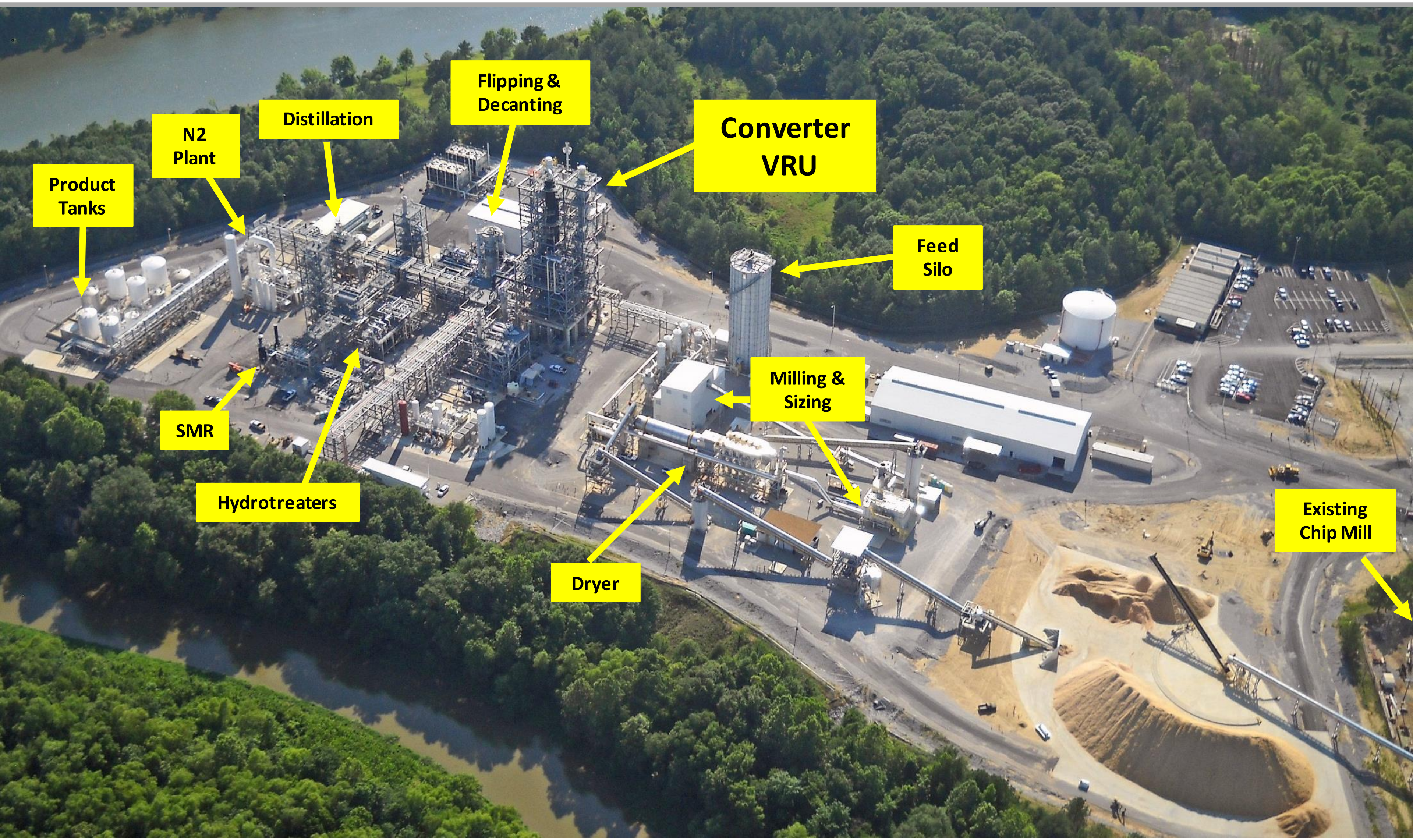
***Formerly KiOR/Inaeris, Currently at ORNL**

Columbus Plant: 500 T/day Biomass



5 Quarters, ~1,000,000 Gallons

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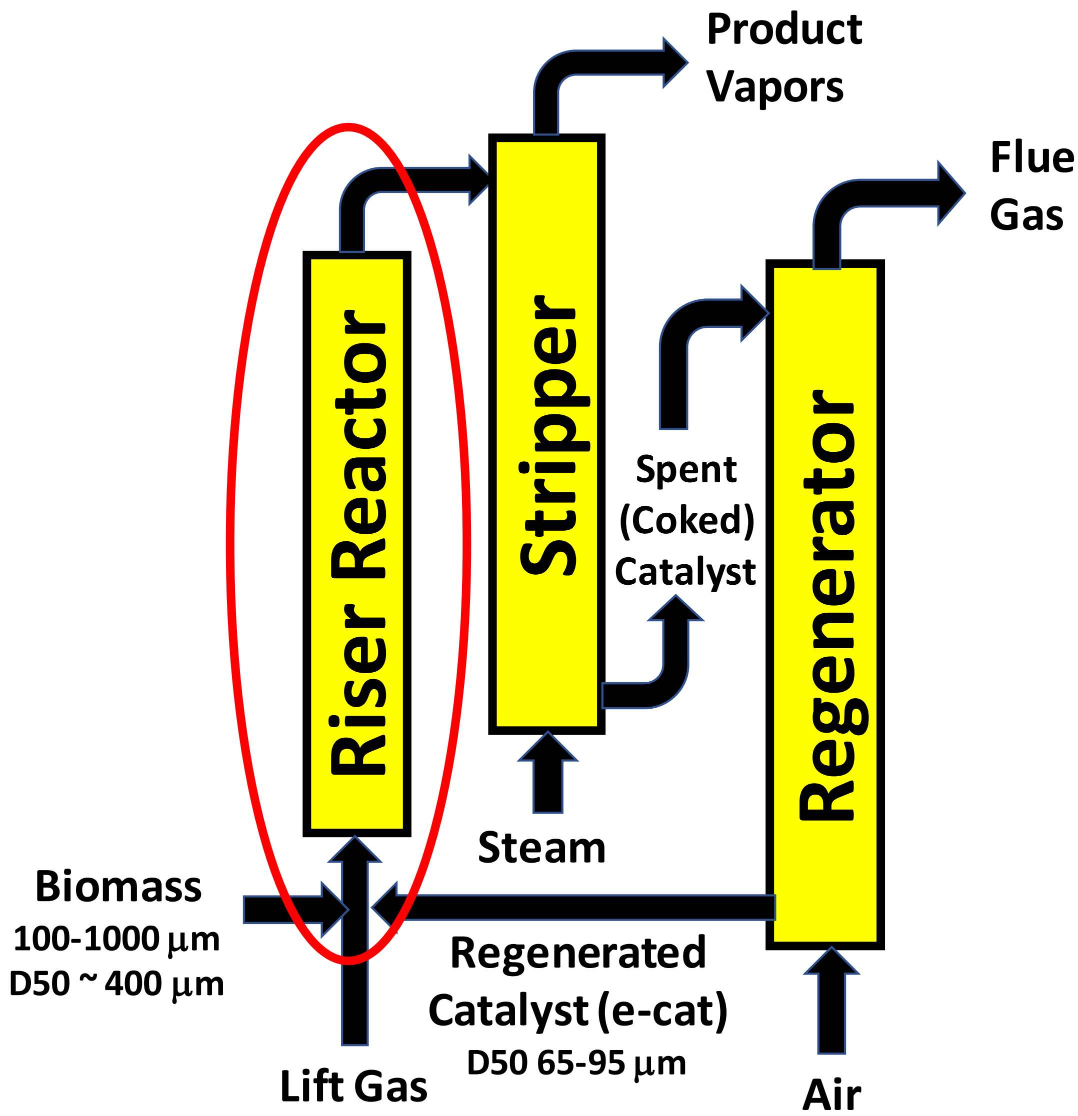
KiOR's *in-Situ* CFP Process is Based on FCC



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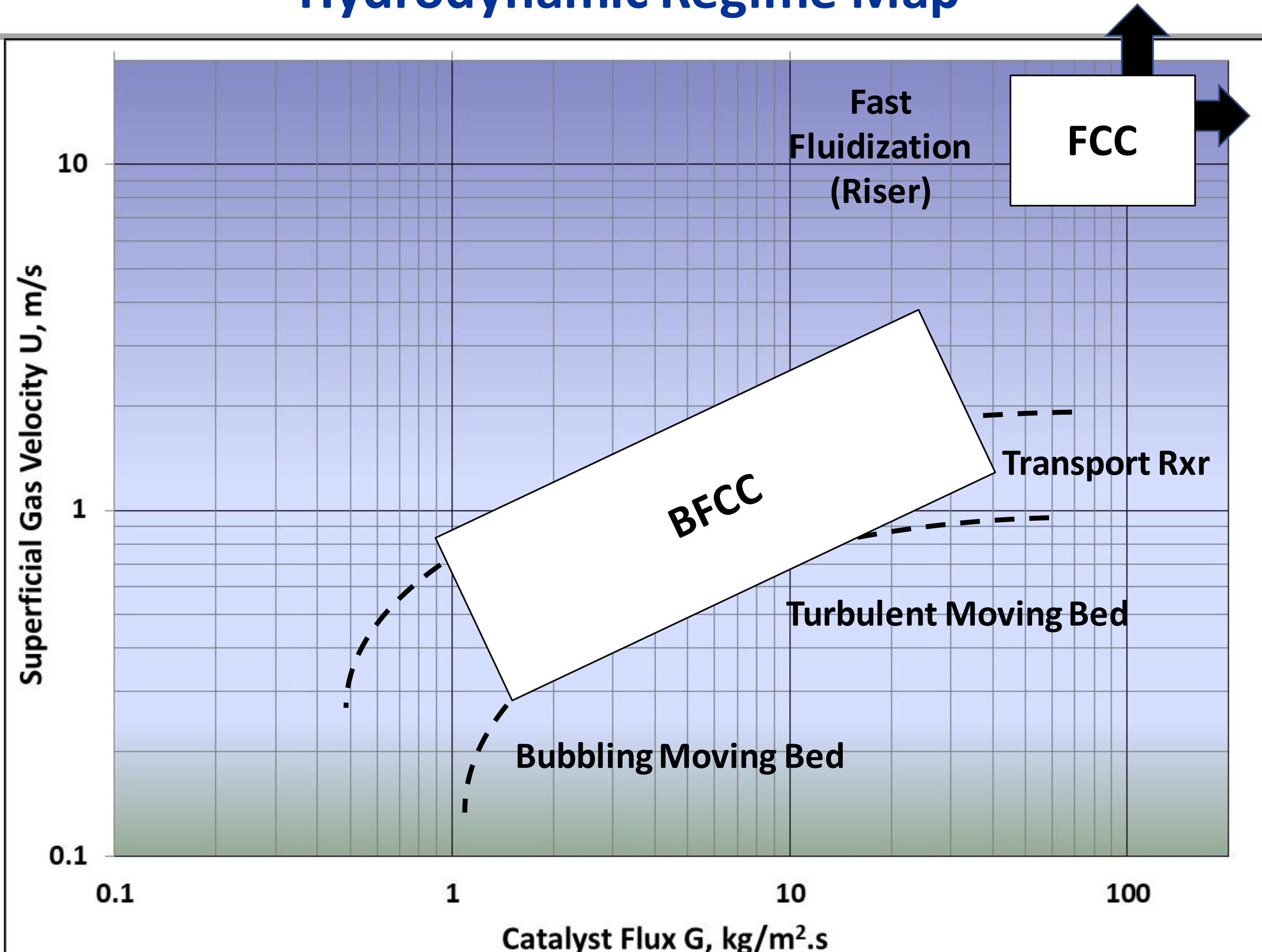
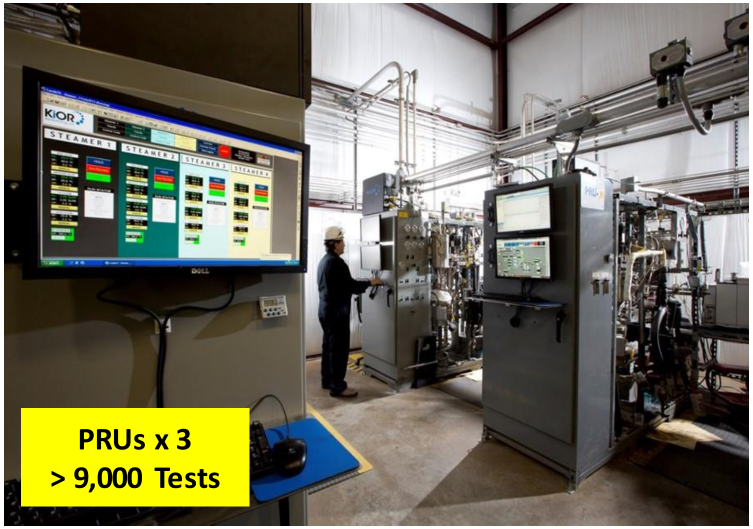
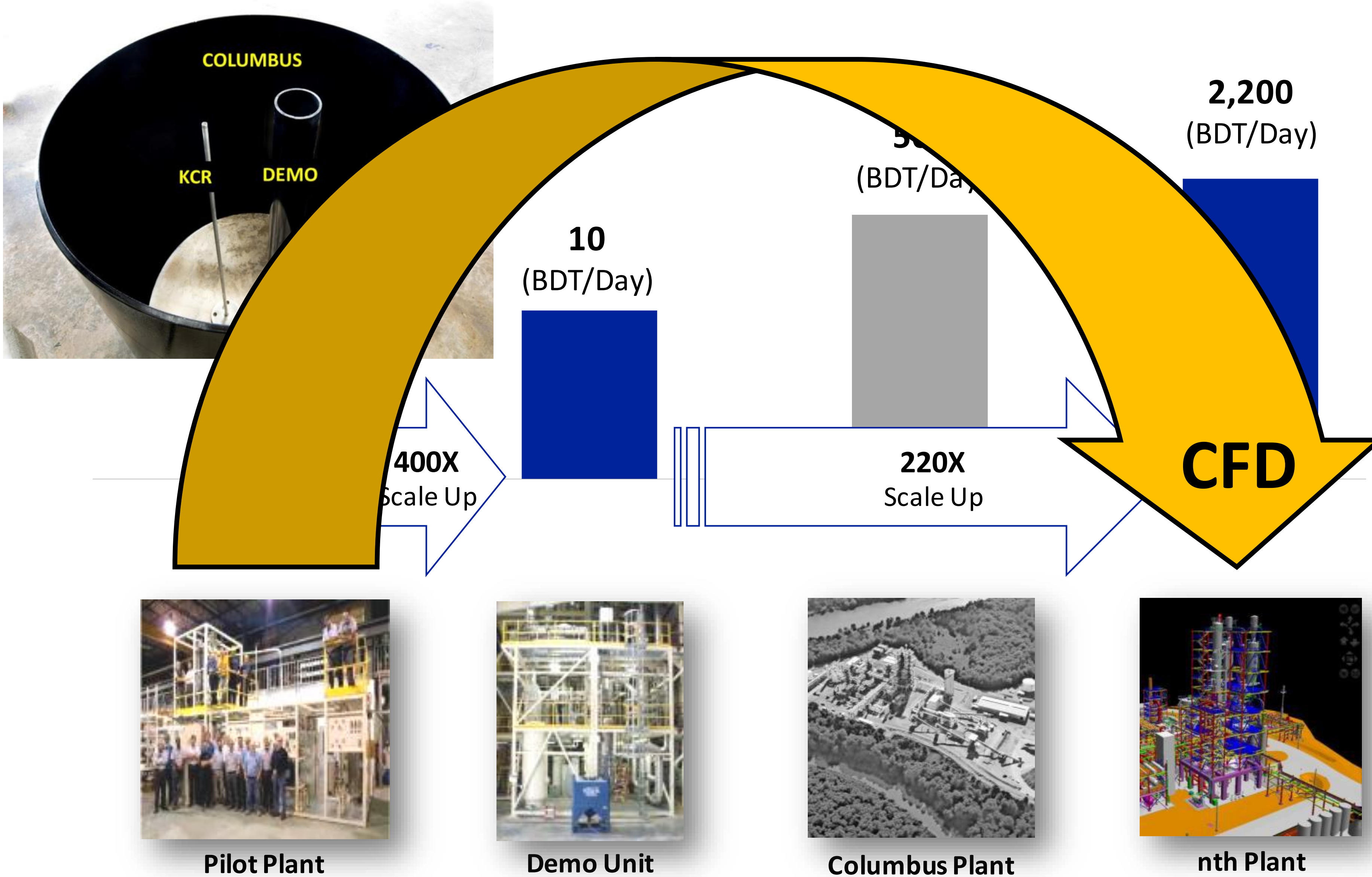
Hydrodynamic Regime Map



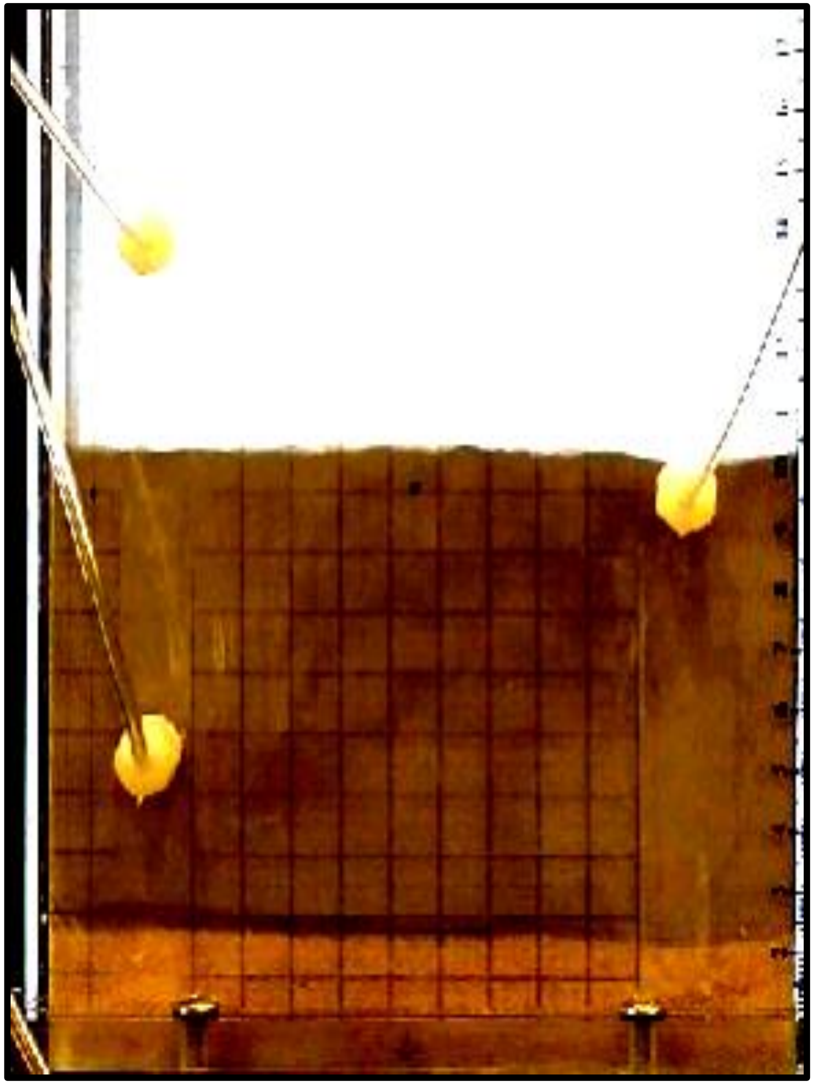
KiOR's Test Units

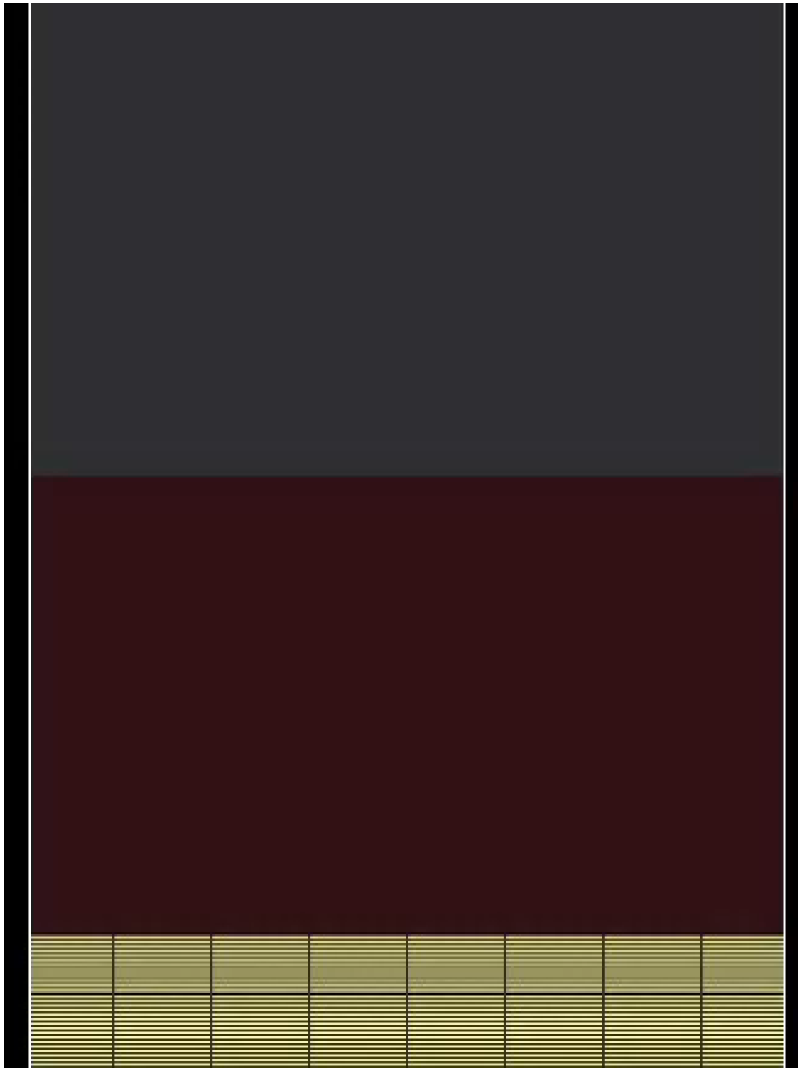


Scaleup Path



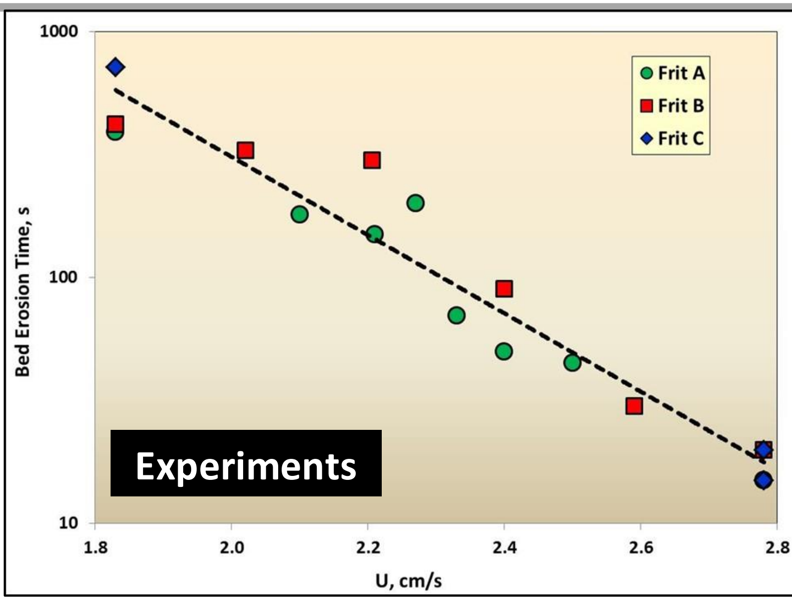
Mix Chamber Part 1



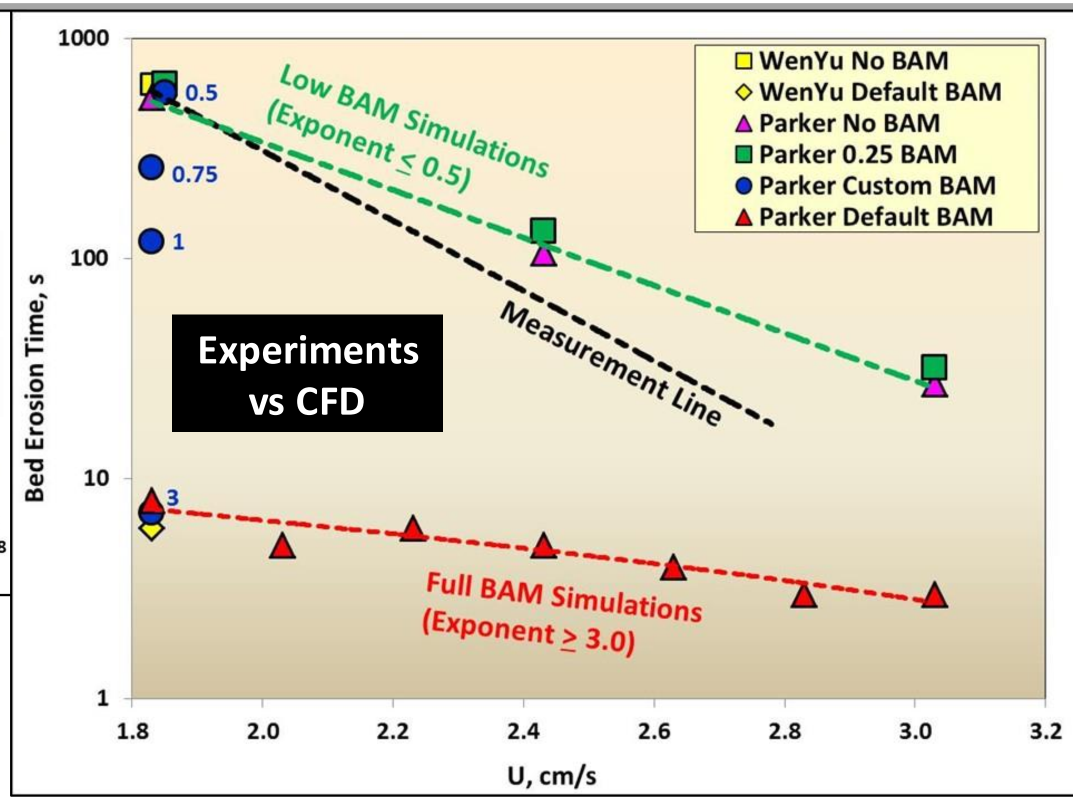


U = 2.8 cm/s

Mix Chamber Part 1



Two orders of magnitude reduction in erosion time, with less than doubling of velocity!



Set the baseline drag model (Parker-2) and Blended Acceleration Model (BAM) exponent

B. Adkins, N. Kapur, J. Parker, P. Blaser, J. Prendergrass, "KiOR Update: Incorporating Barracuda® in Our Development Process"

- **Barracuda Users Conference, Oct 2015**
- **AIChE Annual Meeting, Nov 2015**
- **tcBiomass, Nov 2015**

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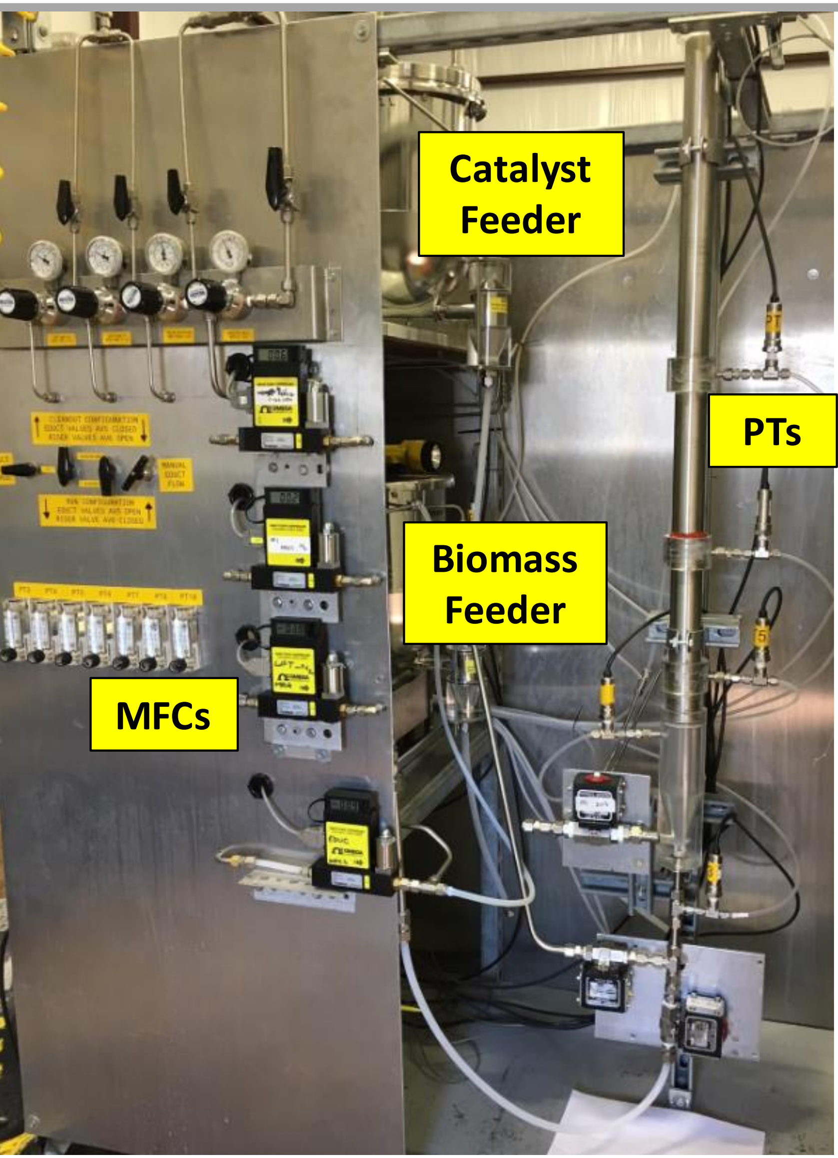
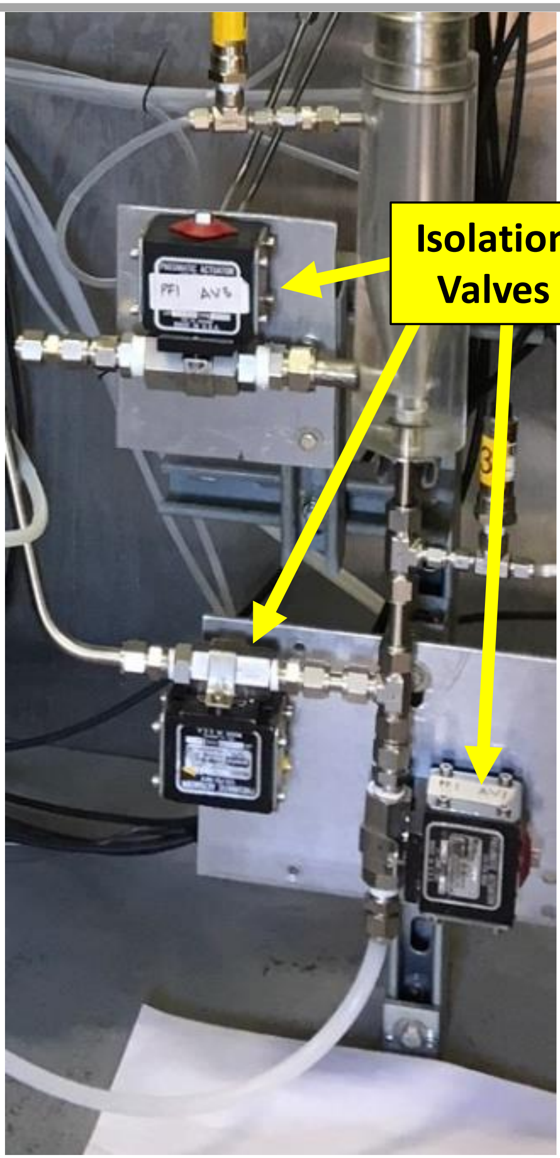
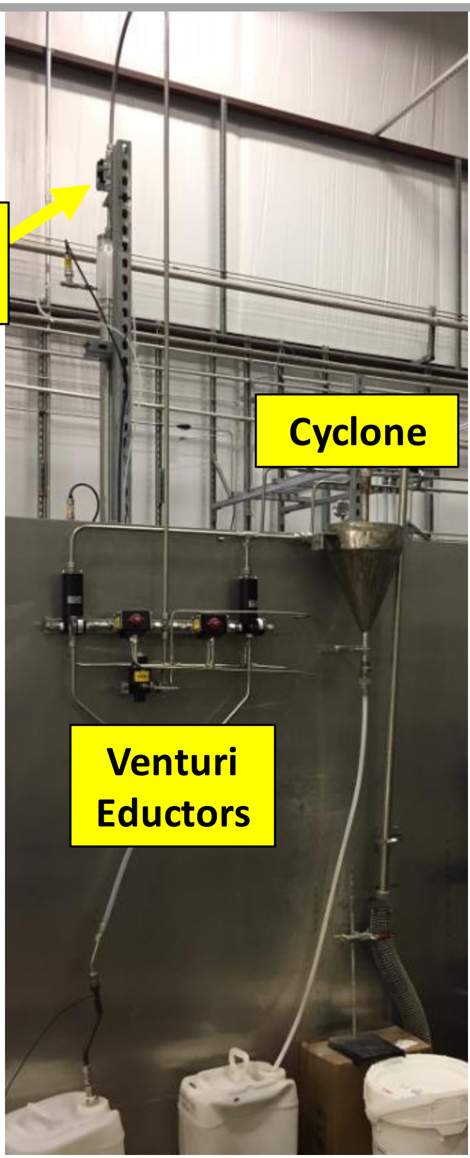
Cold Flow Unit for Producing KCR-Scale CFD Validation Data







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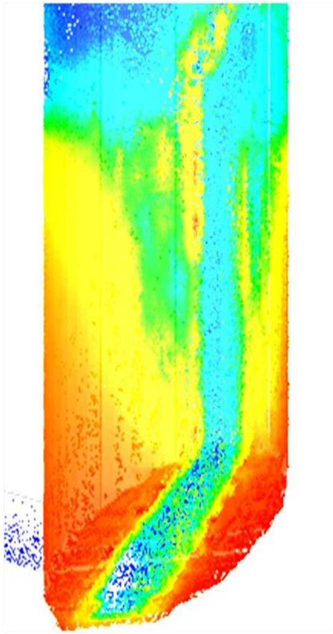
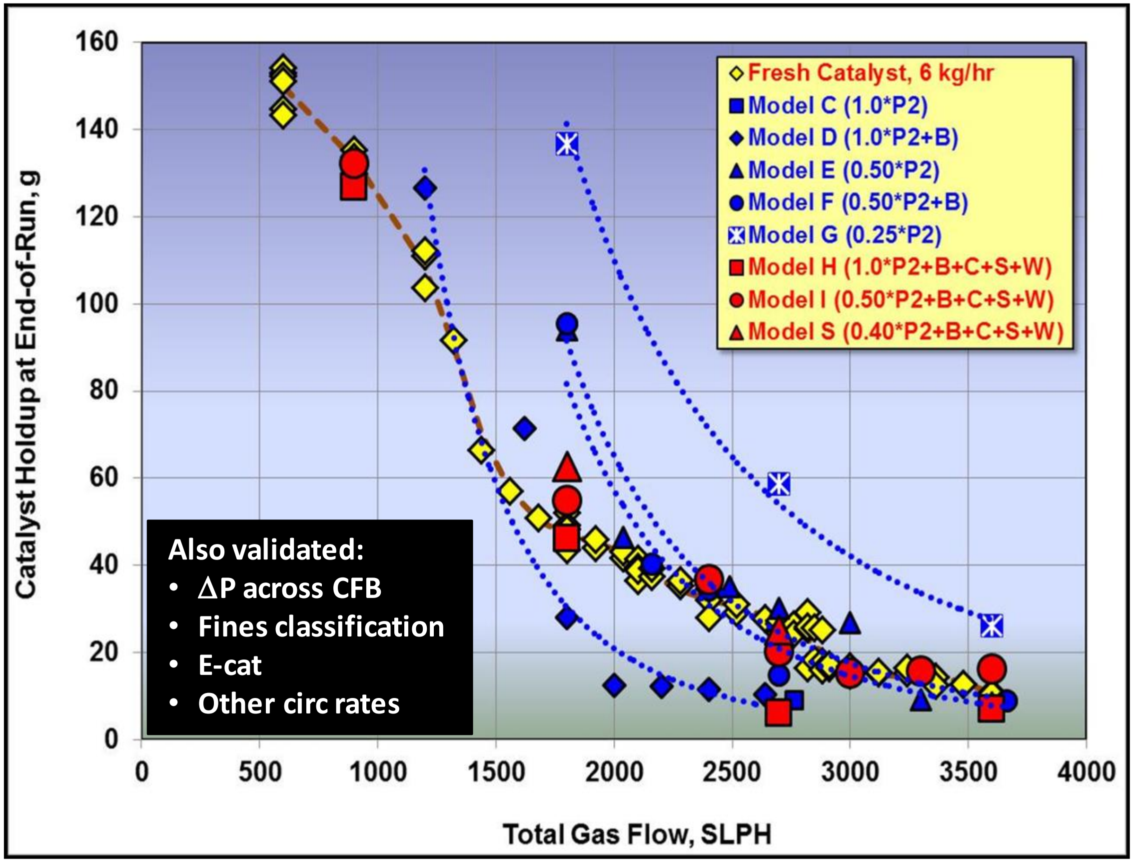
Mix Chamber Part 2: Side Jetted CFB

Jetted-BED CFB Experiments vs CFD





B. Adkins, N. Kapur, T. Dudley, S. Webb, P. Blaser, "Experimental Validation of CFD Hydrodynamic Models for Catalytic Fast Pyrolysis"

- Fluidization XV, May 2016
- Powder Technology v.316 (2017) 725-739

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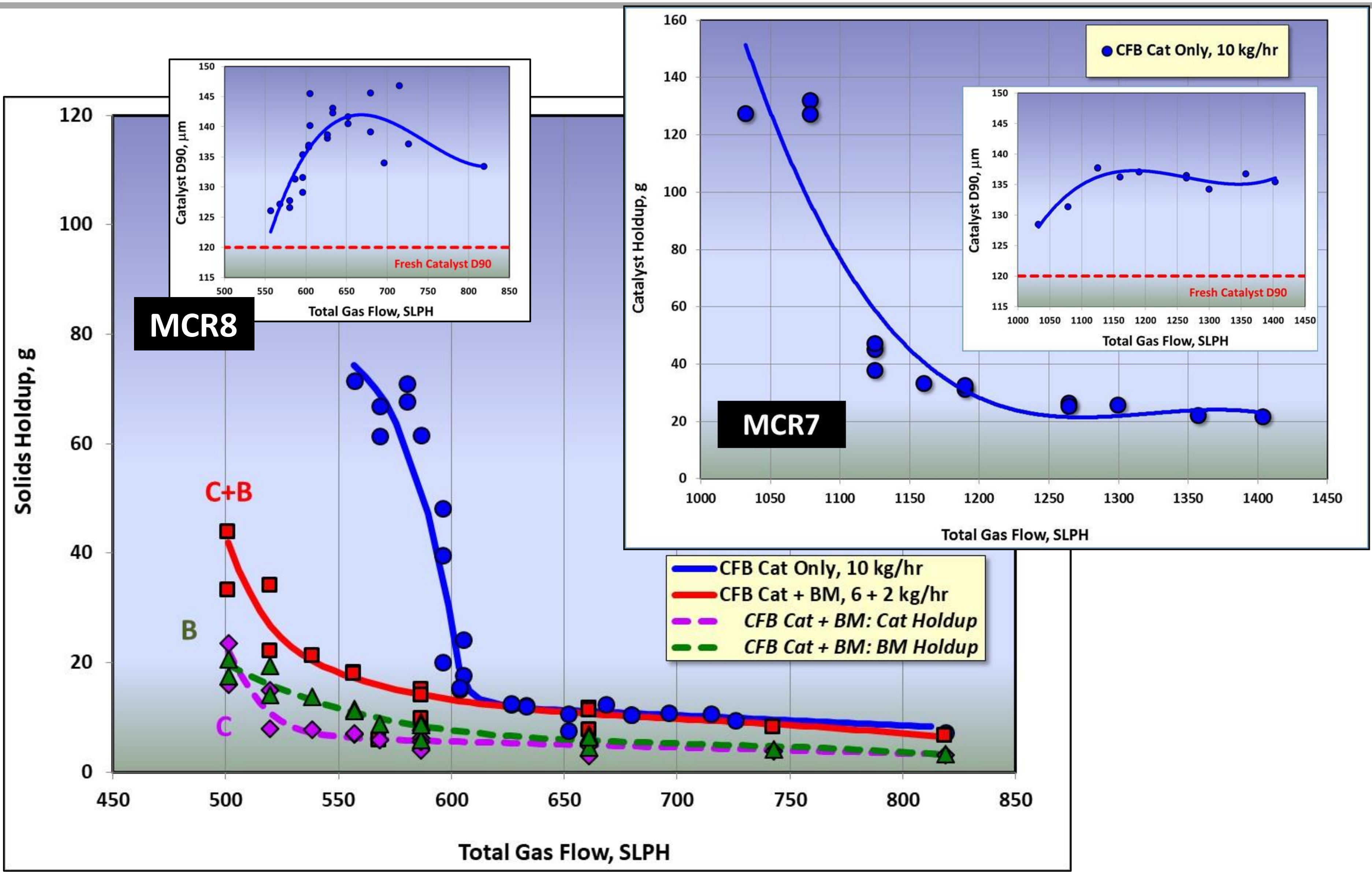
Mix Chamber – Riser (MCR) Experimental Data



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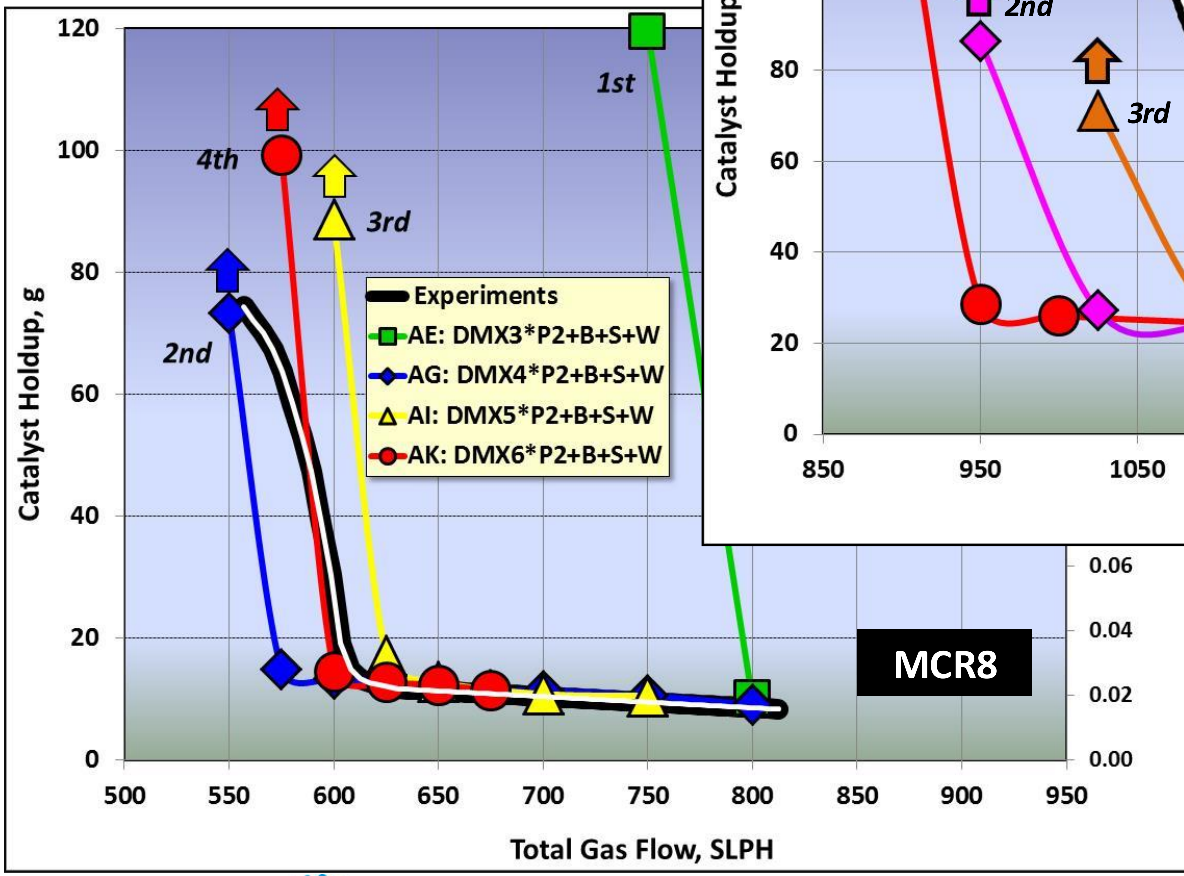
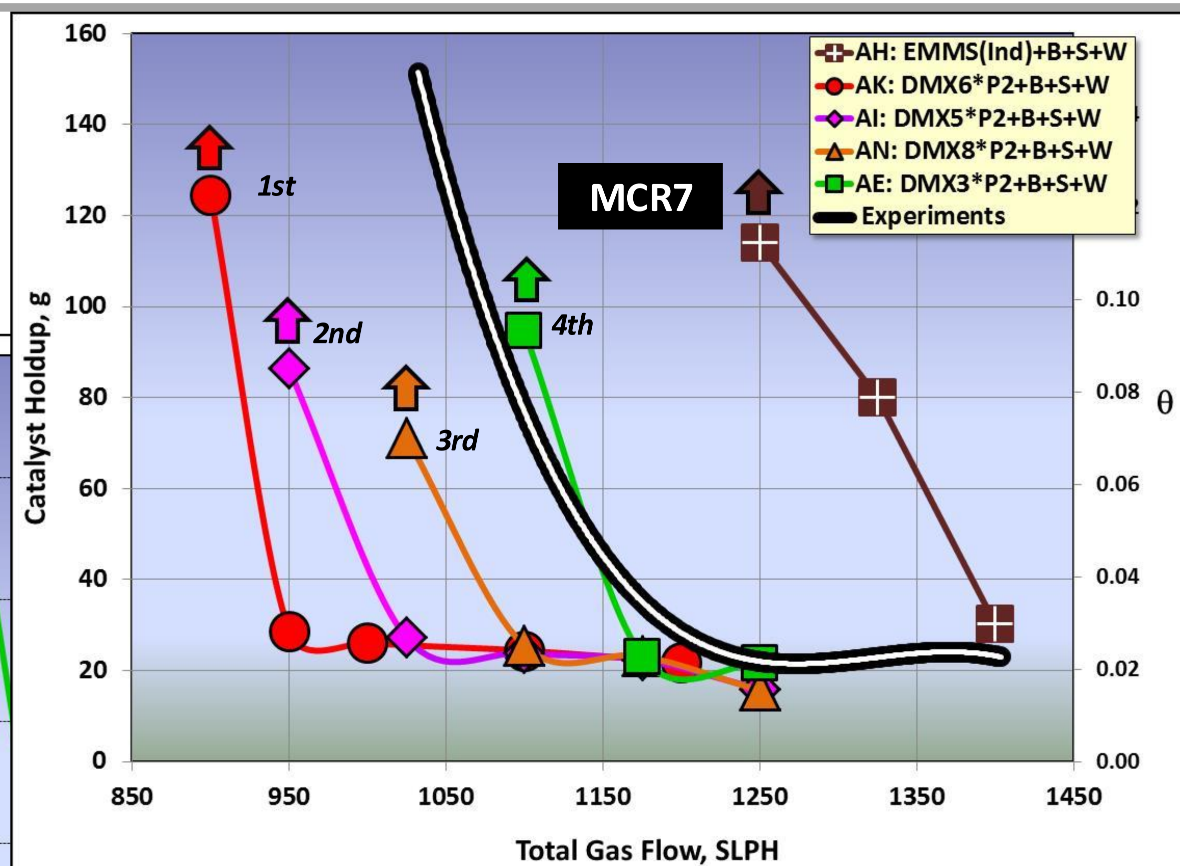
Custom Drag Multiplier (DMX) vs EMMS

Experiments vs CFD
Catalyst Only
Full PSD (35 Size Bins)





Best-Fit DM Curve is a Function of Reactor Size (Just Like EMMS)

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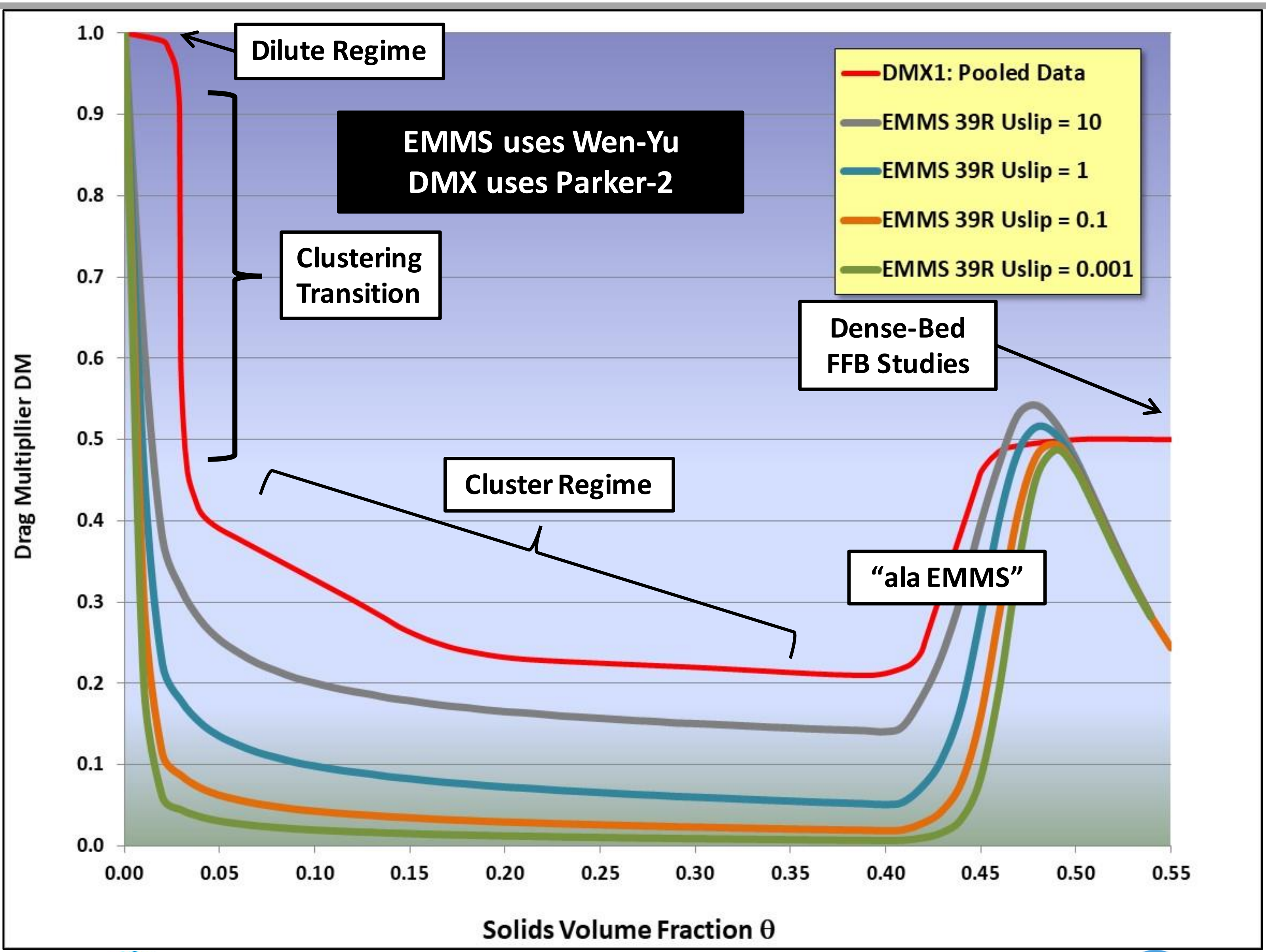
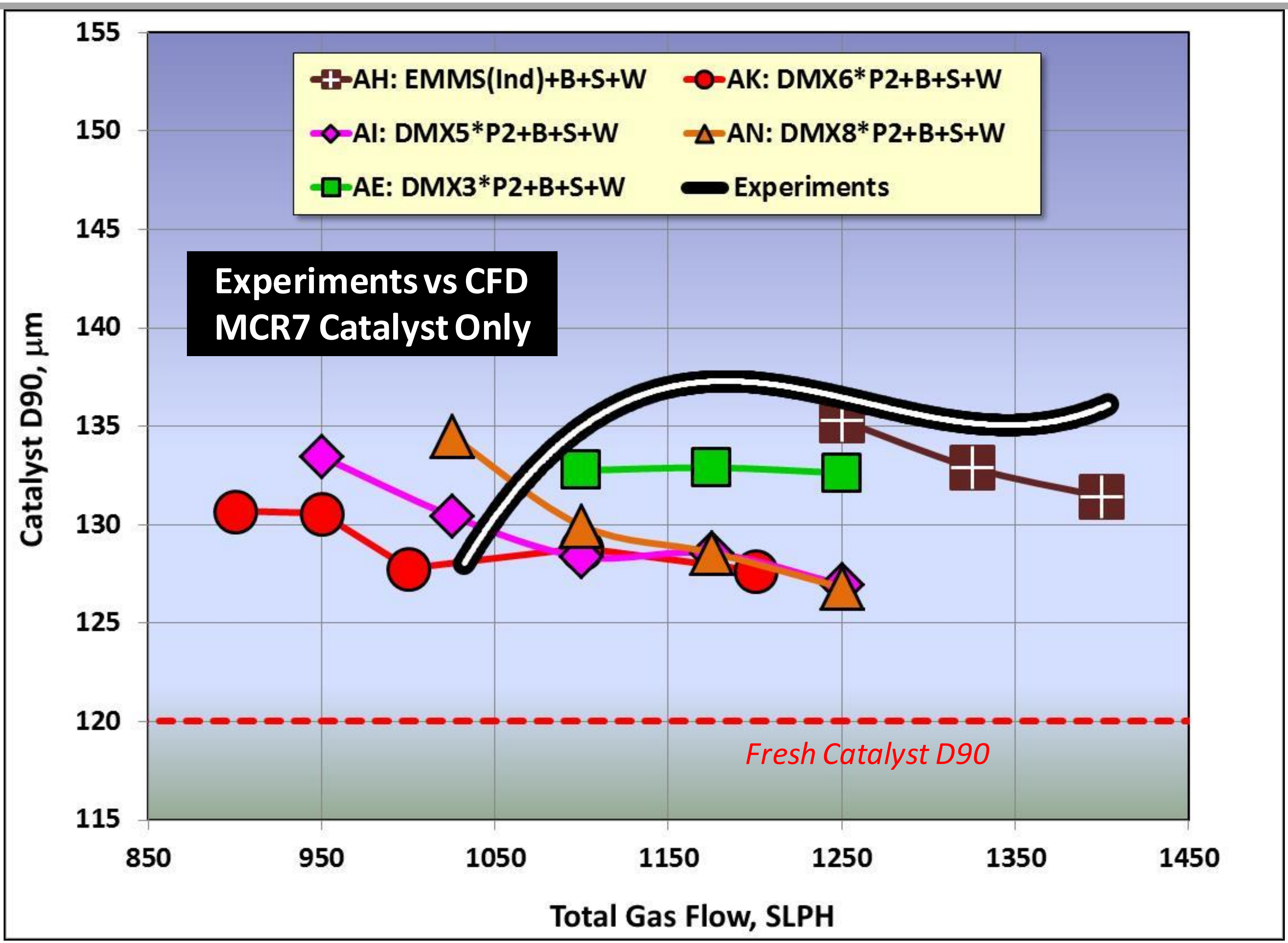
Custom DMX Function vs EMMS



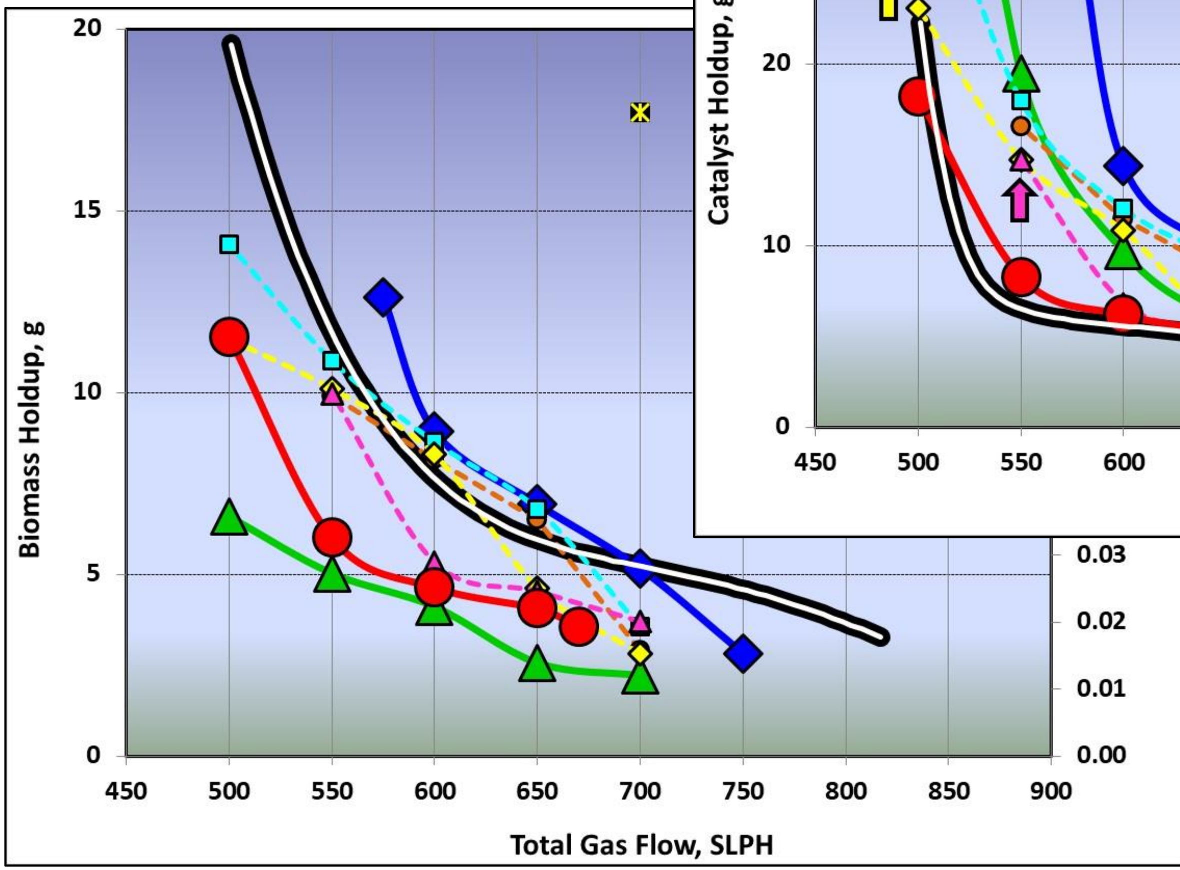
Particle Size Classification Predicted Reasonably Well

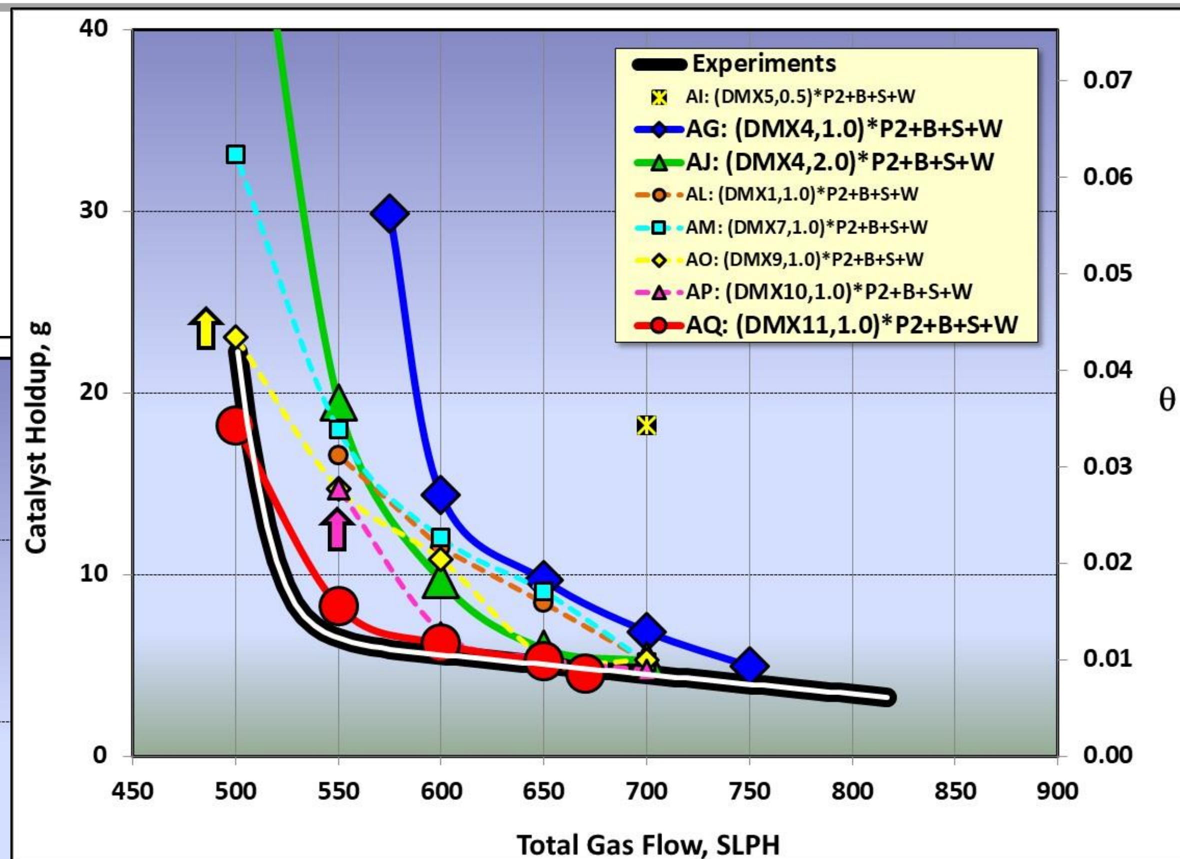


Catalyst-Biomass Mixing: Getting Close…

Experiments vs CFD MCR8

Catalyst + Biomass Full PSDs

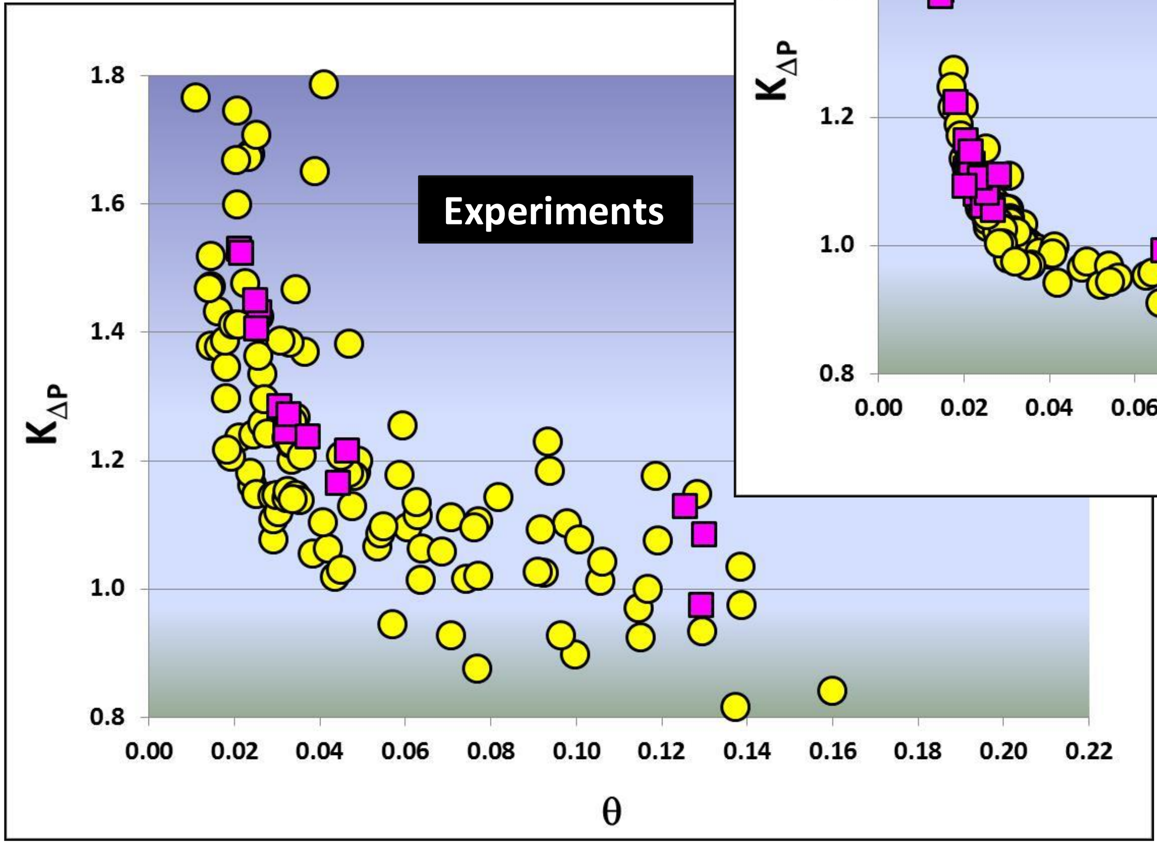


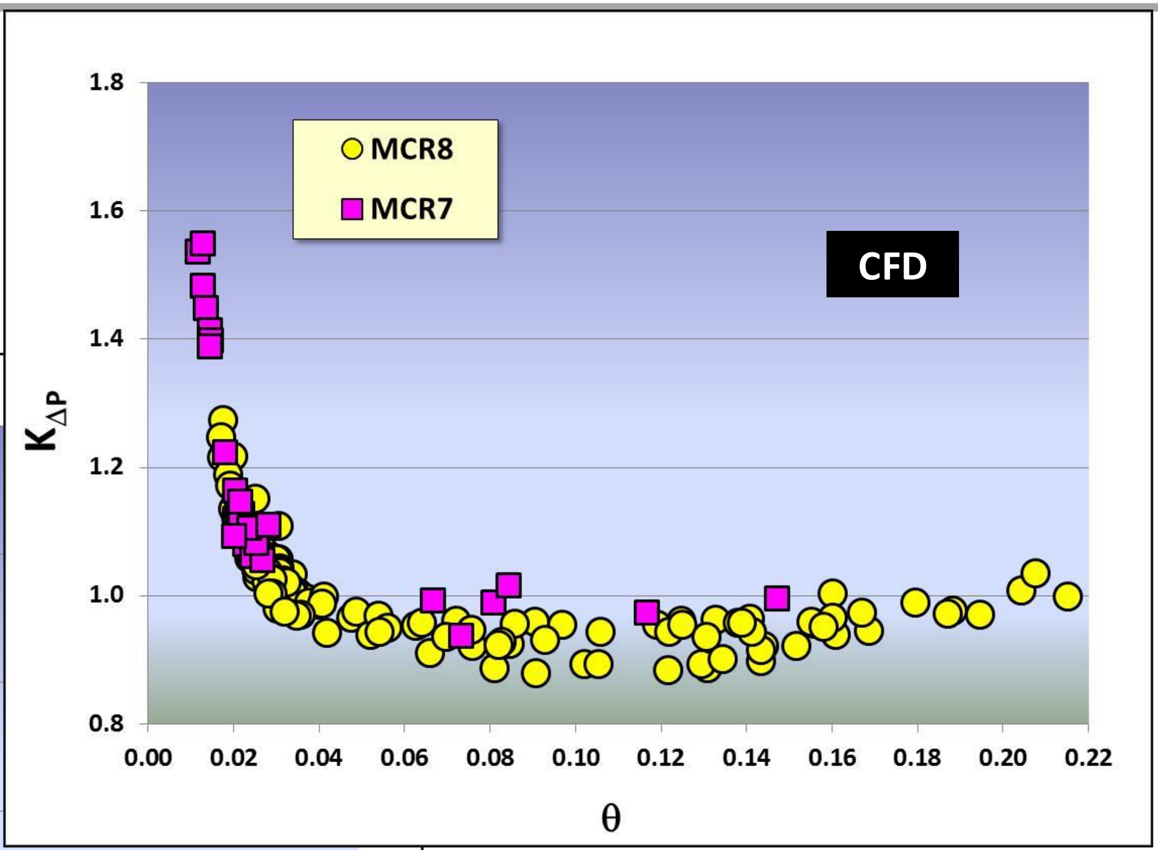


Biomass Drag Model Affects Catalyst Holdup And Vice-Versa

ΔP_{Rxr} Predictions Agree Reasonably With Experiments …

$$K_{\Delta P} = \frac{\text{Total } \Delta P_{Rxr}}{\text{Solids Hydrostatic } \Delta P_{Rxr}}$$





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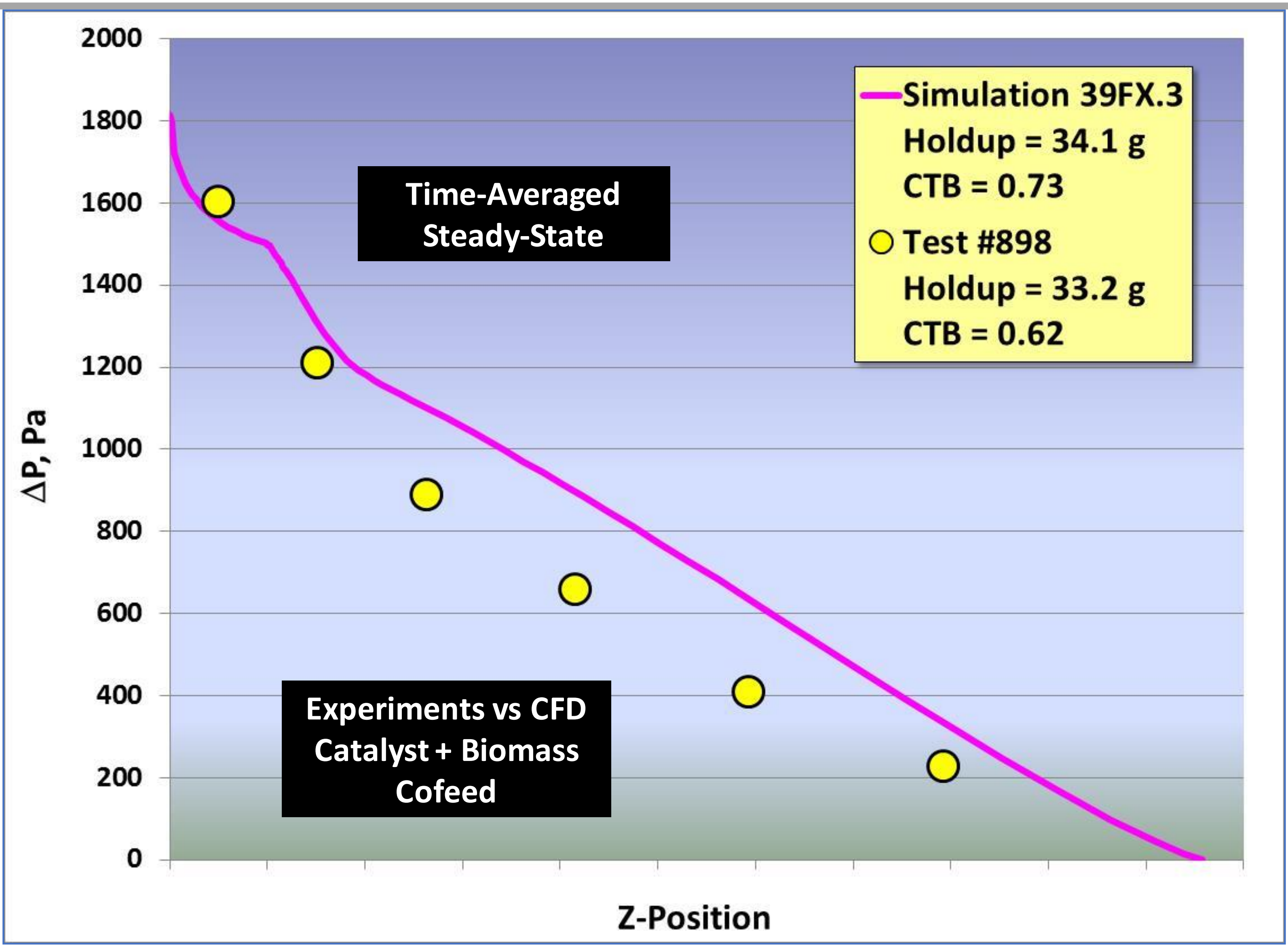
… as do Pressure Profiles, When Holdup is Predicted Correctly



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Conclusions

1. Inaeris Technologies has developed quantitative hydrodynamic models for in-situ CFP reactors using Barracuda Virtual Reactor®. The models:
   - Are sufficiently accurate to assist scale-up
   - Apply equally well to bubbling-bed and MCR fluidization regimes
   - Use full particle size distributions for catalyst and biomass

2. <u>For this system:</u>
   - EMMS drag models do not fit the Inaeris data
   - Custom drag multiplier (DM) tables were developed to fit the data. Like EMMS, these are conceptually based on clustering, and are functions of reactor diameter
   - Catalyst-biomass mixing can be modeled using the DM tables
   - Blended acceleration model (BAM) has value for dense-phase mixing behavior, but only for low value for BAM exponent (0.5-1 iso 6)
   - Other CPFD recommended parameters proved to be sufficient
   - CPFD's BGK "collision" model over-homogenizes velocities of catalyst and biomass particles and was not used

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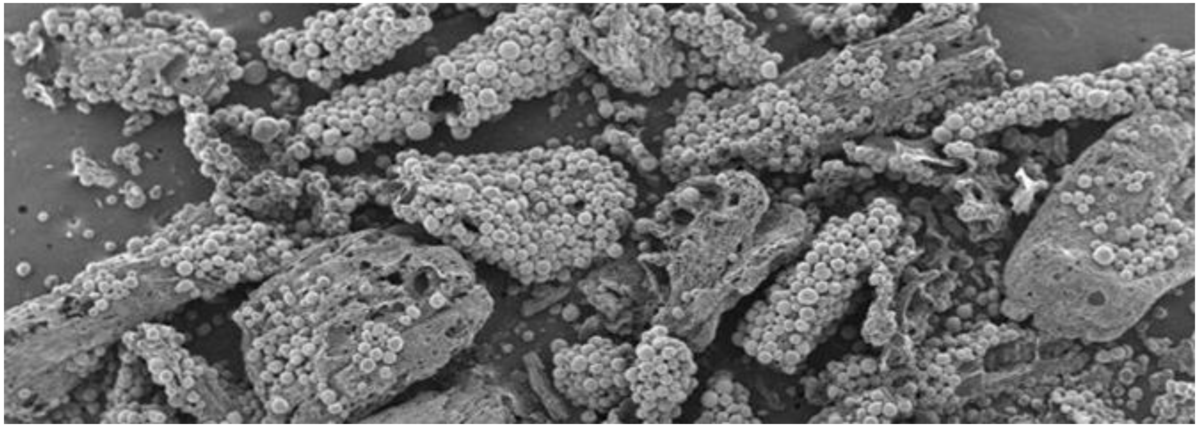
Thank You!

Questions?

BFCC is Not FCC

- BFCC feed is solid, not liquid
  - Pyrolysis is slower and more complex than vaporization
  - Pyrolysis leaves behind the char "skeleton" particle
  - Physical interactions of catalyst and biomass/char particles are important



- Deoxygenation reactions are slower than C-C cracking reactions
  - Need much longer residence times than FCC – especially since modern FCC is short contact time!
  - Need larger catalyst inventories in the reactor