U.S. DEPARTMENT OF ENERGY

Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

Webinar: Cost-Effectively Optimize and Scale Bioenergy Technologies with the Consortium for Computational Physics and Chemistry (CCPC)

Presenters:

- Dr. Jim Parks: CCPC Principal Investigator and Section Head for Energy and Industrial Decarbonization at Oak Ridge National Laboratory
- Dr. Jim Dooley: Chief Technology Officer, Forest Concepts, LLC
- Dr. Kevin Barnett: Chief Technology Officer, Pyran
- Joaquín Alarcón: President and Chief Executive Officer, Catalyxx, Inc.

Feedstock | Algae | Conversion | Systems | Data

October 20, 2022

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About the Bioenergy Communicators (BioComms) Working Group

Sponsor:

- U.S. Department of Energy (DOE)
- Office of Energy Efficiency and Renewable Energy (EERE)
- Bioenergy Technologies Office (BETO)

BETO & DOE National Laboratory Members:

- Bioenergy communicators, laboratory relationship managers, BETO tech team, and education and workforce development professionals

Purpose:

- Communications strategy for BETO-funded bioenergy research and development

Photo by iStock

Today's Agenda

I. Dr. Jim Parks, CCPC Overview

II. CCPC Industry Partners:

   A. Dr. Jim Dooley, Forest Concepts, LLC

   B. Dr. Kevin Barnett, Pyran

   C. Joaquín Alarcón, Catalyxx, Inc.

Photo courtesy of iStock

Today's Presenters

Dr. Jim Parks
Oak Ridge National Laboratory

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Dr. Jim Dooley
Forest Concepts, LLC

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Dr. Kevin Barnett
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Dr. Jim Parks

CCPC Principal Investigator and Section Head for Energy and Industrial Decarbonization

Oak Ridge National Laboratory (ORNL)

CCPC

Consortium for Computational Physics and Chemistry

U.S. DEPARTMENT OF ENERGY

BIOENERGY TECHNOLOGIES OFFICE

Consortium for Computational Physics and Chemistry Overview

Jim Parks (ORNL, parksjeii@ornl.gov), Principal Investigator and Industry Partners

Bioenergy Technologies Office Webinar, October 20, 2022

U.S. DEPARTMENT OF ENERGY

Bioenergy Technologies Office Consortia

The Consortium for Computational Physics and Chemistry (CCPC) is a Bioenergy Technologies Office (BETO) consortium composed of six national labs ***applying multi-scale computational science to enable and accelerate the bioenergy economy.***

CCPC
Consortium for Computational Physics and Chemistry
U.S. DEPARTMENT OF ENERGY
BIOENERGY TECHNOLOGIES OFFICE

Oak Ridge National Laboratory

National Energy Technology Laboratory

Pacific Northwest National Laboratory

A multi-scale problem
… A multi-lab solution

Argonne National Laboratory

INL Idaho National Laboratory

NREL National Renewable Energy Laboratory

Agile BioFoundry

fcic
FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

ChemCatBio
Chemical Catalysis for Bioenergy

BIOPROCESSING SEPARATIONS CONSORTIUM

Co-Optimization of Fuels & Engines
FOR TOMORROW'S ENERGY-EFFICIENT VEHICLES

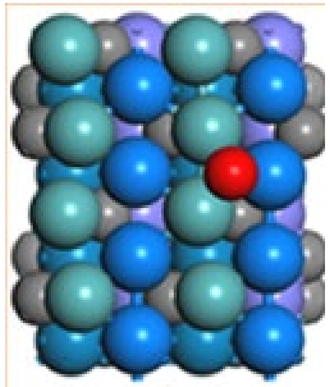
CCPC: A multi-scale problem… A multi-lab solution

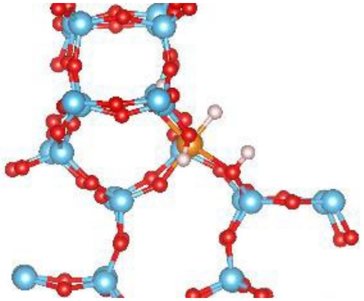
Catalysis Modeling at Atomic Scales

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Argonne
NATIONAL LABORATORY

Pacific Northwest
NATIONAL LABORATORY



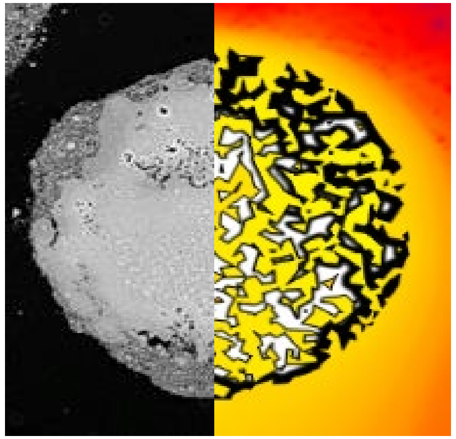


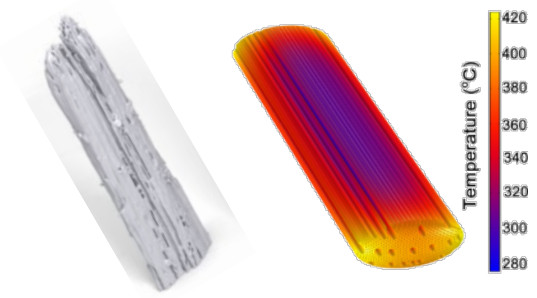
Investigating novel catalyst material combinations and understanding surface chemistry phenomena to guide experimentalists

Biomass and Catalyst Particle Modeling at Meso Scales

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

INL
Idaho National Laboratory





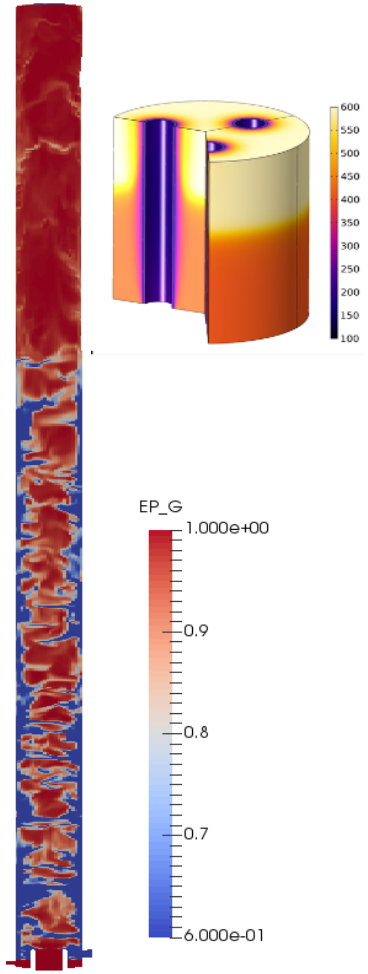
Understanding mass transport of reactants/products, reaction kinetics, and coking and deactivation processes

Conversion Modeling at Reactor Scales

NETL
NATIONAL ENERGY TECHNOLOGY LABORATORY

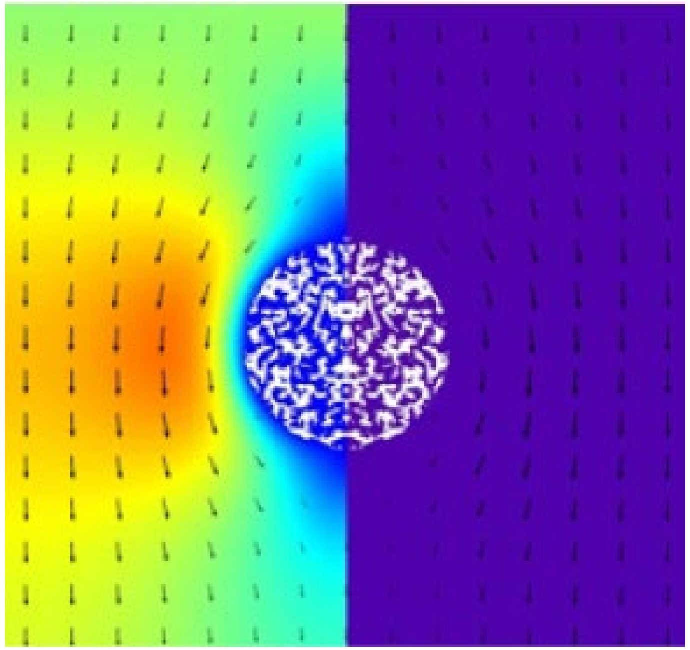
OAK RIDGE
National Laboratory

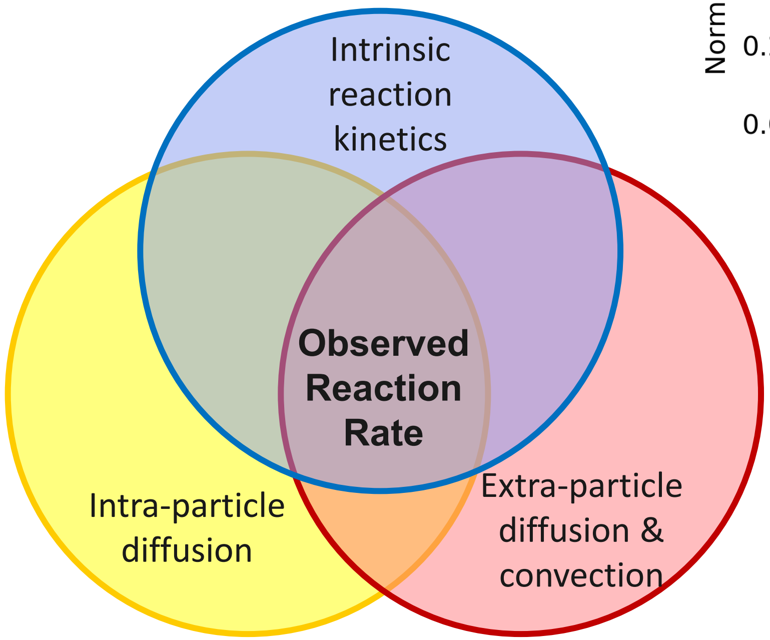
Determining optimal process conditions for maximum yield and enabling scale-up of biomass conversion and catalytic upgrading reactors

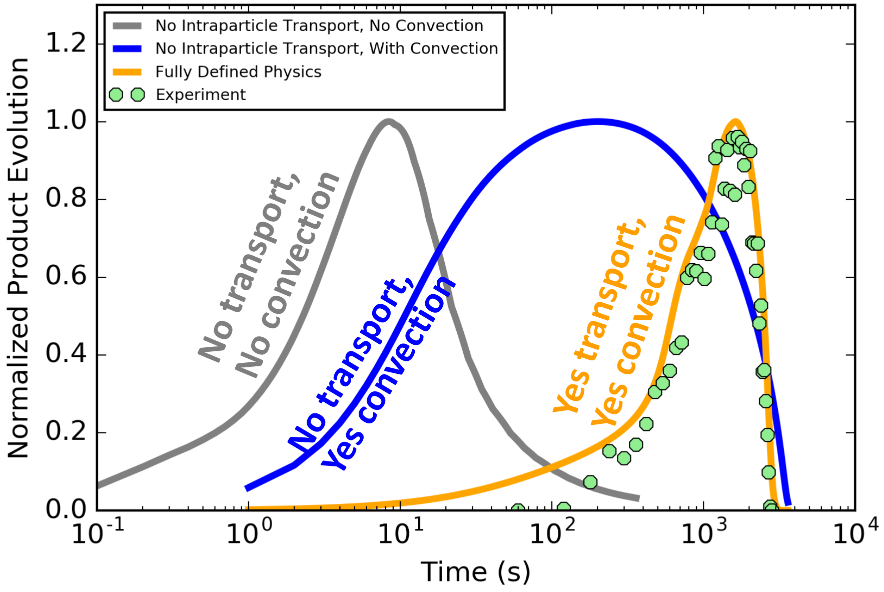


Fixed-Bed Catalyst Reactor for Bioenergy

Heat and Mass Transfer Effects Are Critical to Capturing Accurate Chemical Conversion in Porous Catalyst Particles







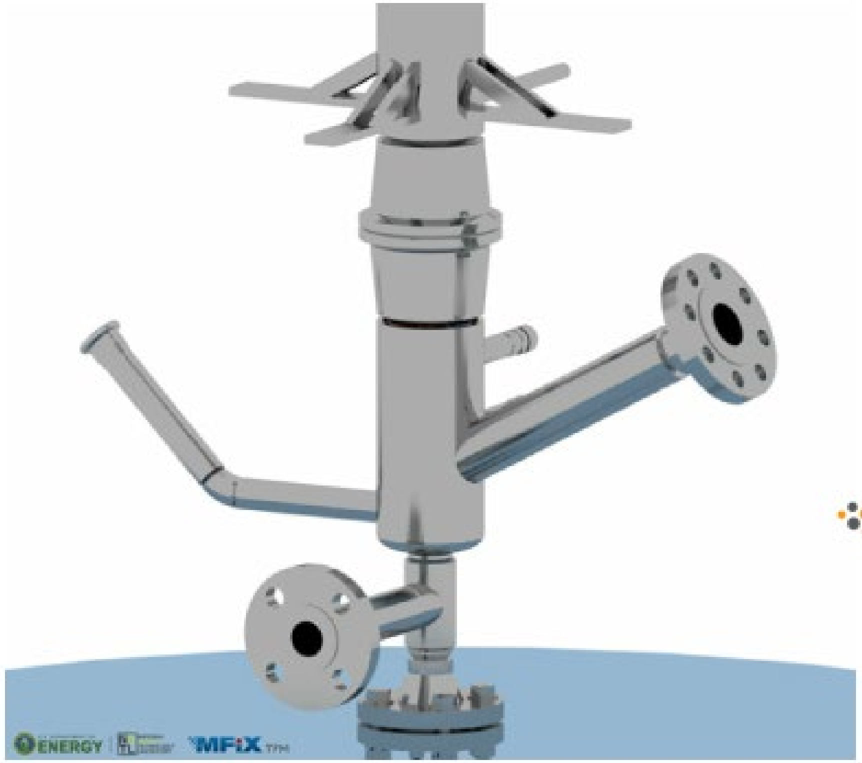
As the process gas flows around the catalyst particle, diffusion of reactants into the catalyst occurs to produce transportation fuel products as well as coke (shown in black) which deactivates the catalyst until coke oxidation regenerates the catalyst

Mass transfer, or diffusion of reactants and products into and out of the catalyst particle, is critical to obtaining accurate representation of conversion processes

Reactor Scale Model of Riser-Type Catalytic Upgrading Reactor

MFiX CFD reactor models capture residence time and mixing effects

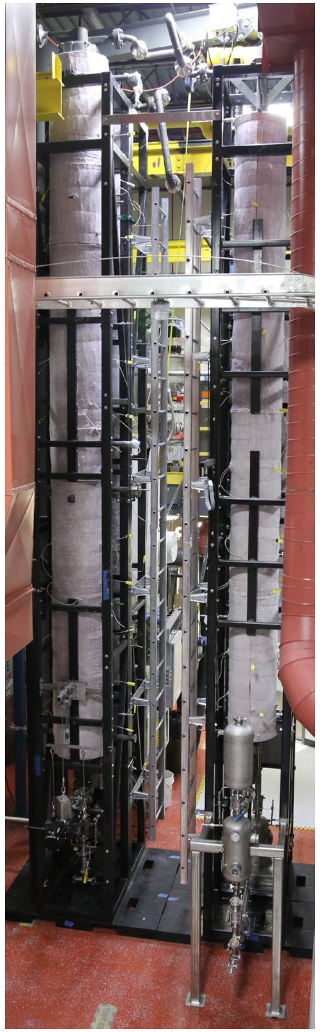
CFD and reduced order models inform BETO reactor teams; experiments validate model results



MFiX model of R-Cubed Catalytic Upgrading Reactor

MFiX

mfix.netl.doe.gov



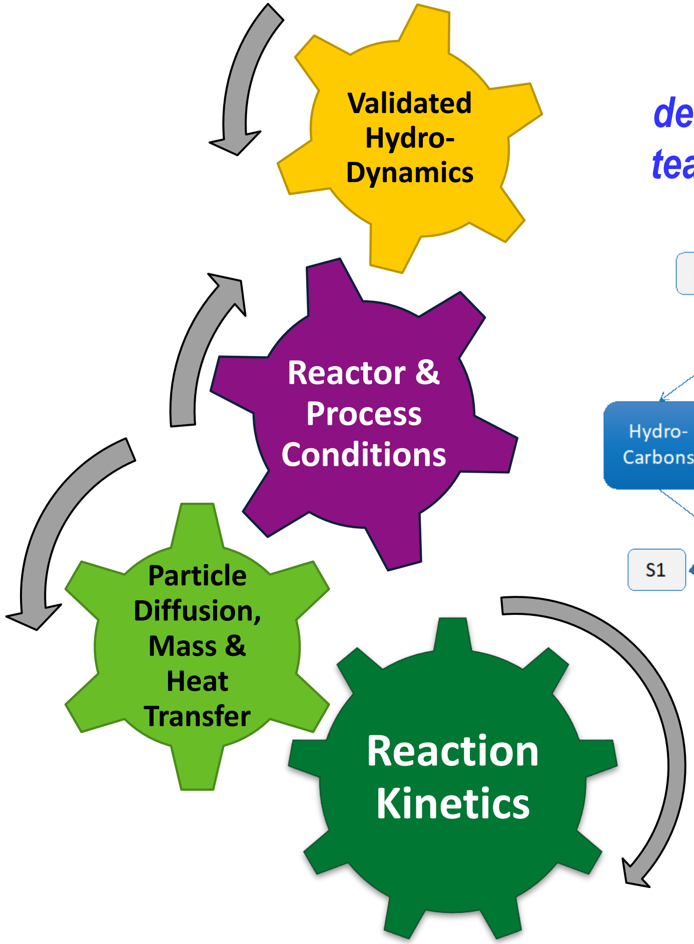
R-Cubed Catalytic Upgrading Reactor at NREL

MFiX (Multiphase Flow with Interphase eXchange) is a computational fluid dynamics (CFD) code developed by DOE's NETL

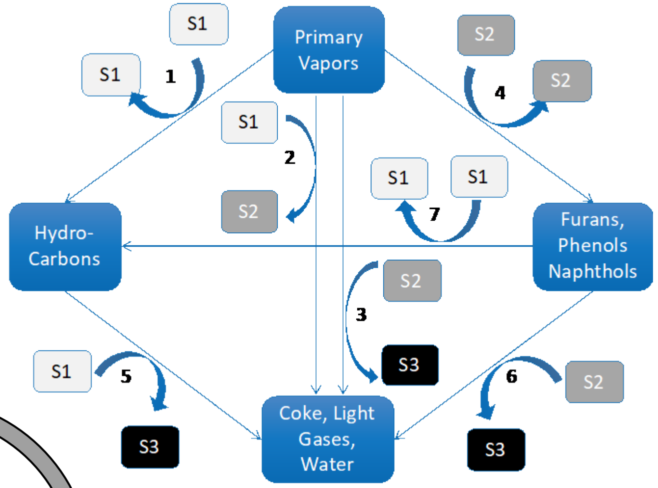
Riser-Type Reactor Model of Catalytic Fast Pyrolysis Upgrading

Bioenergy-specific kinetics implemented in full Computational Fluid Dynamics (CFD) reactor simulation of Catalytic Fast Pyrolysis

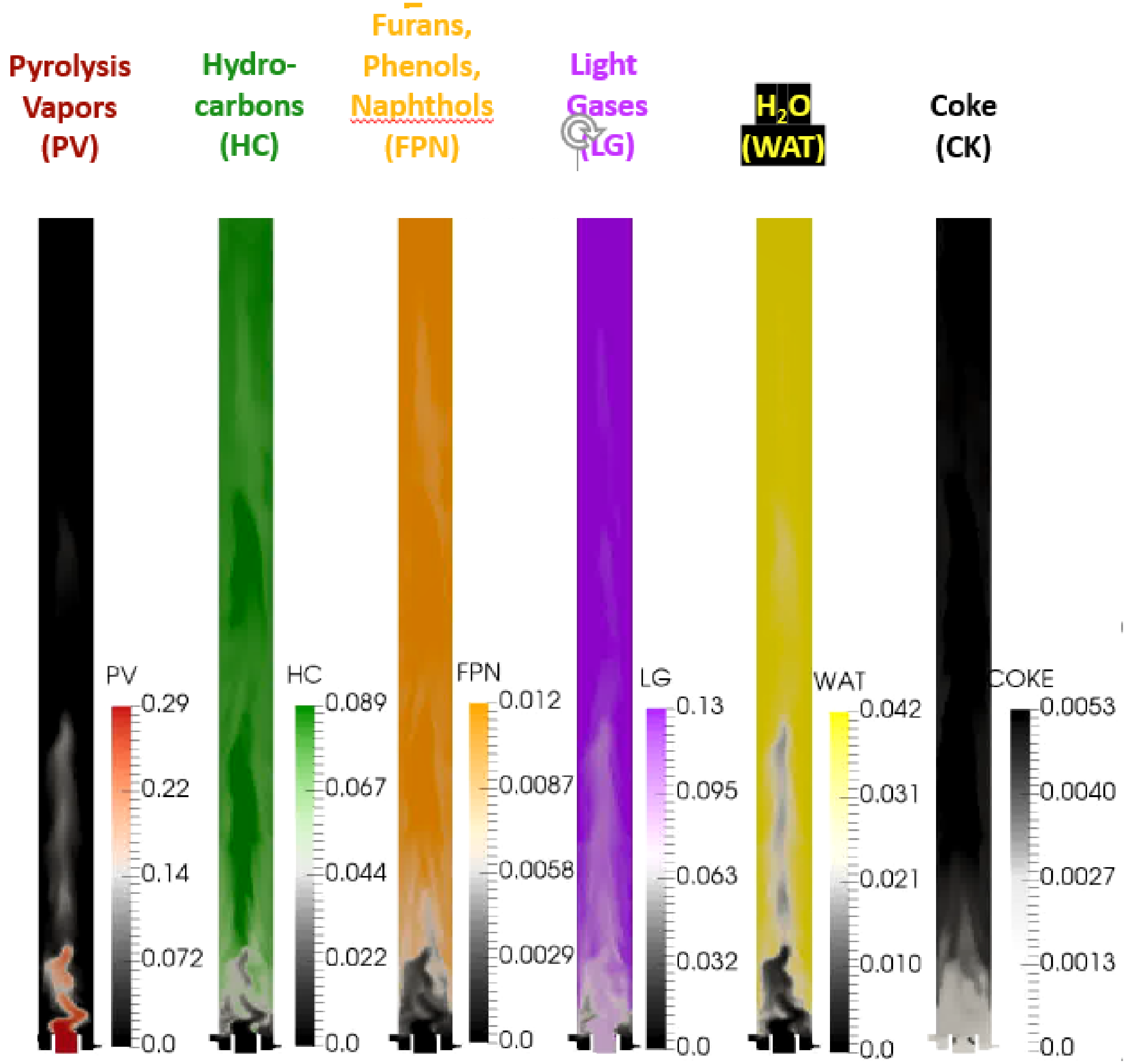
Critical elements to reactor and process model include reaction kinetics



Kinetic reaction pathway developed and applied by CCPC team for Catalytic Fast Pyrolysis



Catalytic Fast Pyrolysis Vapor Upgrading Reactor Model



CCPC Modelers Contributing to Today's Webinar Outcomes

Yidong Xia

Peter Ciesielski

Canan Karakaya

Bruce Adkins

Idaho National Laboratory

NREL NATIONAL RENEWABLE ENERGY LABORATORY

OAK RIDGE National Laboratory

OAK RIDGE National Laboratory

Special thanks for guidance and support from the U.S. Department of Energy Bioenergy Technologies Office and CCPC Technology Manager Trevor Smith.

CCPC Models Enabling Industry Partners

Representative projects supported by the U.S. Department of Energy Bioenergy Technologies Office in the CCPC Direct Funded Opportunity program.

forestconcepts™

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forestconcepts™

Consortium for Computational Physics and Chemistry (CCPC)

Quantifying Improvements in Feedstock Performance Resulting from Forest Concepts' Preprocessing Technology

Jim Dooley

Co-Founder and Chief Technology Officer

Making the World a Better Place With Sound Science, Disciplined Design, & Functional Products

Since 1998, our focus has been on the supply chain for biomass from forests, agricultural, and urban sources.

We develop novel technical solutions to enable the bioeconomy and improve sustainability of industrial bioprocesses.

forestconcepts™

Core Competencies

- Focus on *Big Deal* problems and challenges
- Market assessments frame development programs
- Science before engineering – Know the 1st principles
- Experiment and lab derivation of engineering data
- Disciplined design before the first weld
- Proven production operations and logistics
- Relationship-based sales and marketing
- Close relationships with federal agencies
- Strategic patents: High 1st action allowance rate

The "Forest Concepts' Preprocessing Technology"

- **Functional objectives include:**
  - Minimize comminution energy for high moisture biomass to approach theoretical minimums based on cutting parallel and cross grain
  - Produce uniform particles that have a shape that balances heat transfer and diffusion across the particle with mass-flow of solutes or vapors out the ends of the particles (PNNL, NREL, and WSU science)
  - Maximize mass percentage of biomass that ends up in conversion-ready feedstock.
- **Client constraints include:**
  - Avoid production of dust that requires costly control systems
  - Make it quiet enough to talk around.

The Driving Questions?

2010 – How does the ratio of particle length to thickness matter for pyrolysis?

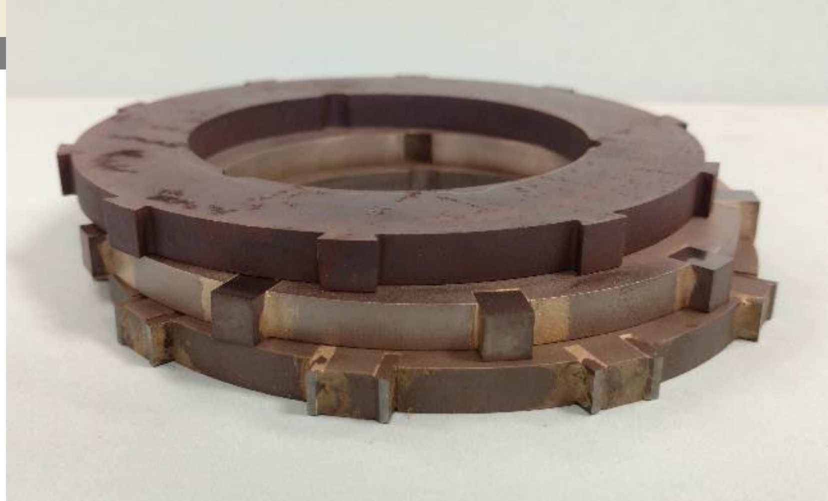
- D. Santosa, A. Zacher, D. Eakin. 2012. Fast Pyrolysis Conversion Tests of Forest Concepts' Crumbles™. Report PNNL-21256
- M. Garcia-Perez, S. Chen, J. de Graaf, D. Gao, J. A. Garcia-Nunez. 2012. Optimization and Low Energy Production of Woody Biomass Particles - Modeling of Pyrolysis Reactions and Modeling of Enzymatic Hydrolysis
- **Answer: When the particle length is more than about three times the thickness, mass flow out becomes limiting over diffusion and heat transfer into the particle.**

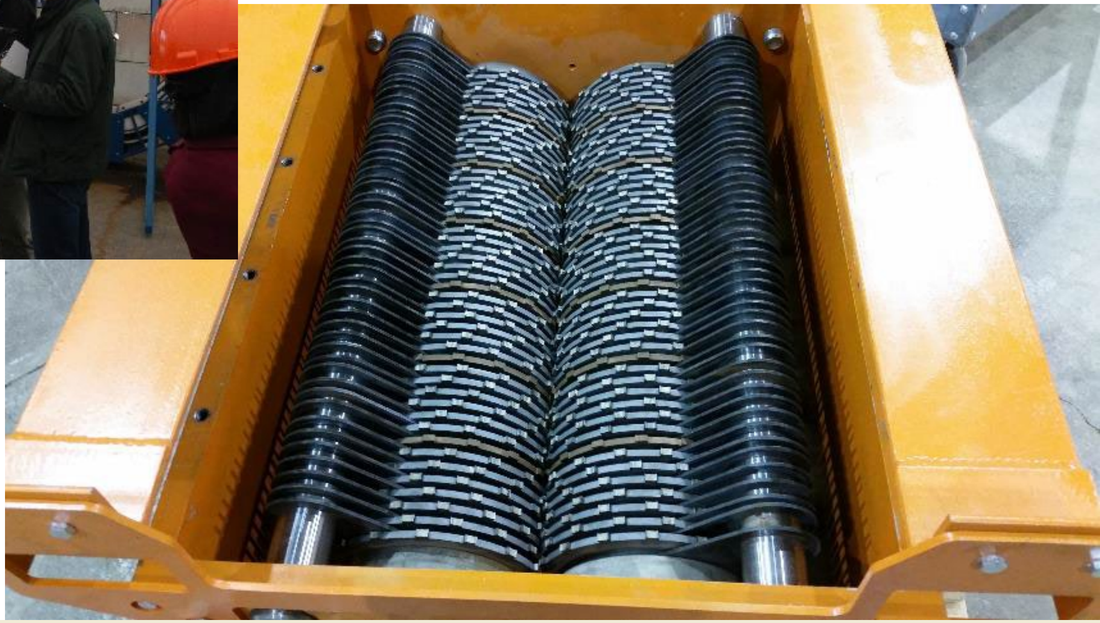
- **Engineering and Operational Interpretations:**
  - **Aspect ratio of 1.0 (perfect cubes) is not needed. Strive for aspect ratio less than 3.0.**
  - **Smaller (thinner) particles will improve reaction rates, but the optimum is a systems question.**

The "Forest Concepts' Crumbler® Rotary Shear"

"Sort of like a paper shredder"

- Cutter thickness controls particle size
- Processes any moisture content from dry to wet
- Specific energy fairly independent of moisture
- Quiet
- Dust control not needed for most materials





Crumbles® Feedstocks

6 mm

2 mm

Crumbles® feedstocks "believers"

Compared to hammermilled biomass of the same "size," rotary sheared material:

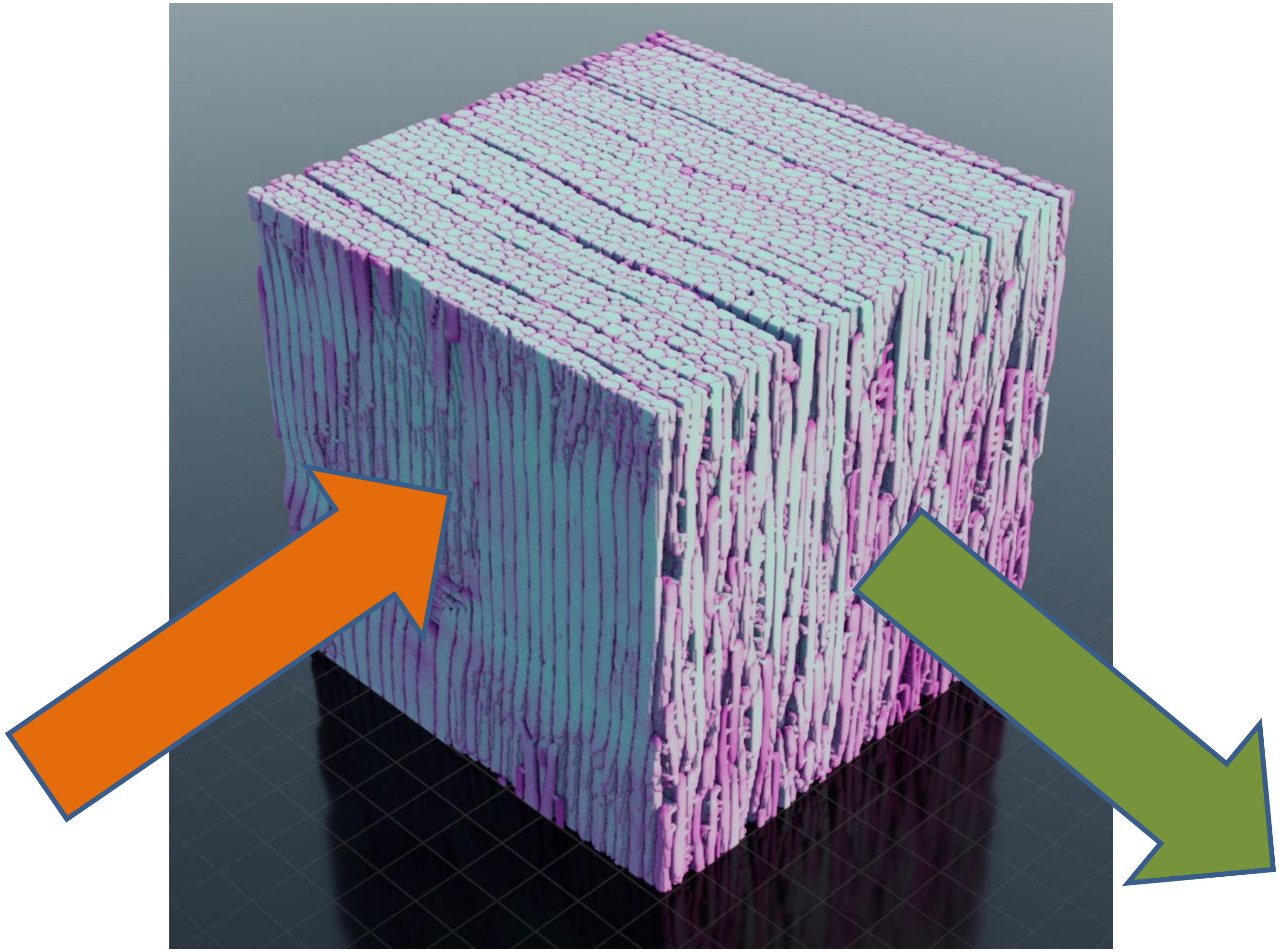
- Flows freely
- Reacts more uniformly, producing less secondary reaction chemicals
- Has higher mass yield of target product

CCPC Questions:

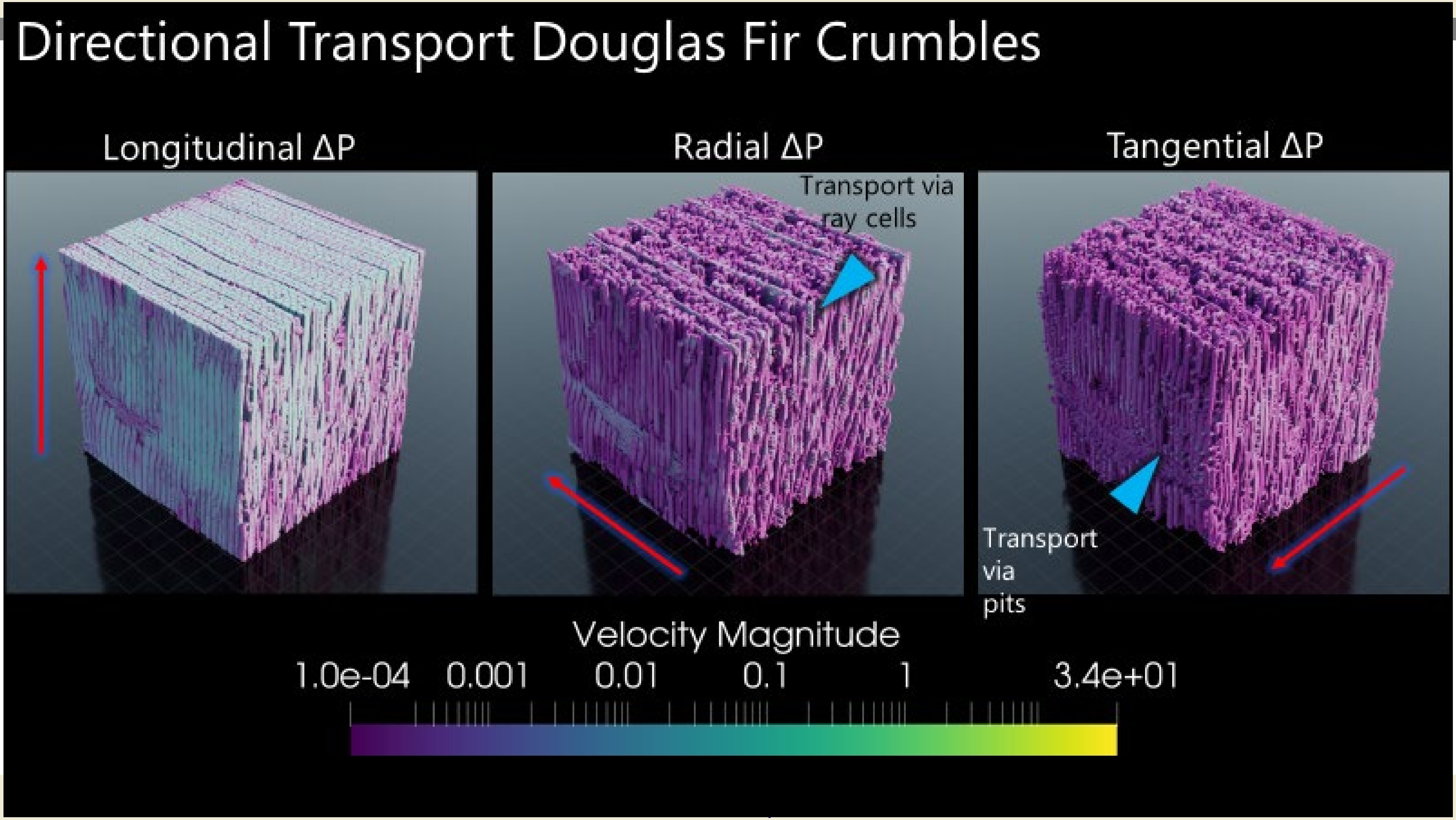
What is it about the Forest Concepts' Crumbles feedstock that explains the observed performance differences?

- Peter Ciesielski – Microstructure
  - Understanding intraparticle transport within individual particles.
- Yidong Xia – Flowability
  - The impact of critical material attributes, including particle size (2–6 mm), particle shape (briquette, chip, clumped-sphere, cube, etc.), and surface roughness on the angle of repose.

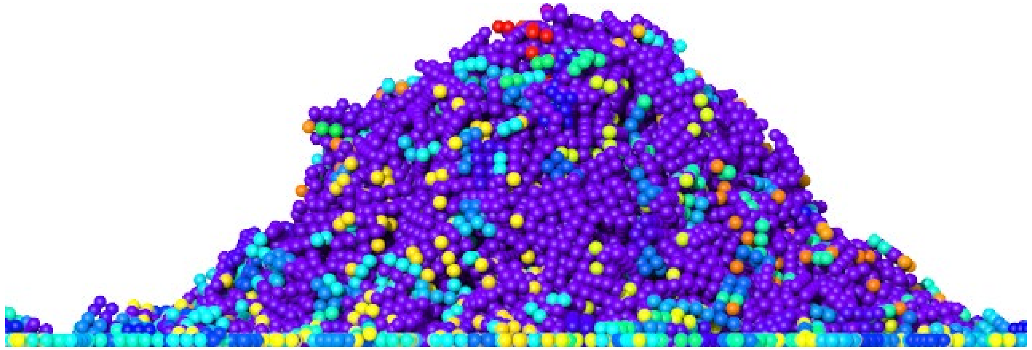
NREL Microstructure Results



It is really way more complex!



Flowability Modeling – Angle of Repose



Application of Discrete Element Modeling to predict angle of repose for bulk biomass.

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Thank You

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Dr. Kevin Barnett

Chief Technology Officer

Pyran

Pioneer in Sustainable Chemistry

October 20, 2022

PYRAN

Pyran – Pioneer in Sustainable Chemistry

Using a simple process and proven catalysts.

- Pyran creates biomass-based substitutes for fossil fuel-derived chemicals in four simple catalytic steps.
- 20%–40% lower production costs than petrochemical processes.

Addressing an attractive market.

- Targeting a $65B market opportunity to replace petrochemical products.
- First commercial product market is $1.5B with a 9.5% CAGR.[1]

Expanding sales through customer validation.

- Toll producing to supply initial customer orders and sample requests for customer qualification.
- Pyran's initial offering exhibits superior qualities to incumbent suppliers in core end markets.

Reducing emissions.

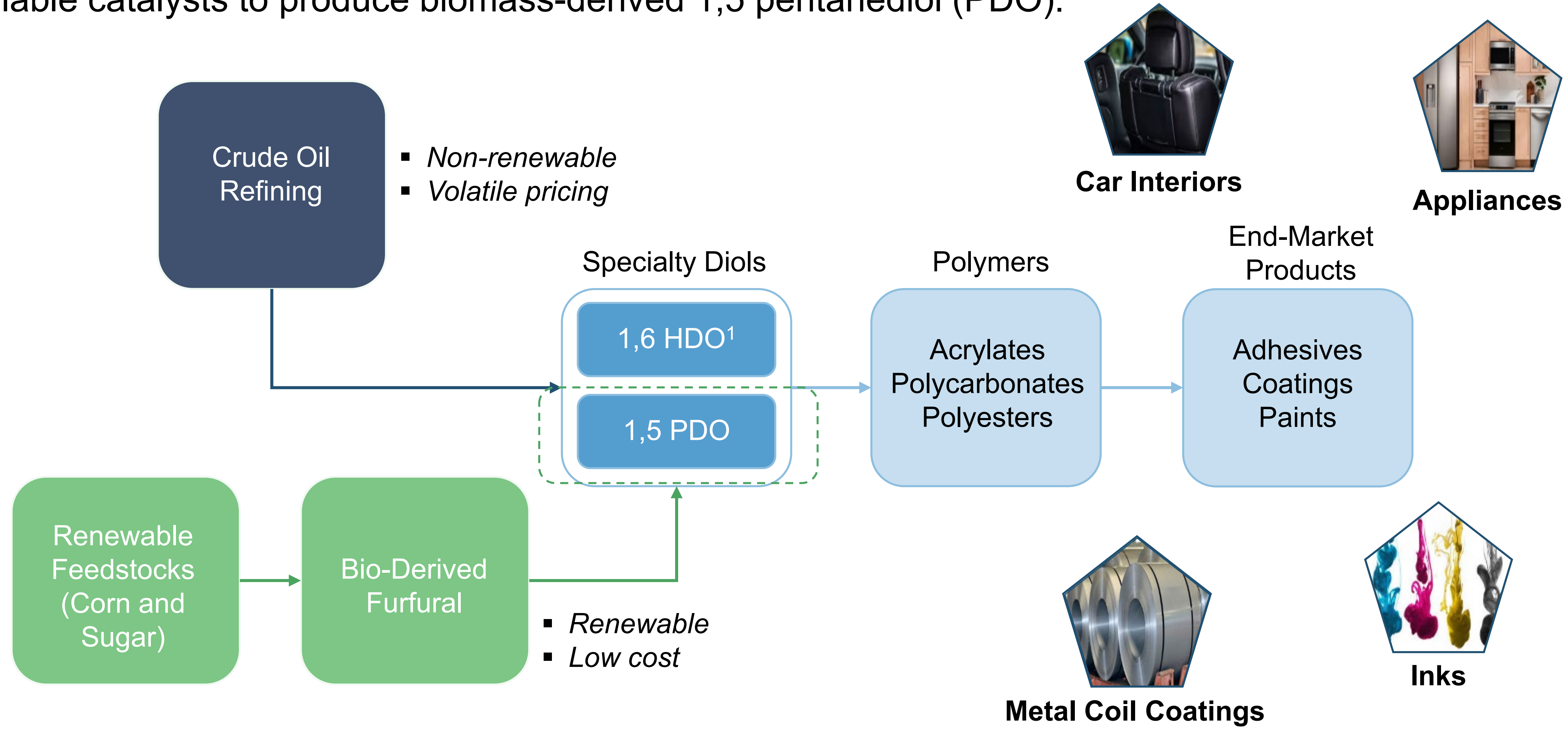
- Pyran's initial product eliminates 95% of cradle-to-gate greenhouse gas (GHG) emissions[2] relative to traditional alternatives.
- Additional products produced using Pyran's patented process affords the potential for further reductions.

PYRAN

1. https://www.marketresearchfuture.com/reports/1-6-hexanediol-market-2434.
2. Pyran, "GHG Internal Analysis," January 2021.

Simple Process and Proven Catalysts

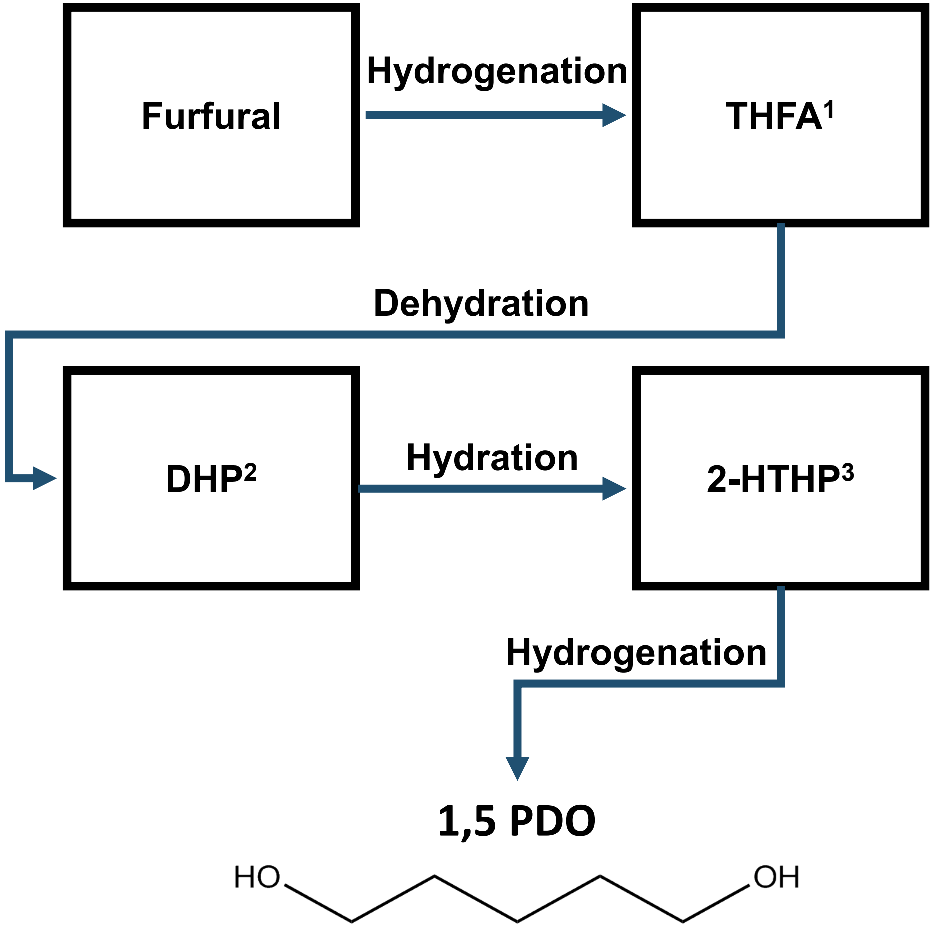
Pyran uses furfural, an agricultural byproduct primarily from corn cobs and sugarcane bagasse, along with readily available catalysts to produce biomass-derived 1,5 pentanediol (PDO).



1. 1,6 Hexanediol.

PYRAN

Simple Process and Proven Catalyst (Cont.)



Four steps outlined here create a **biogenic building block** from furfural with over **85 percent yields**.

Each step has been **demonstrated in continuous** flow reactors with **readily available catalysts.**

It's a simple process.

No recycling

No solvents

No co-products

1. Tetrahydrofurfuryl Alcohol.
2. Dihydropyran.
3. 2-Hydroxytetrahydropyran.

Reducing Emissions

Pyran's PDO could lead to a cumulative reduction in GHG of 6 Gt by 2050 relative to traditional alternatives.

- Adipic acid,[1] the standard building block for HDO, is produced primarily through oil refining – generating ~23 kg CO_2/kg.
- In contrast, Pyran PDO generates ~1 kg CO_2/kg.
- Not surprisingly, specialty chemical companies, particularly consumer-facing ones, have been increasingly vocal about their decarbonization efforts.

Specialty Chemical Sustainability Targets

BASF – We create chemistry

- Net zero emissions by 2050 versus 1990.
- Targeting €22B of "sustainable product" sales by 2025 (vs. €59B of total sales in 2020).

LANXESS – Energizing Chemistry

- 65% reduction in CO_2 emissions by 2025 versus 2004 (75% reduction by 2030).
- "Climate neutral" by 2040.

PPG

- 15% reduction in GHG emissions by 2025 versus 2017.
- Targeting 40% of total sales from "improved sustainability products" by 2025.

UBE

- 17% reduction in GHG emissions by 2030 versus 2017.
- Targeting 50%+ of net sales from "eco-friendly products" by 2050.

1. Corona, "Lifecycle Assessment of Adipic Acid Production," 2018.

Technology Demonstrated at Pilot Scale

Based on contracted offtake, Pyran began manufacturing products earlier this year to supply initial customer orders and sample requests for qualification.

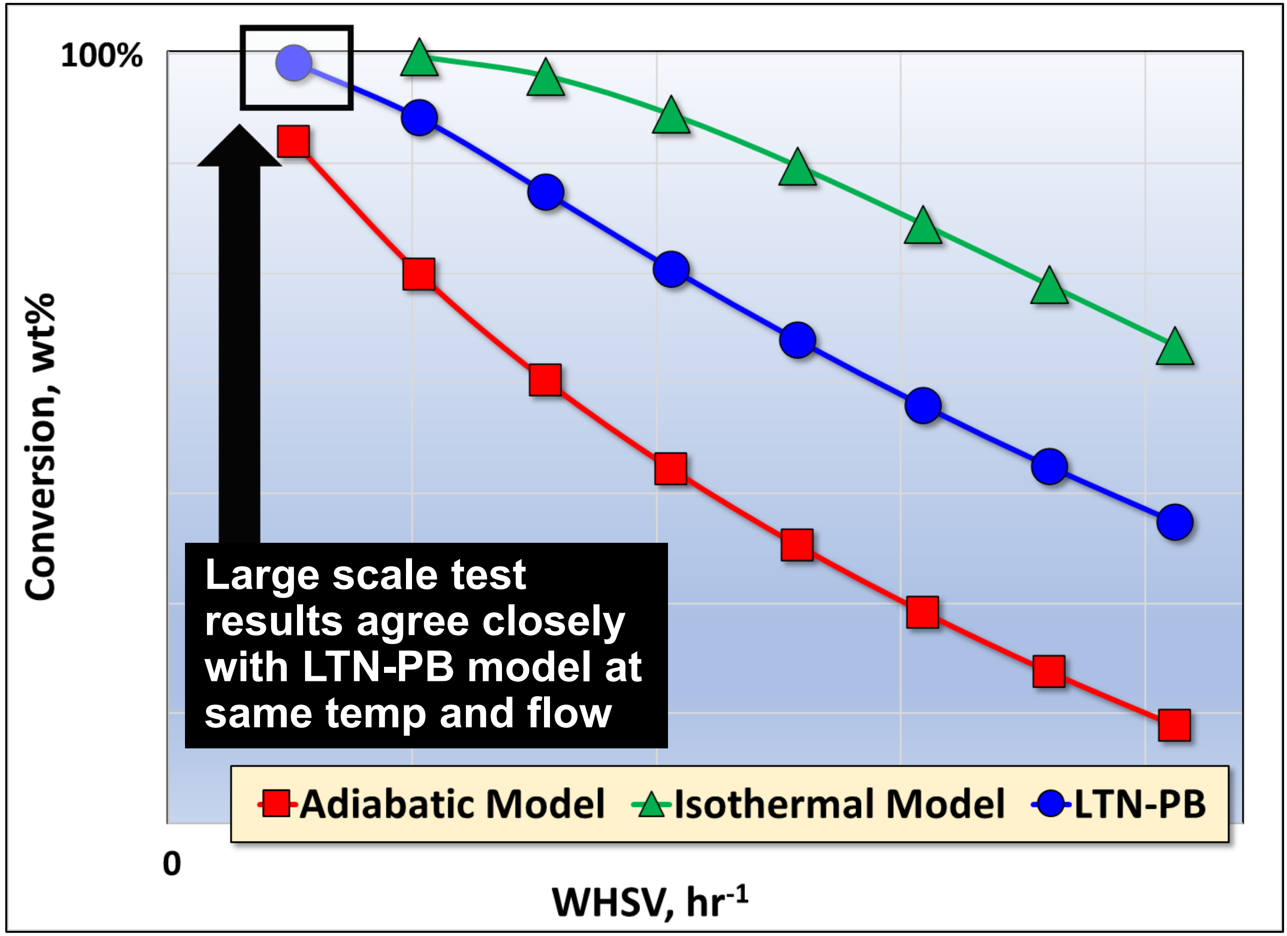
- Target yields have met or exceeded the Company's Aspen pre-production modeling.
- Most importantly, no safety incidents have occurred to date – a record Pyran intends to maintain through the conclusion of on-site work.
- The tolling campaign will ultimately produce 10 metric tons of on-spec PDO to be sold to a combination of contracted parties and new customers.

Test: LTN-PB Model Supports Scaleup Step of ~1,000X!!

Multiple reactor system holds 100's of kgs of catalyst

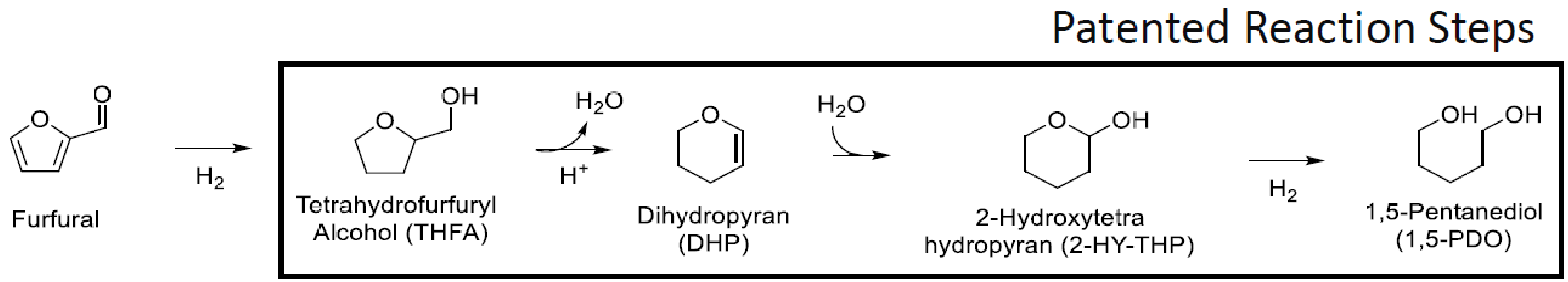
PYRAN
The 5-Carbon Company

RPD Technologies



Beyond the Initial Product

Pyran's process offers 10 key intermediates in addition to PDO.



Two key intermediates serve as the Company's most likely next-generation product(s):

Pyran Product	Incumbent Product	End Use	Global Market[1]
Tetrahydropyran	Tetrahydrofuran	Solvents	$4.2B and 8% CAGR
Pentamethylene Diamine	Hexamethylene Diamine	Corrosion inhibitor, epoxy curing and nylons	$5.7B and 7% CAGR

1. NBID Associates, "Identifying Business Growth Opportunities Intermediates and Derivatives of 1,5 PDO," March 11, 2022.

Thank You

Kevin Barnett – CTO & Co-founder
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PYRAN

Joaquín Alarcón

President and Chief Executive Officer

Catalyxx, Inc.

Modeling of Reactor Design and Optimization for Scale-Up of the Catalyxx Process for Ethanol Conversion to Higher Alcohol

Research Highlights

The Leading Greentech Company to Produce Biochemicals and Biofuels

October 20, 2022

Catalyxx Brief Overview

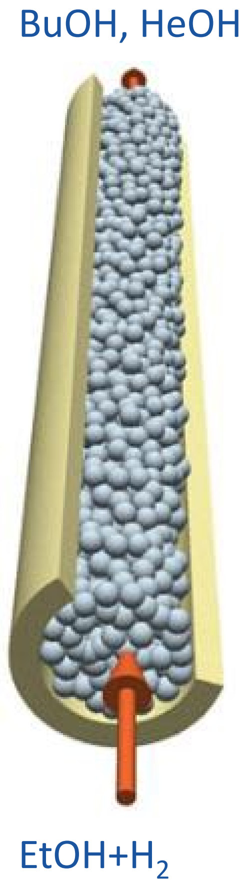
1. Catalyxx, incorporated in 2017, is a **renewable** chemical and fuel technology company that has fully **developed and successfully tested** a new and disruptive technology to produce n-biobutanol and other longer-chain linear alcohols.

2. Butanol is produced by condensing ethanol using Catalyxx's patented catalyst and its thermochemical catalytic process, following the mechanisms of Guerbet's reaction.

3. Economic and environmental **value**:
   - Lower cost of production of butanol. 60% cheaper than the existing petrochemical route.
   - Up to 85% lower CO_2 emissions.

4. The N-butanol is a widely used chemical commodity and has a **market size** of $5bn and is expected to steadily grow in the coming years.

5. The technology is **fully protected** by five international families of patents.

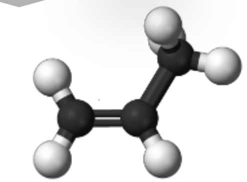


N-Butanol

Traditional petrochemical process

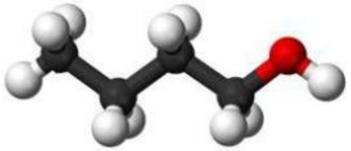
Oil + Natural Gas

Propylene



Oxo process

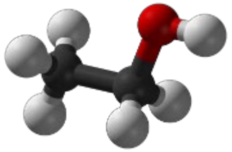
N-butanol



Catalyxx process

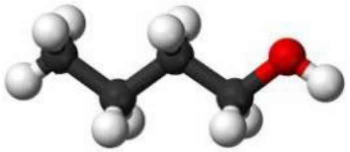
Corn / Sugar Cane / Biomass

Ethanol



Catalytic process

N-butanol



N-butanol is widely used in the chemical industry as a component of:

- **Coatings and paints, plasticizers,** solvent for inks**, cleaning products, adhesives** and caulks, perfumes and synthetic fruit flavoring, textile manufacture, fuel, pesticides, resins.

CCPC Project Objectives

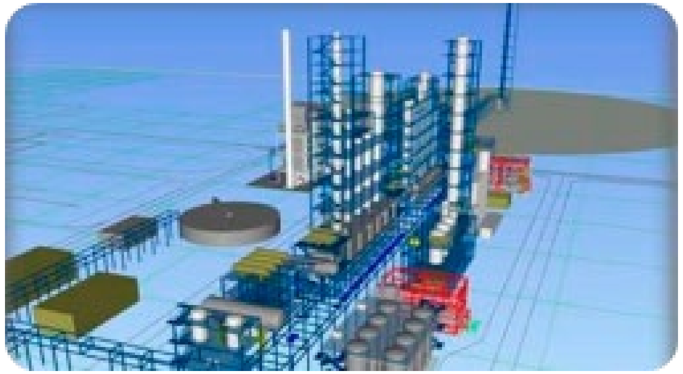
1. Catalyxx and ORNL have worked together to develop the modeling tools to scale up from lab-scale to commercial-scale reactor with successful results.
2. The project’s main objective was to forecast the behavior of a commercial-scale reactor (5 tons of catalyst) based on the data obtained at the three scales where the reaction was tested (lab, bench, pilot, demonstrator).

Lab scale
TRL4

Bench facility
TRL5

Pilot Plant
TRL6

Demonstrator Plant
TRL7



First-of-a-kind Industrial Plant
TRL8

ORNL's modeling efforts helped Catalyxx to design and improve our ethanol upgrading technology

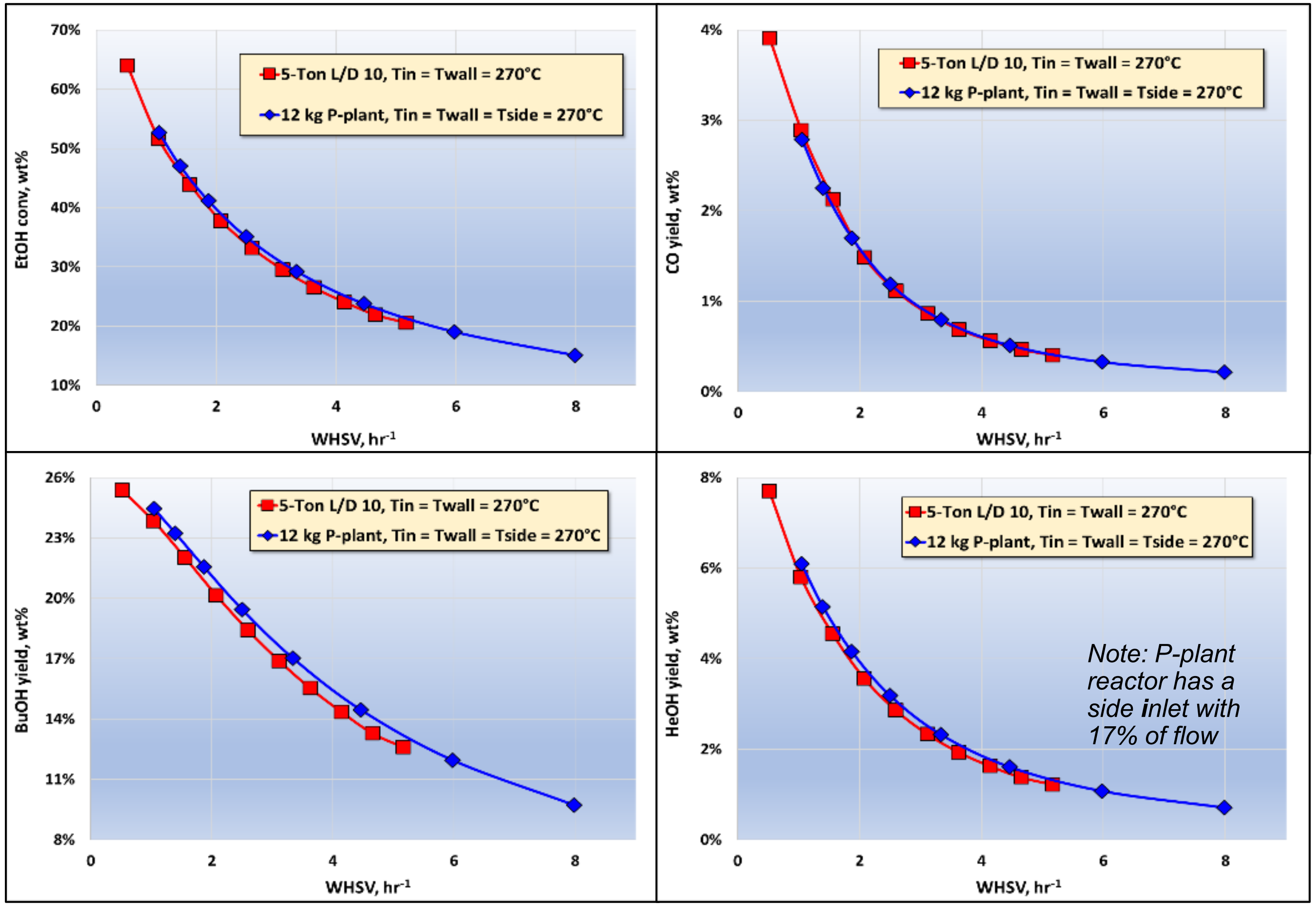
Validated reaction kinetics (Initial kinetics provided by Catalyxx)

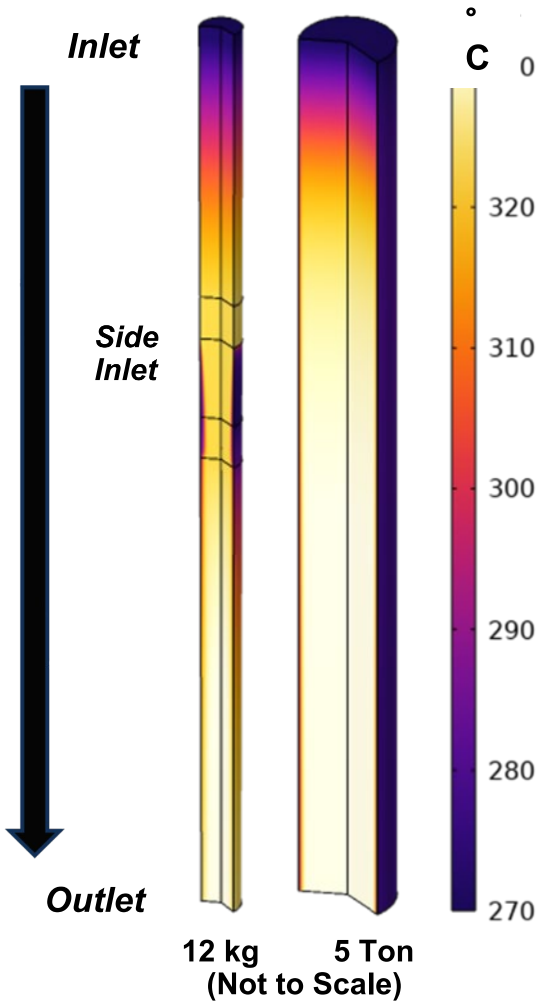
- Complex chemistry is redefined. More than 20 reactions were modeled: Essential for scale-up
- Thermodynamic was built in: Essential for scale-up/heat transfer
- This effort enabled predicting conversion, selectivity, and yield

Validated: Independent of reactor and catalyst configuration 4 gram to 5-ton reactor

- Fully resolved **heat transfer** effects
- Fully resolved **mass transfer** effects
- Verified optimum **operating conditions**: T, p, WHSV
  Suggested: less H_2 feed composition is possible
- Catalyxx's **new experiments** carried out during the project **proved the model**!
  Suggested: Lower temperature adiabatic operation
- Catalyxx's new experiments proved the model!
  ORNL suggested optimum operating T, p, WHSV
- Suggested SED **pellets size** for pilot scale

ORNL's modeling demonstrated 5-ton reactor scale was feasible, with yields similar to pilot-scale beds





The simulation provided Catalyxx with a tool to optimize the 5-ton reactor and reduces scale-up risks, knowing that the model shows similar behaviors independently of scale.

Catalyxx

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Thank you!

Today's Presentation:

Cost-Effectively Optimize and Scale Bioenergy Technologies with the Consortium for Computational Physics and Chemistry (CCPC)

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