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

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Recommended Citation

Bruce D Adkins, Travis Dudley, Neeti Kapur, Peter Blaser, and James Parker, "Experimental validation of CFD hydrodynamic models for catalytic fast pyrolysis (CFP)" in "Fluidization XV", Jamal Chaouki, Ecole Polytechnique de Montreal, Canada Franco Berruti, Western University, Canada Xiaotao Bi, UBC, Canada Ray Cocco, PSRI Inc. USA Eds, ECI Symposium Series, (2016).  
http://dc.engconfintl.org/fluidization_xv/152

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

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*Corresponding author: Bruce.Adkins@inaeristech.com
Inaeris Technologies’ CFP-Based Biomass-to-Fuel Process

Traditional Crude Oil Production

Biomass/Woodchips

Catalytic Fast Pyrolysis (CFP), aka BFCC

Upgrading Process

Drop-in Hydrocarbon Fuels

Standard Refineries
Inaeris Technologies’ Development Program

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

- Complexity
- Coreness

**Reactions and Kinetics**
- Biomass Transport
- Cat-Biomass Mixing
- Char Transport

**Catalyst Circulation**

**Catalyst Fluidization**
Catalysts Used in This Study

![Graph showing particle diameter distribution](graph.png)

![SEM image of catalysts](image.png)

<table>
<thead>
<tr>
<th>Size Range (μm)</th>
<th>Fresh CFP Catalyst</th>
<th>KCR E-Cat</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-20</td>
<td>1.91</td>
<td>0.00</td>
</tr>
<tr>
<td>20-40</td>
<td>10.21</td>
<td>2.02</td>
</tr>
<tr>
<td>40-80</td>
<td>38.76</td>
<td>46.90</td>
</tr>
<tr>
<td>80-150</td>
<td>40.38</td>
<td>48.61</td>
</tr>
<tr>
<td>150+</td>
<td>8.75</td>
<td>2.47</td>
</tr>
</tbody>
</table>

**Other Physical Properties**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Apparent Bulk Density (kg/m³)</td>
<td>760</td>
</tr>
<tr>
<td>Skeletal Density (kg/m³)</td>
<td>2560</td>
</tr>
<tr>
<td>Pore Volume (cm³/g)</td>
<td>0.00</td>
</tr>
<tr>
<td>Particle Density, Eqn (1) (kg/m³)</td>
<td>1380</td>
</tr>
<tr>
<td>( \theta_{cp}, \text{Eqn (2)} )</td>
<td>0.55</td>
</tr>
</tbody>
</table>
## CFD Models Evaluated in Barracuda VR®

<table>
<thead>
<tr>
<th>Model</th>
<th>Drag Model</th>
<th>Drag Multiplier</th>
<th>&quot;B&quot; Blended Acceleration</th>
<th>&quot;C&quot; Collision Model</th>
<th>&quot;S&quot; Stress Model Ps</th>
<th>&quot;S&quot; Stress Model B</th>
<th>&quot;W&quot; Normal Momentum Retention</th>
<th>&quot;W&quot; Tangential Momentum Retention</th>
<th>&quot;W&quot; Diffuse Bounce</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model A: WYE</td>
<td>Wen-Yu Ergun</td>
<td>1.0</td>
<td>No*</td>
<td>No*</td>
<td>1</td>
<td>3</td>
<td>0.30</td>
<td>0.99</td>
<td>0*</td>
</tr>
<tr>
<td>Model B: WYE+B</td>
<td>Wen-Yu Ergun</td>
<td>1.0</td>
<td>Yes</td>
<td>No*</td>
<td>1</td>
<td>3</td>
<td>0.30</td>
<td>0.99</td>
<td>0*</td>
</tr>
<tr>
<td>Model C: Parker</td>
<td>Parker</td>
<td>1.0</td>
<td>No*</td>
<td>No*</td>
<td>1</td>
<td>3</td>
<td>0.30</td>
<td>0.99</td>
<td>0*</td>
</tr>
<tr>
<td>Model D: Parker+B</td>
<td>Parker</td>
<td>1.0</td>
<td>Yes</td>
<td>No*</td>
<td>1</td>
<td>3</td>
<td>0.30</td>
<td>0.99</td>
<td>0*</td>
</tr>
<tr>
<td>Model E: Parker*0.5</td>
<td>Parker</td>
<td>0.5</td>
<td>No*</td>
<td>No*</td>
<td>1</td>
<td>3</td>
<td>0.30</td>
<td>0.99</td>
<td>0*</td>
</tr>
<tr>
<td>Model F: Parker*0.5+B</td>
<td>Parker</td>
<td>0.5</td>
<td>Yes</td>
<td>No*</td>
<td>1</td>
<td>3</td>
<td>0.30</td>
<td>0.99</td>
<td>0*</td>
</tr>
<tr>
<td>Model G: Parker*0.25</td>
<td>Parker</td>
<td>0.25</td>
<td>No*</td>
<td>No*</td>
<td>1</td>
<td>3</td>
<td>0.30</td>
<td>0.99</td>
<td>0*</td>
</tr>
<tr>
<td>Model H: Parker+B+C+S+W</td>
<td>Parker</td>
<td>1.0</td>
<td>Yes</td>
<td>Yes</td>
<td>15</td>
<td>2</td>
<td>0.85</td>
<td>0.85</td>
<td>5</td>
</tr>
<tr>
<td>Model I: Parker*0.5+B+C+S+W</td>
<td>Parker</td>
<td>0.5</td>
<td>Yes</td>
<td>Yes</td>
<td>15</td>
<td>2</td>
<td>0.85</td>
<td>0.85</td>
<td>5</td>
</tr>
</tbody>
</table>

* = Default Values in Barracuda VR 17.02
FFB Results: Simulations vs Experimental Results
CFB Visual Comparison: KCR e-cat, 12.0 kg/hr, N\textsubscript{2} Flow 40 SLPM

Experiment

Simulation
CFB Results: Bed-Building Kinetics
CFB Results: End-of-Run (EOR) Catalyst Holdup Measurements

- Graph showing catalyst holdup measurements vs. nitrogen flow (SLPM).
- Data points for Fresh, E-Cat, and different flow rates (3 kg/hr, 6 kg/hr, 12 kg/hr).
- regions A, B, and C indicated on the graph.
CFB Results: Time-Averaged $\Delta P$ (PT2-PT3)
CFD Results: Fresh Catalyst, 6.0 kg/hr: EOR Holdup
CFB Results: Fresh Catalyst, 6.0 kg/hr: Time-Averaged $\Delta P$

![Graph showing CFB results with various models and N₂ flow vs. average steady-state $\Delta P$.](image-url)
CFB Results: Fresh Catalyst, 6.0 kg/hr: EOR Fines Content

Fresh Catalyst 0-40 μm = 12.1%
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.