Advancing Catalytic Fast Pyrolysis through Integrated Experimentation and Multi-Scale Computational Modeling

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Catalytic Fast Pyrolysis (CFP) Overview

CFP is an adaptable pathway for the conversion of woody biomass and waste carbon sources into fuel blendstocks and chemical co-products

Approach to Catalytic Fast Pyrolysis

Fluidized Bed Zeolite CFP
Pilot and demonstration scale data demonstrate the technical feasibility of the approach

Challenge: Rapid coking lowers yields, necessitates frequent regeneration, and drives up fuel costs

Fixed Bed Hydrodeoxygenation
Fundamental research highlights opportunities for enhanced performance

Gap: Lack of realistic reaction testing data increases risk and uncertainty

Technical approaches include different catalysts and reactor configurations
Integrated Reaction Testing With Biomass

**Feedstock**
Debarked Loblolly Pine and Forest Residues

**Idaho National Lab**

**Catalyst**
0.5-2.0 wt% Pt/TiO₂ on Technical Supports

**Conditions**

Pyrolysis Temperature: 500 °C  
Upgrading Temperature: 435-450 °C  
Catalyst Mass: 100 g

WHSV: 1.4 g biomass/gcat*h  
Biomass:Catalyst Ratio: 3-13.2  
Hydrogen Concentration: 83%

> 10 L of CFP-oil produced over 100+ reaction cycles
Pt/TiO$_2$ exhibited **improved carbon yields** at similar oxygen content compared to ZSM-5.

- **Pt/TiO$_2$**: Exhibited stable performance over 100+ reaction/regeneration cycles.

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The Pt/TiO$_2$ CFP-oil was hydrotreated using a single stage system for 80+ hours without fouling or plugging.

Fractionation indicates high selectivity to the distillate range:
- 45 wt% in gasoline range
- 39 wt% in diesel range

Fuel testing reveals need for continued R&D:

<table>
<thead>
<tr>
<th></th>
<th>Measured</th>
<th>Target</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gasoline AKI</td>
<td>65</td>
<td>85</td>
</tr>
<tr>
<td>Diesel DCN</td>
<td>24</td>
<td>40</td>
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</tbody>
</table>

CFP provide opportunity to improve fuel quality by controlling hydrogenation and promoting ring opening reactions.

NiMo Sulfide, LHSV: 0.2-0.3, 13 MPa

Conceptual process models indicate a minimum fuel selling price of $3.80, with an opportunity for further reduction through refinery integration and the generation of chemical co-products.

Overall Process
Carbon Yield:
36% for Pt/TiO₂
≤ 22% for ZSM-5

Considerable reduction in carbon intensity

Summary and Research Needs

Integrated reaction testing confirmed potential for improved performance from fixed bed hydrodeoxygenation and motivates investigation of process scale up.

High Yields

Improved Economics

Low Emissions

Process Stability

Scalability

Leverage partnerships to perform particle and reactor scale computational modeling to directly address open questions about reaction kinetics and process scale-up.
Teasing out fundamental information from bench top packed bed reactor experiments with multiscale modeling
Introduction

• Promising bioenergy technologies often *fail at scale-up*

• Modeling can guide engineers moving from bench to pilot
  • Simultaneous transport phenomena at multiple scales

• Multiscale frameworks enable the use of DOE’s high-performance computing (HPC) capacity

• In this work, we apply multi-scale modeling to catalytic fast pyrolysis vapor phase upgrading over platinum on titania
Multiscale phenomena in catalysis

Multiscale phenomena in catalysis

Multiscale phenomena in catalysis

Multiscale phenomena in catalysis

Multiscale phenomena in catalysis

Observed reaction rate: Physics at all scales

- Intra-particle diffusion
- Extra-particle diffusion and convection
- Observed reaction rate
- Intrinsic reaction kinetics
Experimental setup for CFP

Bench scale *ex-situ* catalytic fast pyrolysis system utilized in this work with a packed bed (fixed bed) of catalyst.
Problem description

Packed bed vapor phase upgrading reactor

Relevance:

- Coke profiles predicted by the simulation enable detailed simulation of regeneration cycles.

- Transport-independent kinetic parameters enable computational scaling studies and in-silico reactor optimization.

Pecha, Iisa, Griffin, Mukarakate, French, Adkins, Bharadwaj, Crowley, Foust, Schaidle, and Ciesielski. “Ex situ upgrading of pyrolysis vapors over PtTiO 2: extraction of apparent kinetics via hierarchical transport modeling.” Reaction Chemistry and Engineering, 2020
Yields can be broken down into lumps

A. Bioenergy Technologies Office

<table>
<thead>
<tr>
<th>LMW PV Ketones/Aldehydes</th>
<th>OX Cyclopene/anones Phenol(s) Methylphenols Furanics Additional Light condensables</th>
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<tbody>
<tr>
<td>Acids</td>
<td></td>
</tr>
<tr>
<td>Methoxyphenols</td>
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<tr>
<td>Sugars</td>
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<tr>
<td>Other oxygenates</td>
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<tr>
<td>LG</td>
<td></td>
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<tr>
<td>CH₄</td>
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<tr>
<td>CO</td>
<td></td>
</tr>
<tr>
<td>CO₂</td>
<td></td>
</tr>
<tr>
<td>C₂-C₄ from FBR</td>
<td></td>
</tr>
</tbody>
</table>

B. 2” FBR pyrolysis reactor, 50/50 CP/FR

- Pyrolysis 500 °C
  - HMW PV 15%
  - Light condensables (LC) 2.3%
  - Light gas (LG) 15.2%
  - H₂O 13.3%

- wt.% yields from dry wood
  - char 10.7%
  - LMW PV 45.8%

B. 2” FBR pyrolysis reactor, 100 CP

- Pyrolysis 500 °C
  - HMW PV 15%
  - Light condensables (LC) 0.5%
  - Light gas (LG) 13.9%
  - H₂O 17.5%

- wt.% yields from dry wood
  - char 11.8%
  - LMW PV 41.7%

Packed bed VPU

- B:C 6, 0.5% Pt loading
  - Test case
    - HC 5.9%
    - OX 26.1%
    - LMW PV 19.4%
    - LG 25.8%
    - WAT (H₂O) 18.9%
    - coke 3.9%

- Base case
  - HC 5.2%
  - OX 30.2%
  - LMW PV 19.1%
  - LG 24.0%
  - WAT (H₂O) 18.4%
  - coke 3.1%

- B:C 21, 0.5% Pt loading
  - Test case
    - HC 4.8%
    - OX 32.8%
    - LMW PV 22.1%
    - LG 22.9%
    - WAT (H₂O) 14.8%
    - coke 2.5%

- B:C 3, 1% Pt loading
  - Test case
    - HC 9.7%
    - OX 34.3%
    - LMW PV 2.7%
    - LG 34.5%
    - WAT (H₂O) 12.9%
    - coke 6.0%
Deactivation and multiple active sites

On-stream MS shows rapid deactivation

Lumped reaction scheme describes organic fraction of pyrolysis vapors over PtTiO2

How do changes to catalyst properties and operating conditions impact process performance metrics (yield, composition, catalyst lifetime)?
**Problem:** Accurately model multi-step reactions requires heavy computational resources, not suitable for iterative parameter extraction

**Hypothesis:** An analytical solution to diffusion-reaction-deactivation is mathematically feasible and will accurately represent multi-step reactions

**Solution:** Extend the effectiveness factor

**State of the art** for accounting for diffusion limitations in porous catalysts: Thiele (1930s) + Aris (1970s)

\[
\phi = \sqrt{\frac{ka^2}{D_{\text{eff}}}}
\]

\[
\eta = \frac{3C_{Bi}}{\phi^2} \left( \phi \coth(\phi) - 1 \right)
\]

\[
C_{Bi} = \frac{Bi}{(\phi \coth(\phi) - 1 + Bi)}
\]

No coupling of intraparticle sequential reactions
Extending the Thiele effectiveness factor: A bridge between scales

1) Unsteady advection-diffusion-reaction
\[ \frac{\partial C_i}{\partial t} + u \cdot \nabla (C_i) = \nabla \cdot J_i - \sum_{j=1}^{N} \dot{r}_{ij} + \sum_{m=1}^{N} \dot{r}_{im} \]

2) Assume no advection, sphere
\[ \frac{\partial C_i}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 D_{i,\text{eff}} \frac{\partial C_i}{\partial r} \right) - \sum_{j=1}^{N} \dot{r}_{ij} + \sum_{m=1}^{N} \dot{r}_{im} \]

3) Nondimensionalize, cons. & prod. TM
\[ \hat{C}_i = \frac{C_i}{C_{i,\infty}}, \quad \hat{r} = \frac{r}{R_p}, \quad \hat{t}_i = t \frac{D_{i,\text{eff}}}{R_p^2}, \quad \phi_i = \sqrt{\frac{R_p^2 \psi^t \sum_{j=1}^{N} k_{ij}}{D_{i,\text{eff}}}}, \quad \phi_{im} = \sqrt{\frac{R_p^2 \psi^t k_{im}}{D_{i,\text{eff}}}} \]

4) Quasi-steady state + BCs in sphere (\(\Omega\))
\[ \frac{d^2 \hat{C}_i}{dr^2} + \frac{2}{\hat{r}} \frac{d \hat{C}_i}{d\hat{r}} - \phi_i^2 \hat{C}_i = -\sum_{m} \phi_{im}^2 \hat{C}_m \quad \text{in} \ \Omega \]
\[ \frac{d \hat{C}_i}{d\hat{r}} = 0 \quad \text{on} \ \partial \Omega_1 \]
\[ \frac{d \hat{C}_i}{d\hat{r}} = Bi \left( 1 - \hat{C}_i \right) \quad \text{on} \ \partial \Omega_2 \]

5) Use matrix-vector form (matrix of Thiele moduli for consumption-production)
\[ \frac{d^2 \hat{C}}{dr^2} + \frac{2}{\hat{r}} \frac{d \hat{C}}{d\hat{r}} - \phi^2 \hat{C} = 0 \]

6) When eigenvalues ($\lambda$) are real, solution is hyperbolic function

$$\dot{U}_i = A_1 \sinh(\sqrt{\lambda_i} \hat{r}) + A_2 \cosh(\sqrt{\lambda_i} \hat{r}) \quad \lambda_i > 0$$

7) Converting back to concentration & BCs
(P is eigenvector matrix)

$$\dot{\hat{C}} = \mathbf{PD} \left( \frac{C_{Bi} \sinh(\sqrt{\lambda} \hat{r})}{\sinh(\sqrt{\lambda}) \hat{r}} \right) \mathbf{P}^{-1} \dot{\hat{C}}_{Rat,\infty}$$

8) Volume-averaging the rates

$$< \dot{r}_{ij} > \equiv \frac{4\pi R_p^3 \psi k_{ij} C_{1,\infty}}{4/3\pi R_p^3} \int_0^1 \dot{\hat{C}}_i \hat{r}^2 \, d\hat{r} = \psi k_{ij} C_{1,\infty} \eta_i,$$

9) Multi-step effectiveness vector! (MEV)

$$\eta = \mathbf{PD} \left( \frac{3C_{Bi}}{\lambda} \left( \sqrt{\lambda} \coth(\sqrt{\lambda}) - 1 \right) \right) \mathbf{P}^{-1} \dot{\hat{C}}_{Rat,\infty}$$

10) Individual rates with MEV!

$$< \dot{r}_i > \equiv \sum_m < \dot{r}_{im} > - \sum_j < \dot{r}_{ij} > = \psi C_{1,\infty} \left( \sum_m k_{im} \eta_m - \sum_j k_{ij} \eta_i \right)$$

Apply multistep effectiveness vector to PBR

Packed bed transport equations

\[
\frac{\partial PV_{LMW}}{\partial t} = -u \frac{\partial PV_{LMW}}{\partial x} + D_{PV} \frac{\partial^2 PV_{LMW}}{\partial x^2} - R_{PV,LMW,eff} \left(1 - \varepsilon_p\right)
\]

\[
\frac{\partial OX}{\partial t} = -u \frac{\partial OX}{\partial x} + D_{OX} \frac{\partial^2 OX}{\partial x^2} - R_{OX,eff} \left(1 - \varepsilon_p\right)
\]

\[
\frac{\partial HC}{\partial t} = -u \frac{\partial HC}{\partial x} + D_{HC} \frac{\partial^2 HC}{\partial x^2} - R_{HC,eff} \left(1 - \varepsilon_p\right)
\]

\[
\frac{\partial LG}{\partial t} = -u \frac{\partial LG}{\partial x} + D_{LG} \frac{\partial^2 LG}{\partial x^2} - R_{LG,eff} \left(1 - \varepsilon_p\right)
\]

\[
\frac{\partial WAT}{\partial t} = -u \frac{\partial WAT}{\partial x} + D_{WAT} \frac{\partial^2 WAT}{\partial x^2} - R_{WAT,eff} \left(1 - \varepsilon_p\right)
\]

\[
\frac{\partial S1}{\partial t} = R_{S1,eff} \left(1 - \varepsilon_p\right)
\]

\[
\frac{\partial S2}{\partial t} = R_{S2,eff} \left(1 - \varepsilon_p\right)
\]

\[
\frac{\partial CK}{\partial t} = R_{CK,eff} \left(1 - \varepsilon_p\right)
\]

\[PV_{LMW} = PV_{LMW,0}, \ x = 0\]

\[HC = OX = LG = WAT = 0, \ x = 0\]

\[
\frac{dPV}{dt} = \frac{dOX}{dt} = \frac{dHC}{dt} = \frac{dLG}{dt} = \frac{dWAT}{dt} = 0, \ x / L = 1
\]
Catalyst characterization

Multiscale imaging of the Pt/TiO2 catalyst particles

(a) Light microscopy of catalyst particles showing the spherical bulk geometry with narrow size distribution. (b) Scanning electron microscopy (SEM) of the particle surface reveals a porous support structure formed by the agglomeration of TiO2 nanoparticles. (c) Transmission electron microscopy shows the presence of ~5 nm Pt particles visualized as dark spots on the surface of the larger TiO2 support structure.

TEM Tomography of the TiO2 catalyst particle mesostructure

(a, b) Slices through the tomographic volume are shown at two different magnifications. Pt particles are clearly identified by their higher electron density (indicated by red arrows in panel b). (c, d) 3D visualizations of the reconstructed volume are shown at two different magnifications.
Apparent rate constants fit to real data

Initial guess for 10 apparent rate parameters + experimental data

Simplex parameter optimizer + PBR model

New parameters from optimizer

Multiscale packed bed model

Objective function (yield vs time)

Best-fit lumped rate constants fit for base case

<table>
<thead>
<tr>
<th>RATE CONSTANT</th>
<th>FITTED VALUE</th>
</tr>
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<tbody>
<tr>
<td>$k_1$ [s$^{-1}$]</td>
<td>76</td>
</tr>
<tr>
<td>$k_{1g}$ [s$^{-1}$]</td>
<td>50.5</td>
</tr>
<tr>
<td>$k_{1w}$ [s$^{-1}$]</td>
<td>39</td>
</tr>
<tr>
<td>$k_2$ [s$^{-1}$]</td>
<td>5.4</td>
</tr>
<tr>
<td>$k_{2g}$ [s$^{-1}$]</td>
<td>0.7</td>
</tr>
<tr>
<td>$k_{2w}$ [s$^{-1}$]</td>
<td>7.9E-10</td>
</tr>
<tr>
<td>$k_3$ [s$^{-1}$]</td>
<td>7E-14</td>
</tr>
<tr>
<td>$k_4$ [s$^{-1}$]</td>
<td>3.7E-4</td>
</tr>
<tr>
<td>$\Theta_{S_1}$</td>
<td>1.2E-3</td>
</tr>
<tr>
<td>$\Theta_{S_2}$</td>
<td>15.2</td>
</tr>
</tbody>
</table>
Results: Model validation

Yields from low MW pyrolysis vapors, VPU only

0.5% Pt, 0.5mm, 50/50 clean pine/FR, B:C=6

Yields from dry wood for pyrolysis + VPU

0.5% Pt, 0.5mm, 50/50 clean pine/FR, B:C=12

0.5% Pt, 0.5mm, 50/50 clean pine/FR, B:C=21

1% Pt, 0.5mm, clean pine, B:C=3
Results: Predictions and extrapolations

- **Pressure drop vs Particle Diameter**
  - Dependence on reactor diameter
  - Different reactor diameter values: Drxr = 0.016 m, Drxr = 0.024 m, Drxr = 0.032 m, Drxr = 0.040 m, Drxr = 0.048 m, Drxr = 0.056 m, Drxr = 0.064 m

- **Catalytic Conversion vs Particle Diameter**
  - Final timestep
  - Dependence on reactor diameter
  - Different reactor diameter values: Drxr = 0.016 m, Drxr = 0.024 m, Drxr = 0.032 m, Drxr = 0.040 m, Drxr = 0.048 m, Drxr = 0.056 m, Drxr = 0.064 m

- **Coke concentration vs reactor length**
  - 0.5%Pt, B:C=12
  - Different times: l=0h, 0.8h, 1.5h, 2.2h, 3.1h, 3.8h, 4.5h, 5.3h, 6.1h, 7.1h

The graphs illustrate the changes in concentration, pressure drop, and catalytic conversion over different periods and reactor diameters.
Conclusions

• New multiscale simulation framework was capable of capturing
  • multiple cascading reactions
  • multiple operating conditions
  • catalyst loadings
  • active site deactivation

• Fast, accurate, can be used to mine old *good* data

• Future work will extend the model to other catalyst shapes, other technologies

• In the next slides, you will see how results from this work were used to design a catalytic regeneration system at a much larger scale with a different set of modeling tools.
Packed Bed Reactor Scale-up Using High Fidelity Reactor Models
Lab Scale Packed Bed Reactor (PBR) and Catalyst

**Upgrading**

- **Biomass Feed, g/hr**: 150
- **Inlet Pressure, kPa**: 110
- **Inlet Temperature, °C**: 410
- **H2 Flowrate, SLPM**: 13.5
- **N2 Flowrate, SLPM**: 2.4
- **WHSV, hr⁻¹**: 1.5
- **Duration, B/C (hr)**: 12 (8)

**Oxidative Regeneration**

- **Inlet Temperature, °C**: 410
- **Outlet Temperature, °C**: 450
- **N2 Flowrate, SLPM**: 15.6
- **Air Flowrate, SLPM**: 0.42
- **Duration, hr**: 8

**0.5 mm Pt/TiO₂ Spheres**

- **Purge Gas**
- **BM Hopper**
- **2” Bubbling-Bed Pyrolyzer**
- **Char Cyclone**
- **Char Pot**
- **1.37” Tubular Reactor**
- **Product Gases**
- **Condenser**
- **Liquid Products**
- **ESP**

**Images and Diagrams**

- Diagram showing the process flow of the PBR and catalyst regeneration.
- Image of 0.5 mm Pt/TiO₂ Spheres.
Scaling Up the PBR

- TCPDU-PBR
  - 6 kg cat
  - 9 kg/hr biomass
  - WHSV 1.5 hr⁻¹

- Constraints
  - PBR ΔP 20 kPa or less
  - No wall heat removal (mimic industrial scale)
  - Gas temperature ≈ 400°C to minimize cycle time and ensure quick light-off
  - B/C = 12 corresponds to 25 wt% coke (g C / g fresh)
• Split the 6 kg bed between 3 existing reactors, 2 kg each
• Per-bed scale-up = 20 X
• N2 flow limit = 1200 SLPM, 400 kg per bed
• Each reactor has 3 heating rods which can be converted to cooling tubes
• Air flow limit = 1800 SLPM, 200 per tube
Model Details

TCPDU
18M Pellets

2FBR
900k Pellets

\[ n_{\text{cell}} = 152k \quad n_{\text{pellet/cell}} = 120 \]

\[ n_{\text{cell}} = 434k \quad n_{\text{pellet/cell}} = 42 \]

<table>
<thead>
<tr>
<th>N2 Flow, SLP (SLPM)</th>
<th>Cooling Air Flow, SLP (30°C)</th>
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<tbody>
<tr>
<td>600</td>
<td>300</td>
</tr>
<tr>
<td>400</td>
<td>Case 1</td>
</tr>
<tr>
<td>300</td>
<td>Case 4</td>
</tr>
<tr>
<td>200</td>
<td>Case 7</td>
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</table>
2FBR Data Used in Model Development

**Catalyst / Bed Parameters**

<table>
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<tr>
<th>Parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>$A_f$, m$^3$/mol.s</td>
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<tr>
<td>$E_a$, J/mol</td>
<td><strong>5x10^4</strong></td>
</tr>
<tr>
<td>ABD, kg/m$^3$</td>
<td><strong>900</strong></td>
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<tr>
<td>$\rho_{skel}$, kg/m$^3$</td>
<td><strong>3,900</strong></td>
</tr>
<tr>
<td>$\rho_{pe}$, kg/m$^3$</td>
<td><strong>1,900</strong></td>
</tr>
<tr>
<td>Pellet porosity</td>
<td><strong>0.592</strong></td>
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<tr>
<td>Bed voidage</td>
<td><strong>0.437</strong></td>
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<tr>
<td>Total voidage</td>
<td><strong>0.770</strong></td>
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<tr>
<td>BET, m$^2$/g</td>
<td><strong>54</strong></td>
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<tr>
<td>Pore diam, nm</td>
<td><strong>27</strong></td>
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**Thermal Parameters**

<table>
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<th>Parameter</th>
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<tr>
<td>$\Delta H$, J/mol</td>
<td><strong>3.94x10^5</strong></td>
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<tr>
<td>Thermal conductivity, W/(m.K)</td>
<td>$k_{s,eff}$</td>
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<tr>
<td>Wall heat transfer, W/(m$^2$.K)</td>
<td>$h_w$</td>
</tr>
<tr>
<td>Bulk heat capacity, J/(kg.K)</td>
<td><strong>680</strong></td>
</tr>
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</table>

**CO$_2$ in effluent gas**

**Outlet temperature**

**Coke profile predicted by kinetics model**
Biggest Unknown: Heat Transfer Parameters

![Diagram showing relationship between Wall Heat Transfer Coefficient (h_w) and Effective Solids Thermal Conductivity (k_{s,effect})](image)

- **Gases**
- **Catalysts in Literature**
- **Bulk Oxides**

The graph illustrates a significant decrease in Wall Heat Transfer Coefficient as the Effective Solids Thermal Conductivity increases, indicating a challenge in heat transfer parameters in bioenergy technologies.
TCPDU Model Predictions

Temperature, °C  \n\∇T, °C/cm  \ndT/dt, °C/s

400 SLPM N₂
No Cooling Air

200 SLPM N₂
600 SLPM
Cooling Air

Rapid Cooldown

Sharp Gradients

Air Flow Direction

t = 3 hrs
TCPDU Model Predictions (2)

200 SLPM N2, 600 SLPM Cooling Air

B.D. Adkins et.al, Predicting thermal excursions during in-situ oxidative regeneration of packed bed catalytic fast pyrolysis catalyst, submitted to Reaction Chemistry and Engineering
Conclusions

1. Risk of catalyst damage and/or accelerated irreversible deactivation from thermal excursion is high in proposed TCPDU design
   - Pressure drop associated with small catalyst particle size (0.5 mm) constrains bed depth and process gas flow rate, both of which constrain heat removal

2. Potential design improvements
   - Construct reduced order models and thoroughly map catalyst / bed design space
   - Evaluate moving bed alternatives to packed bed. Not fluid bed: more like Continuous Catalytic Reformers (CCRs)

3. Although small by industry standards, a scale-up factor of 20 can be substantial, as demonstrated here
1. Firm up conclusions from regen model by addressing key unknowns
   - Thermal conductivity of catalyst pellets
     - Experimental measurements
     - High resolution mesoscale modelling of heat transfer
   - Coke distribution
     - Bed dissection
     - Carbon distribution in pellet interiors

2. Expand model to include stacked beds with multiple catalysts
Stacked Bed Model

Exothermic

\[ + 3 \text{H}_2 \xrightarrow{\Delta H_1} \text{A}_{f,1} \text{E}_{a,1} \]

Endothermic

\[ + \text{H}_2 \xrightarrow{\Delta H_2} \text{A}_{f,2} \text{E}_{a,2} \]

Bed-Specific Parameters

- Mass of catalyst
- ABD
- Skeletal density
- Particle size
- Particle shape
- Pore volume
- Surface area
- Pore diameter
- Porosity
- Void fraction
- Thermal conductivity
- Heat capacity
- Wall heat transfer coeff.
- Reaction rate constants
- Reaction enthalpy
- ...
Stacked Bed Model

\[ \log(A_{f,1}) \leftarrow \log(A_{f,2}) \rightarrow \]

<table>
<thead>
<tr>
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<th>Mass Fractions</th>
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<td>benzene</td>
<td>0.8</td>
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<tr>
<td>cyclohexane</td>
<td>0.08</td>
</tr>
<tr>
<td>ethylene</td>
<td>0.25</td>
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<td>butane</td>
<td>0.5</td>
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## Acknowledgements

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<th>Hydrotreating (PNNL)</th>
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<td>Joshua Schaidle</td>
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<td>Anne Starace</td>
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<td>Susan Habas</td>
<td>Vivek Bharadwaj</td>
<td>Feedstock Logistics (INL)</td>
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<td>Connor Nash</td>
<td>Meagan Crowley</td>
<td>Damon Hartley</td>
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<td>Carrie Farberow</td>
<td>Tom Foust</td>
<td>Jordan Klinger</td>
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<td>Matt Yung</td>
<td>Aaron Lattanzi</td>
<td>Fuel Properties (NREL)</td>
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<td>Mark Nimlos</td>
<td>Zach Mills</td>
<td>Nolan Wilson</td>
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<td>Anne Starace</td>
<td>Austin Ladshaw</td>
<td>Earl Christensen</td>
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<td>James Parks II</td>
<td>Lisa Fouts</td>
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Packed Bed Modeling (NREL)

- Vivek Bharadwaj
- Meagan Crowley
- Tom Foust
- Aaron Lattanzi

Packed Bed Modeling (ORNL)

- Zach Mills
- Austin Ladshaw
- James Parks II
Thank you. Let’s Discuss.

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