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Experimental validation of CFD hydrodynamic models for catalytic fast pyrolysis (CFP)

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EXPERIMENTAL VALIDATION OF CFD HYDRODYNAMIC MODELS FOR CATALYTIC FAST PYROLYSIS (CFP)

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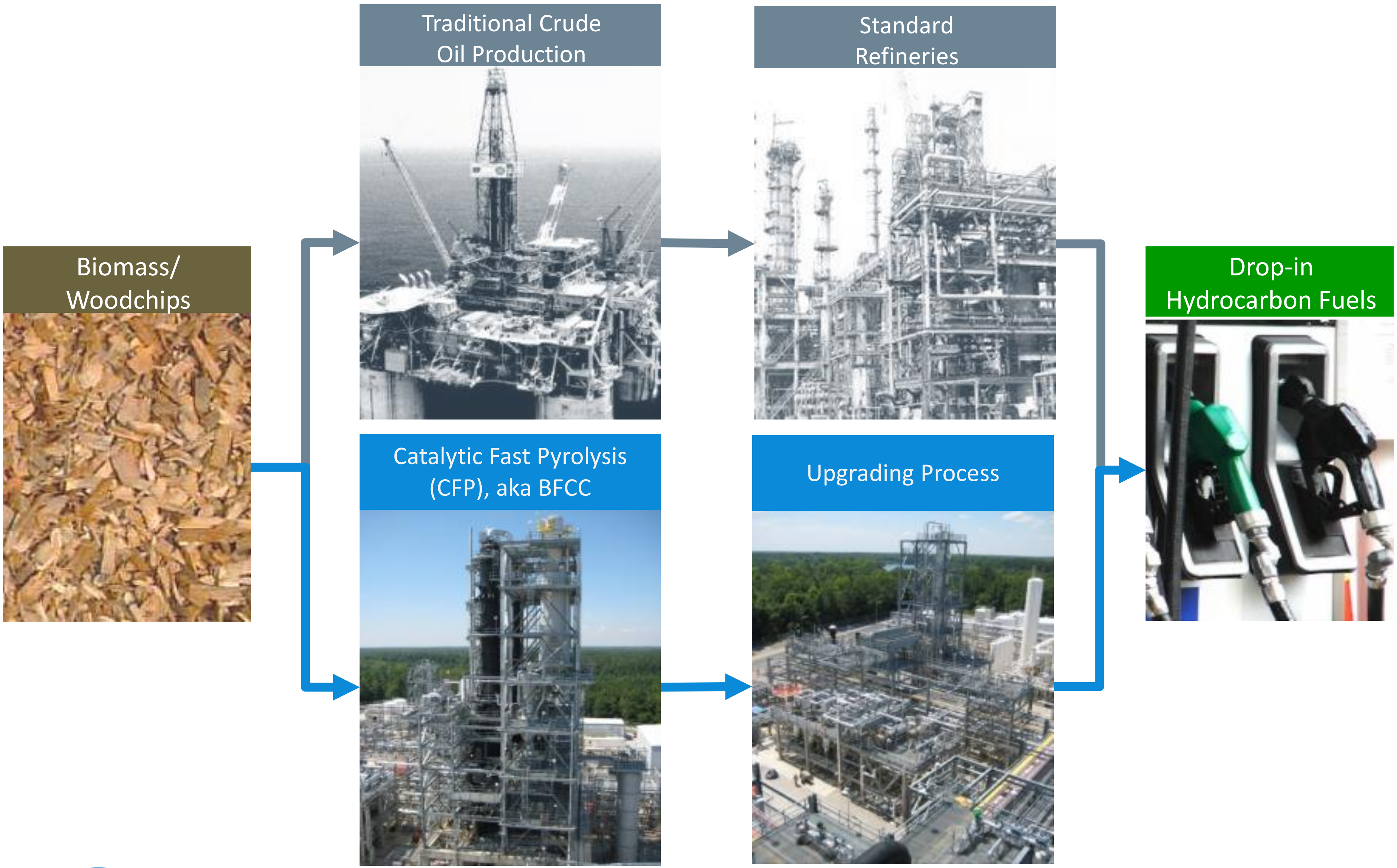
Inaeris Technologies' CFP-Based Biomass-to-Fuel Process



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cpfd COMPUTATIONAL PARTICLE FLUID DYNAMICS

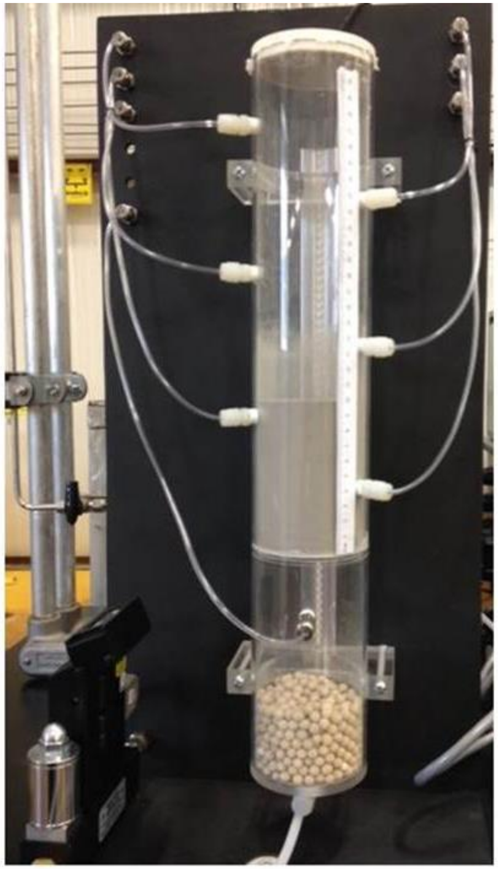
Inaeris Technologies' Development Program

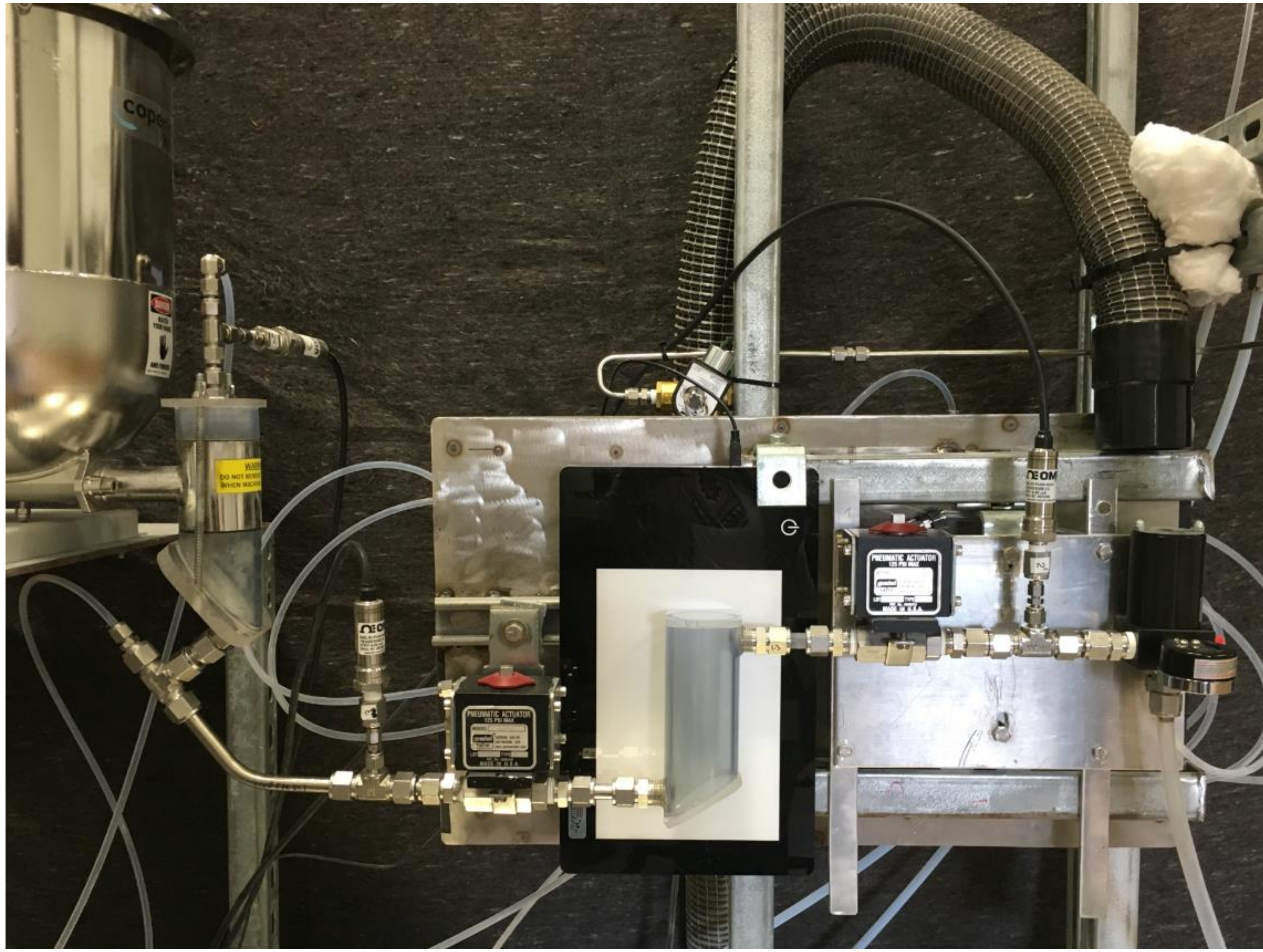
PRU (Process Research Unit) 3 Batch Units, ~ 1 kg catalyst → KCR (KiOR Circulating Riser) 2 Units, ~ 10 kg catalyst → Demonstration Unit 5 tons catalyst → Commercial Scale

CFD (Barracuda VR®) →

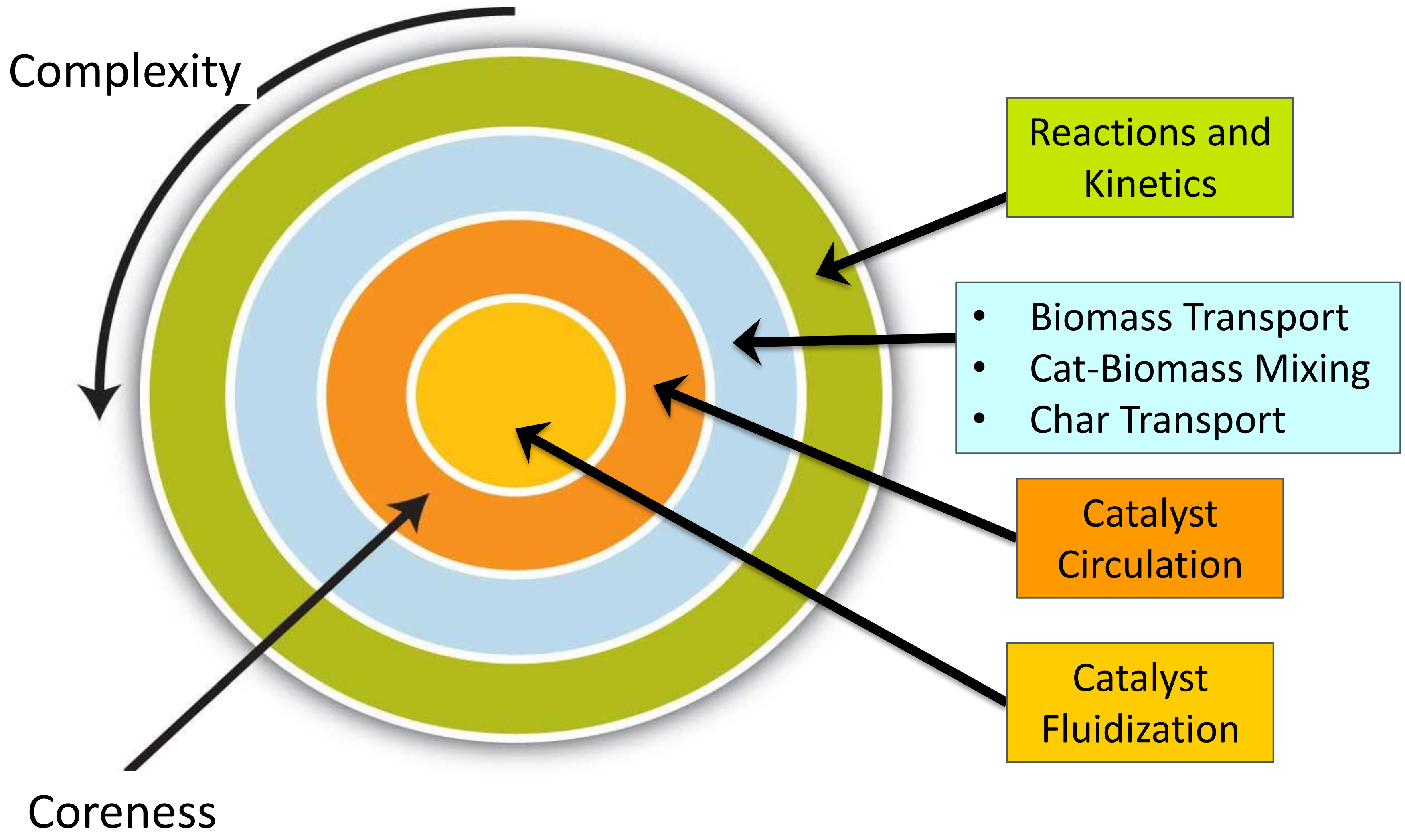
1. Add a Parallel Path to our Development Process
2. Speed Scale-up and Commercialization

Simple Cold-Flow Units for Model Validation

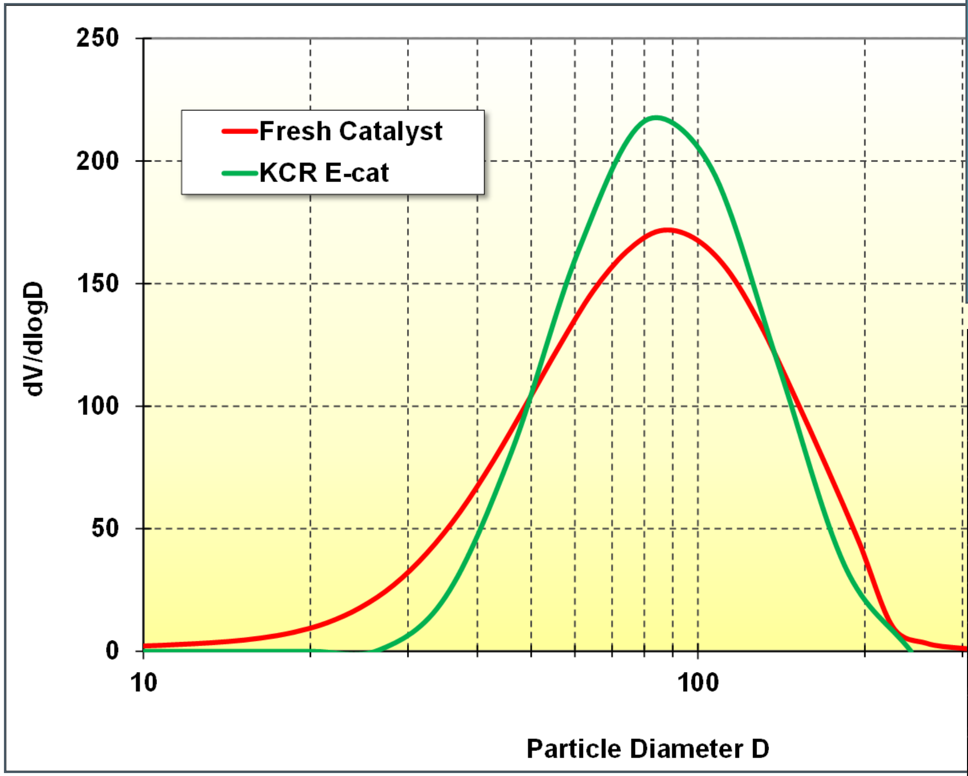


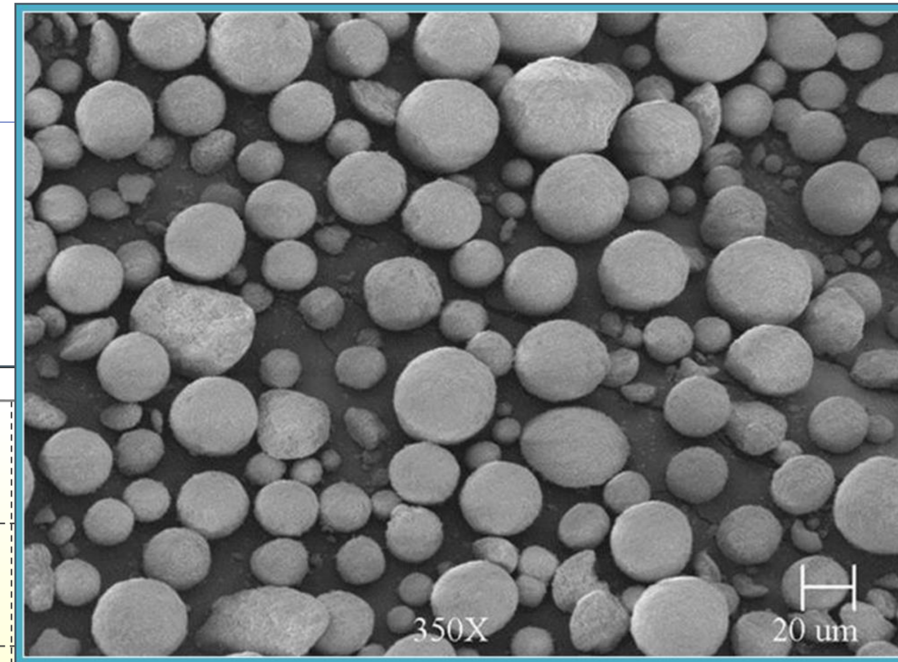


Hierarchical Modeling Program



Catalysts Used in This Study





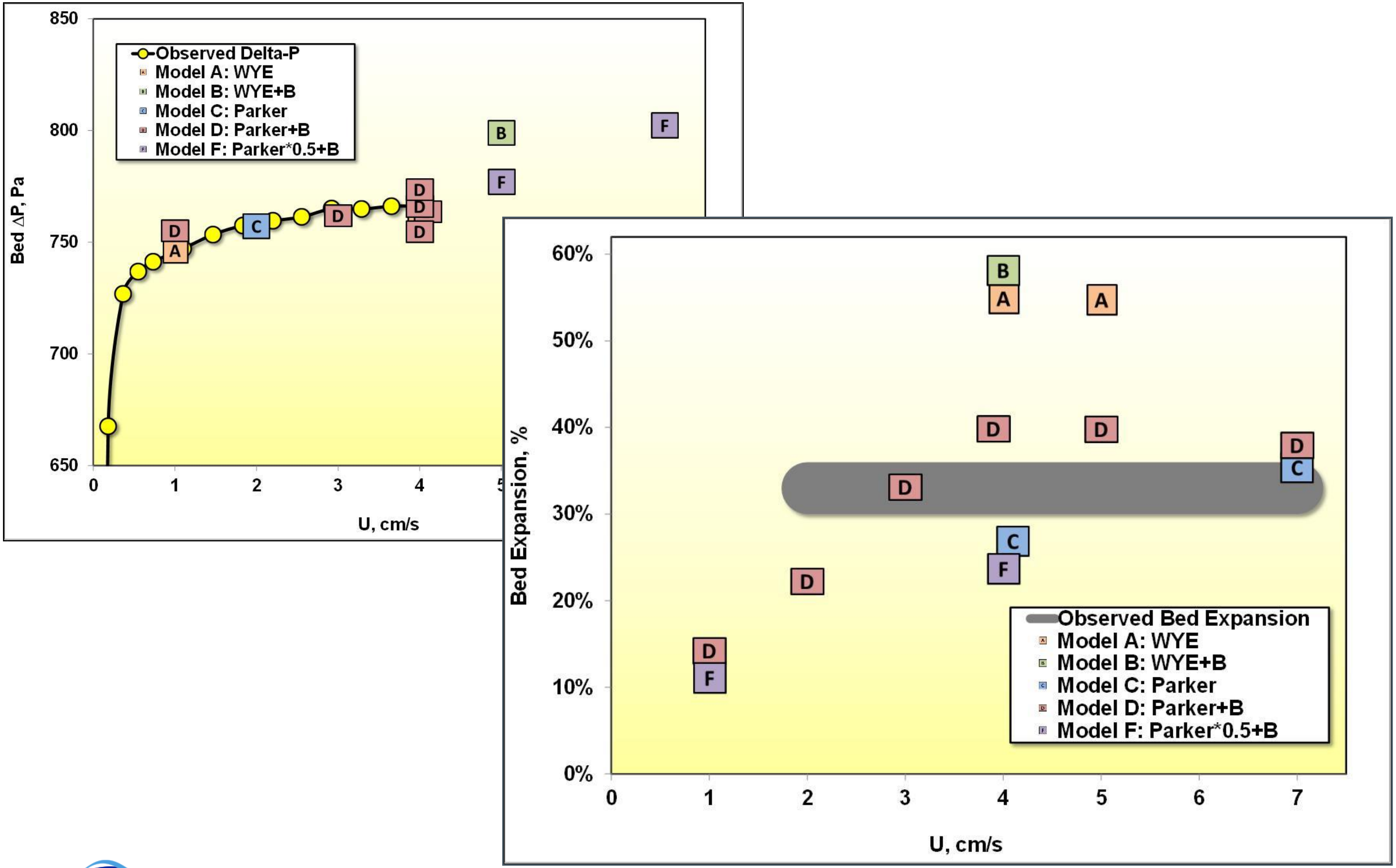
	Fresh CFP Catalyst	KCR E-Cat
Particle Size Distribution (wt%)		
Size range 0-20 (μm)	1.91	0.00
20-40 (μm)	10.21	2.02
40-80 (μm)	38.76	46.90
80-150 (μm)	40.38	48.61
150+ (μm)	8.75	2.47
Other Physical Properties		
Apparent Bulk Density (kg/m^3)	760	
Skeletal Density (kg/m^3)	2560	
Pore Volume (cm^3/g)	0.00	
Particle Density, Eqn (1) (kg/m^3)	1380	
θ_{cp}, Eqn (2)	0.55	

CFD Models Evaluated in Barracuda VR®

Legend	Drag Model	Drag Multiplier	"B" Blended Acceleration	"C" Collision Model	"S" Stress Model Ps	"S" Stress Model B	"W" Normal Momentum Retention	"W" Tangential Momentum Retention	"W" Diffuse Bounce
Model A: WYE	Wen-Yu Ergun	1.0	No*	No*	1*	3*	0.30	0.99	0*
Model B: WYE+B	Wen-Yu Ergun	1.0	Yes	No*	1*	3*	0.30	0.99	0*
Model C: Parker	Parker	1.0	No*	No*	1*	3*	0.30	0.99	0*
Model D: Parker+B	Parker	1.0	Yes	No*	1*	3*	0.30	0.99	0*
Model E: Parker*0.5	Parker	0.5	No*	No*	1*	3*	0.30	0.99	0*
Model F: Parker*0.5+B	Parker	0.5	Yes	No*	1*	3*	0.30	0.99	0*
Model G: Parker*0.25	Parker	0.25	No*	No*	1*	3*	0.30	0.99	0*
Model H: Parker+B+C+S+W	Parker	1.0	Yes	Yes	15	2	0.85	0.85	5
Model I: Parker*0.5+B+C+S+W	Parker	0.5	Yes	Yes	15	2	0.85	0.85	5

* = Default Values in Barracuda VR 17.02

FFB Results: Simulations vs Experimental Results



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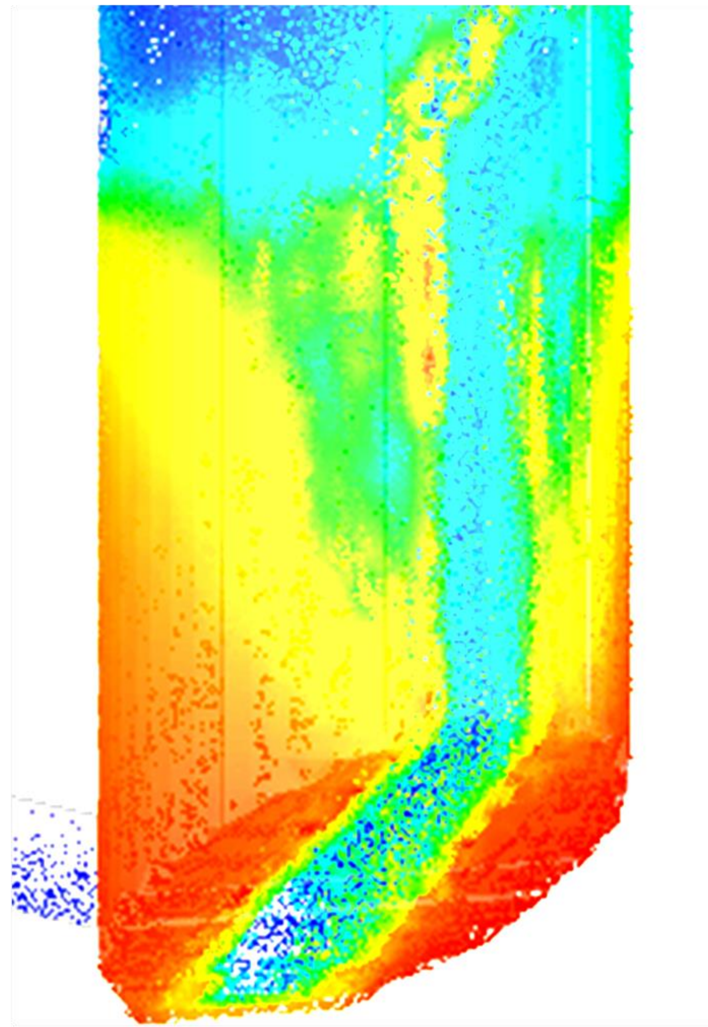
CFB Visual Comparison: KCR e-cat, 12.0 kg/hr, N_2 Flow 40 SLPM

4.8 cm

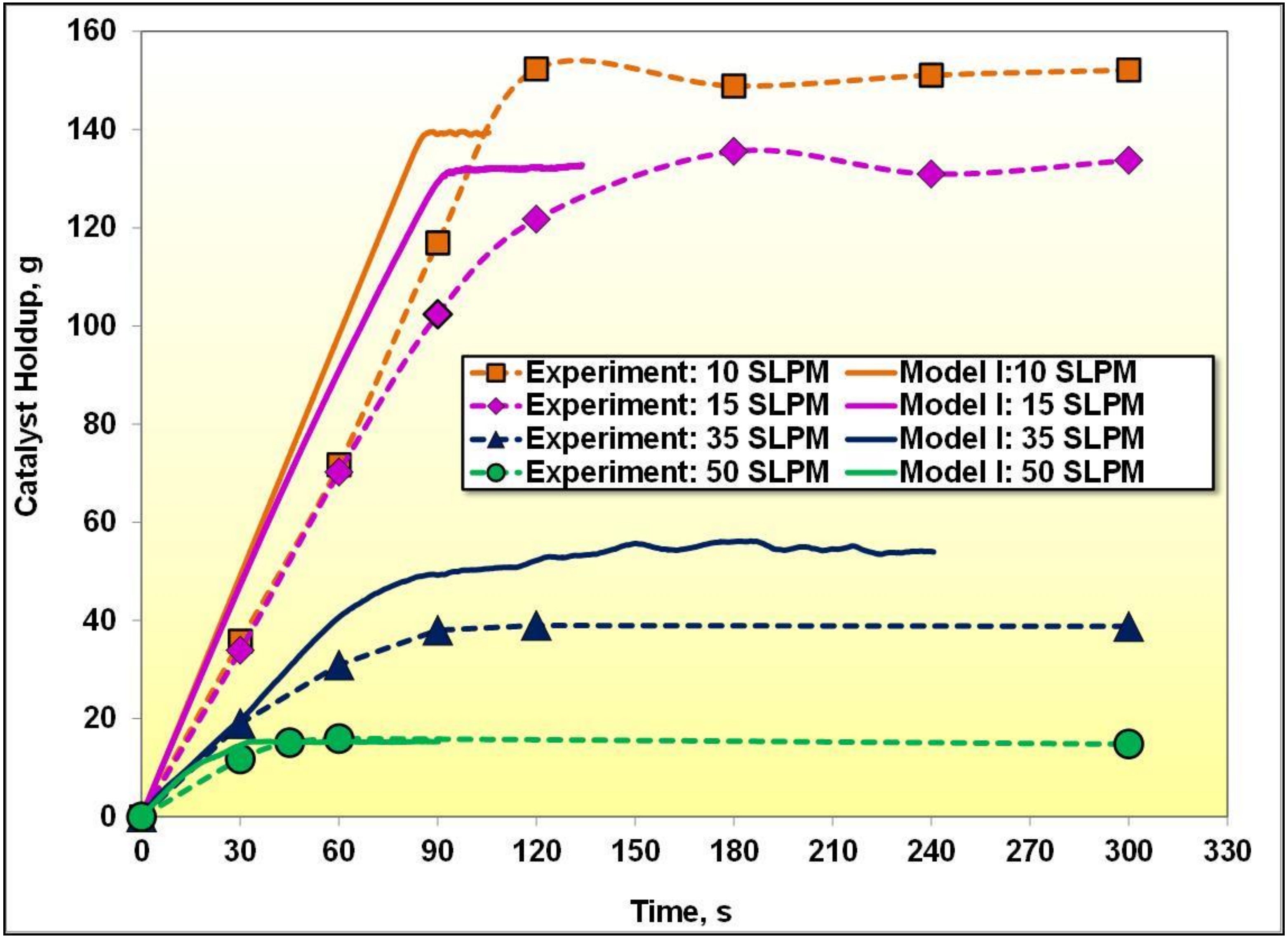
Experiment

4.8 cm

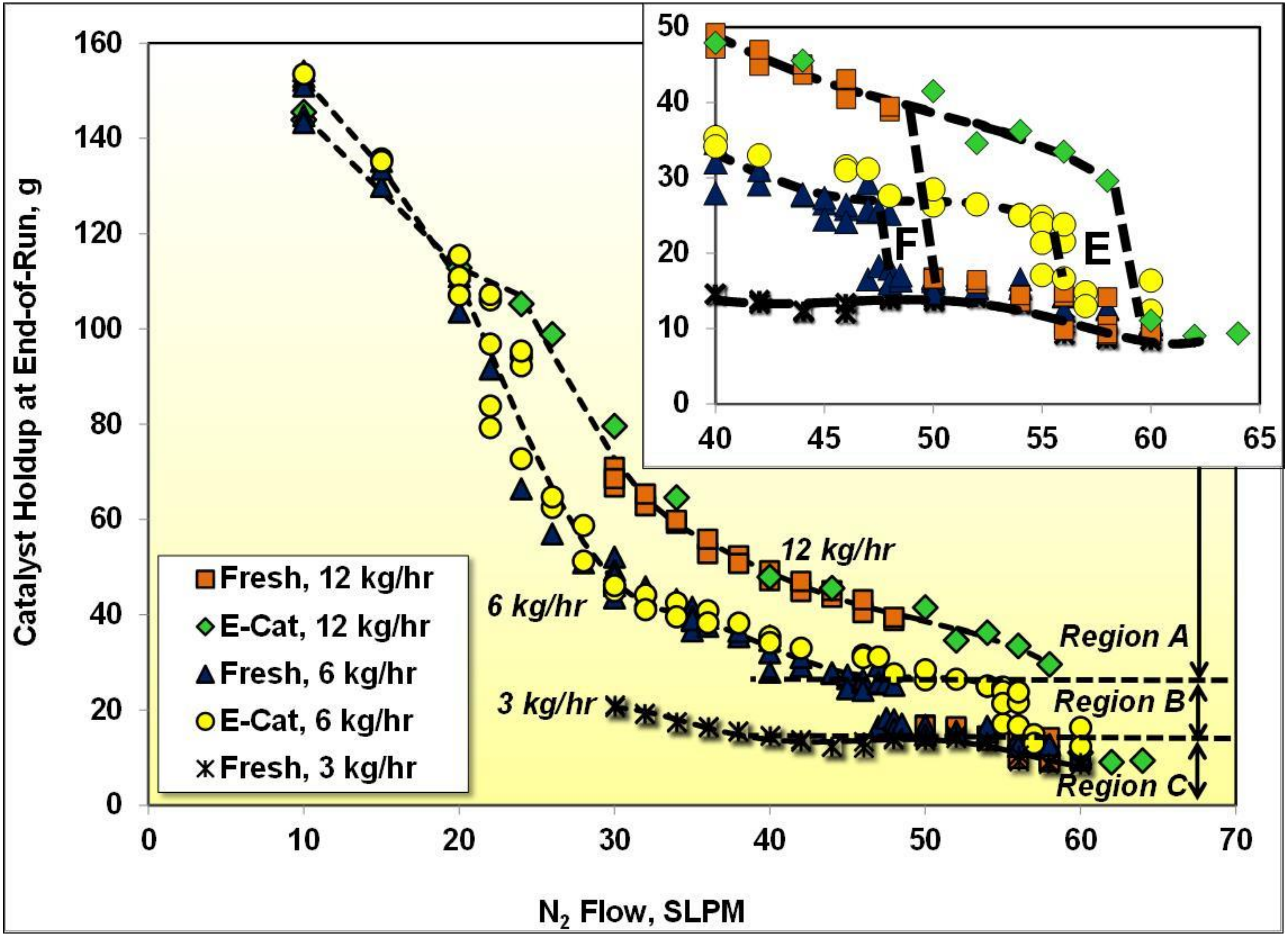


Simulation

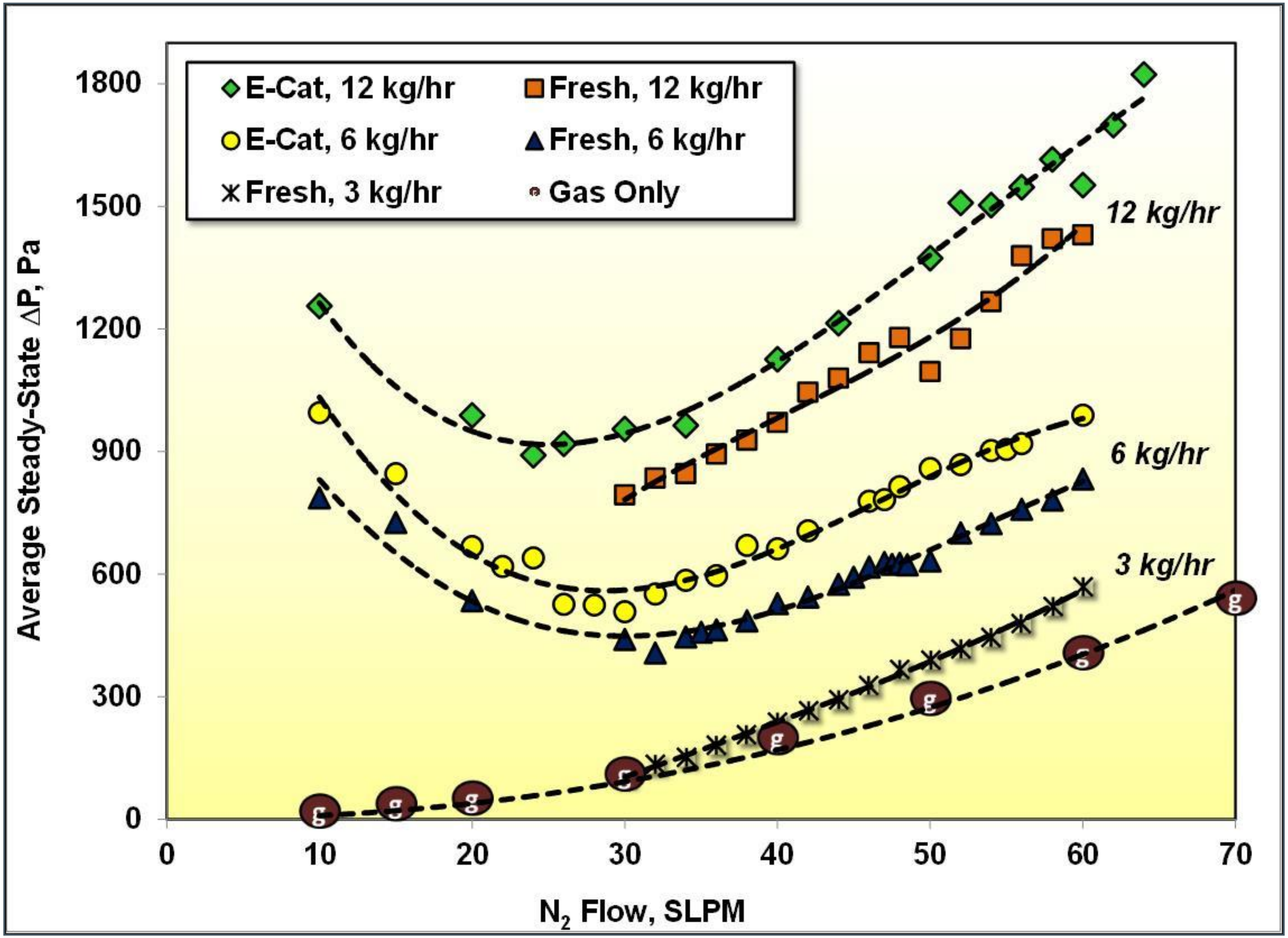
CFB Results: Bed-Building Kinetics



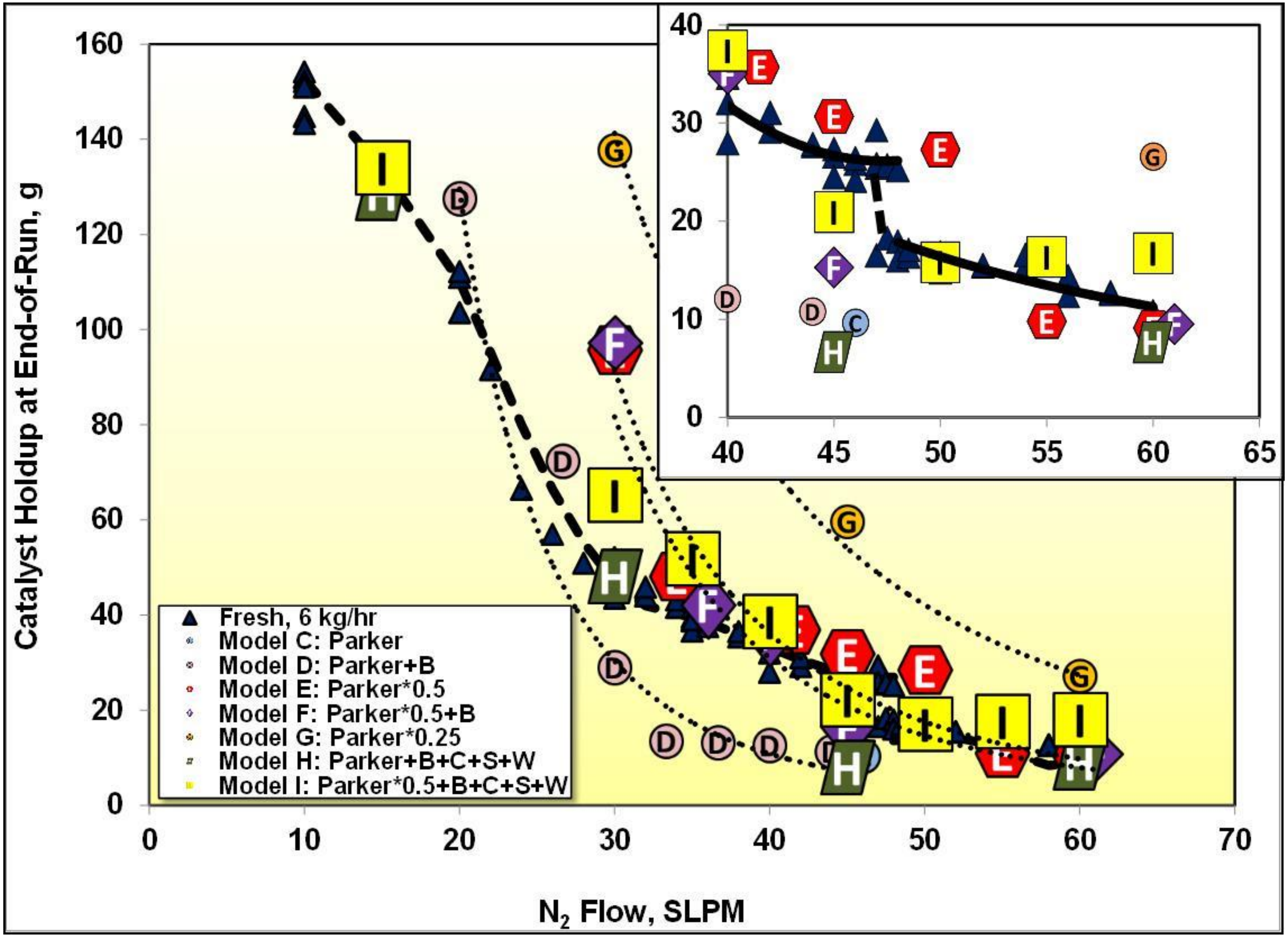
CFB Results: End-of-Run (EOR) Catalyst Holdup Measurements



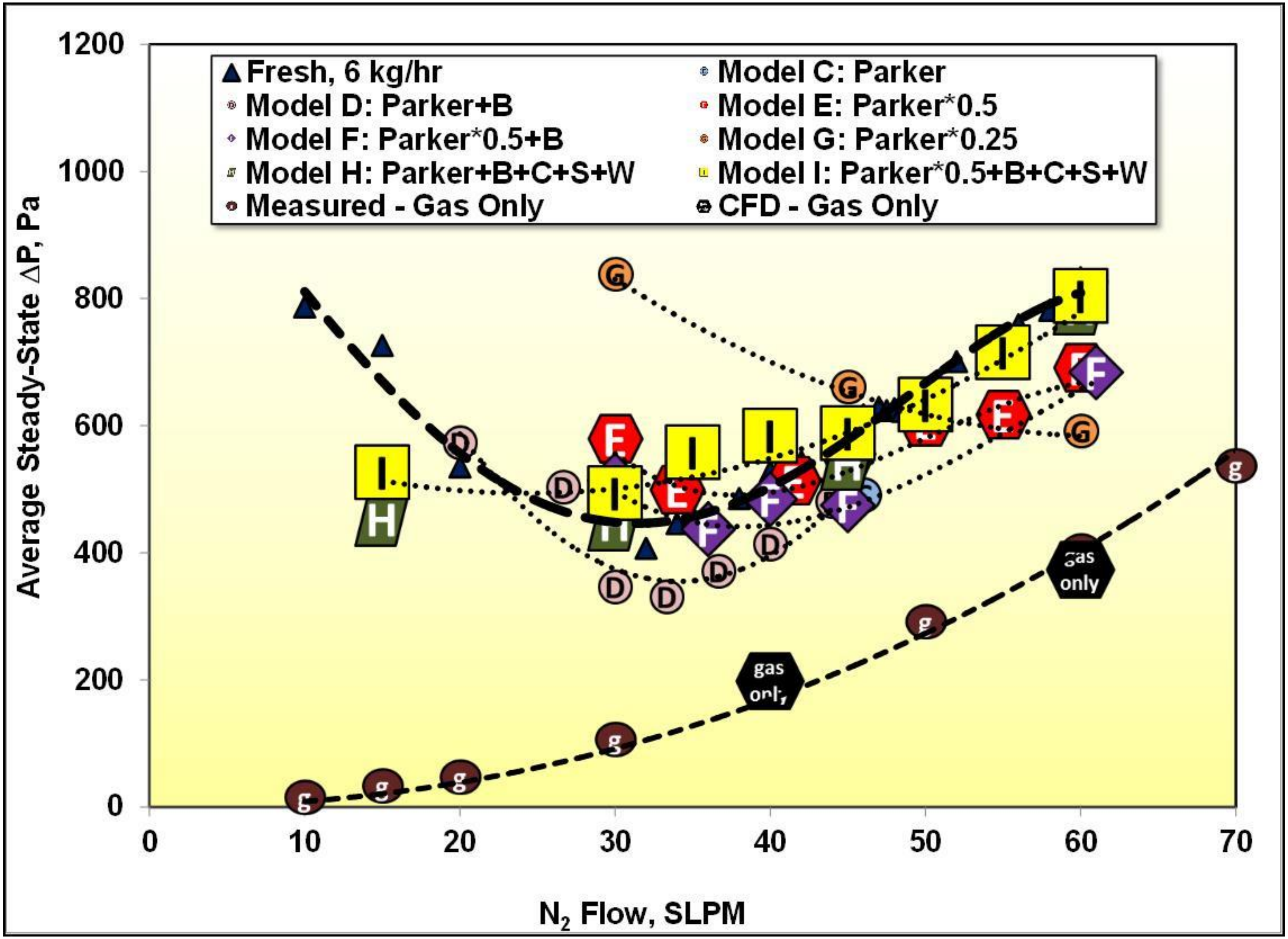
CFB Results: Time-Averaged ΔP (PT2-PT3)



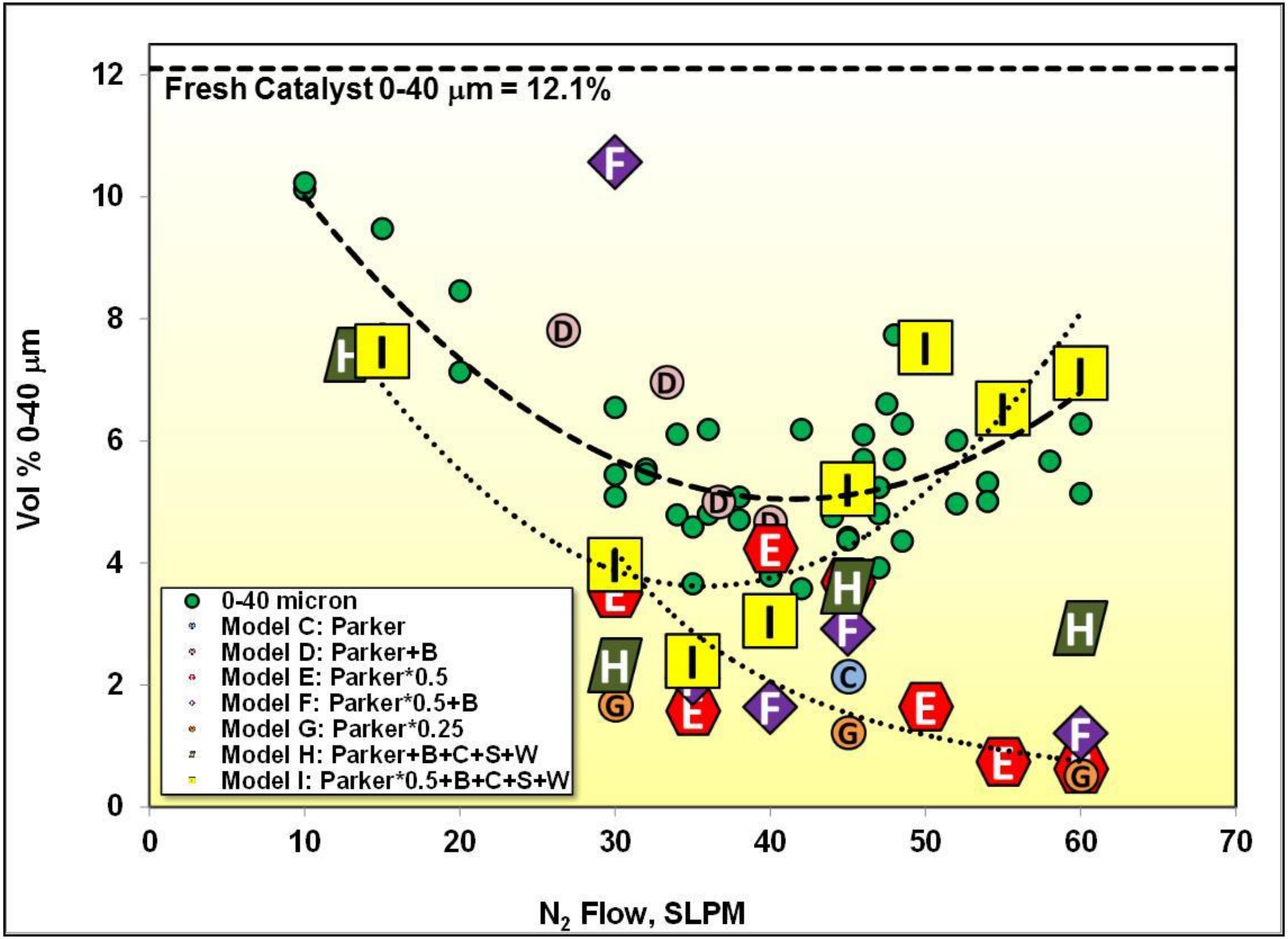
CFD Results: Fresh Catalyst, 6.0 kg/hr: EOR Holdup



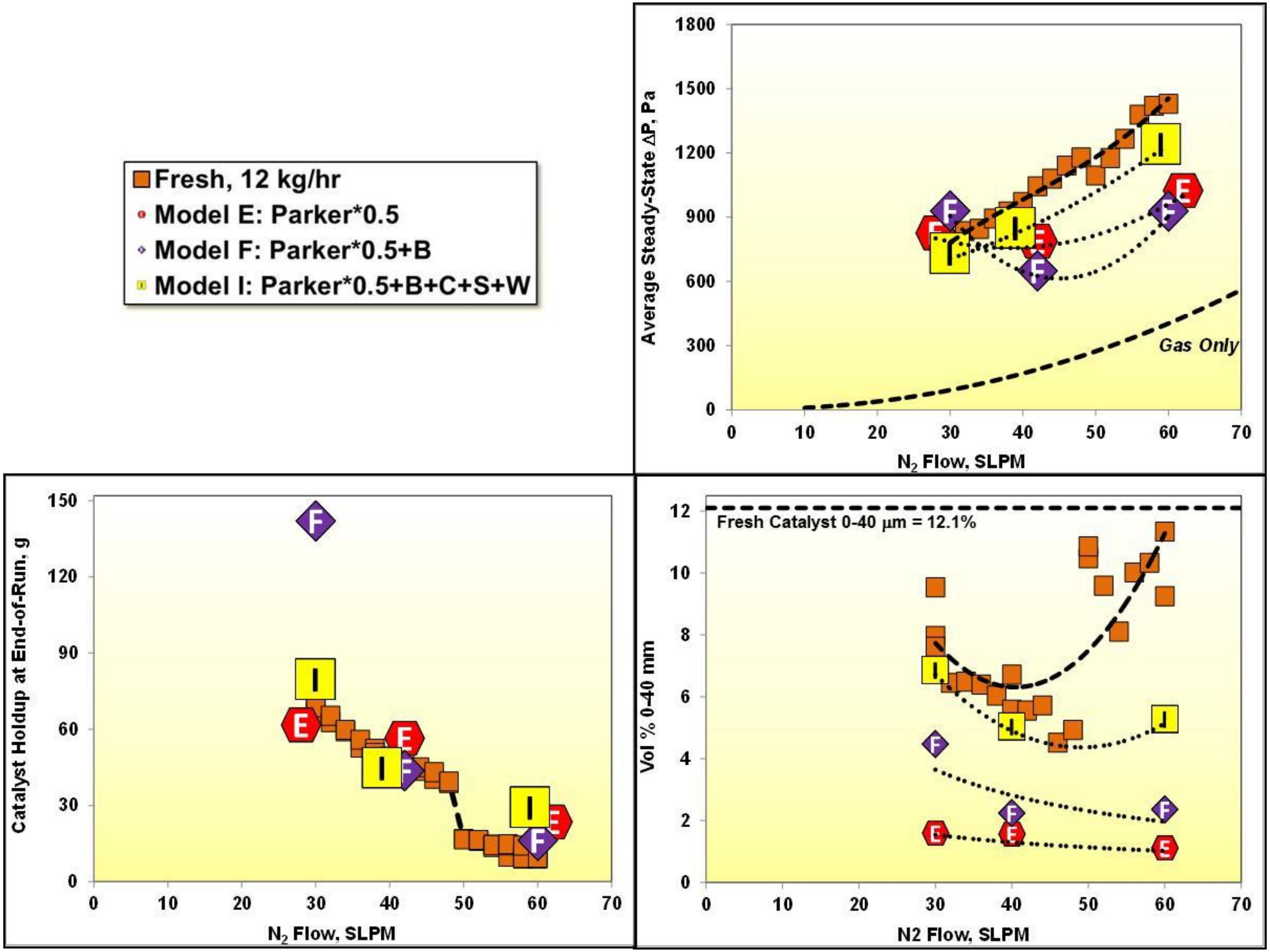
CFB Results: Fresh Catalyst, 6.0 kg/hr: Time-Averaged ΔP



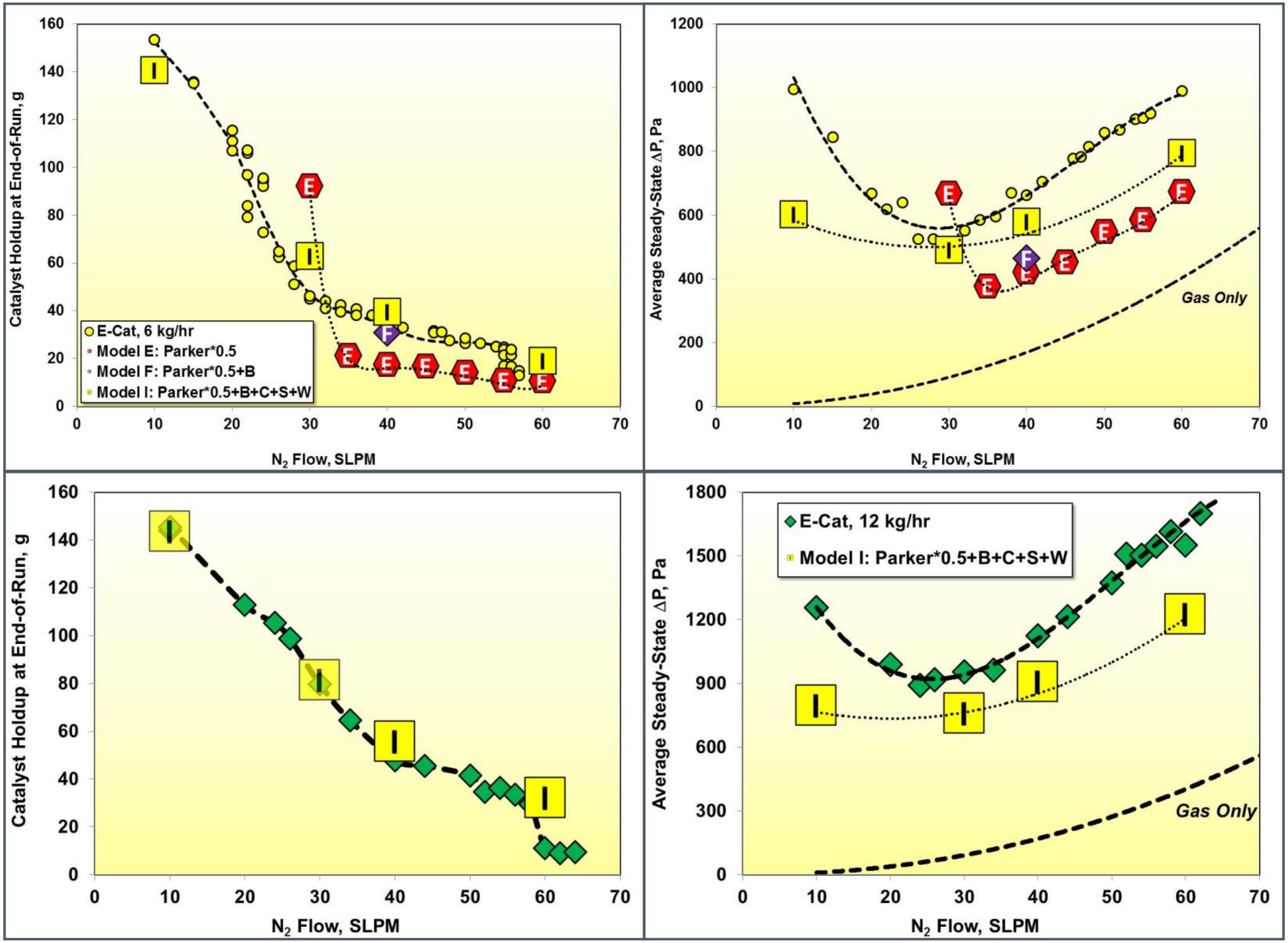
CFB Results: Fresh Catalyst, 6.0 kg/hr: EOR Fines Content



CFB Results: Fresh Catalyst, 12.0 kg/hr



CFB Results: E-Cat at 6.0 and 12.0 kg/hr



Conclusions

- Wen-Yu-Ergun drag correlation over-estimates drag forces in CFP catalyst fluidization and circulation. A modified drag correlation by Parker (CPFD) improves the correspondence between data and simulation but does not fit the overall shape of the holdup, ΔP and classification curves adequately
- Applying simple drag multipliers to the "basic Parker" models shifts the CFB holdup mass and ΔP curves to the right (to higher gas flowrates) without changing the shapes of the curves to better fit the data. All five "basic Parker" models over-predict the extent of classification at higher gas flows
- Adding an extended set of Barracuda parameters (B+C+S+W) to the "basic Parker" models significantly improves the match between data and simulation. Of all nine models tested in this study, only Model I (0.5*Parker+B+C+S+W) adequately predicts the shapes of all three data curves – holdup mass, ΔP and classification – for all three catalyst flowrates and both catalysts
- The effects of PSD differences (mainly fines) between fresh catalyst and e-cat are limited to the location of a "jump" flowrate between two flow regimes. In the bed-building region, the PSD differences have no effect on holdup, and only slight effects on ΔP. Only Model I predicts these findings correctly