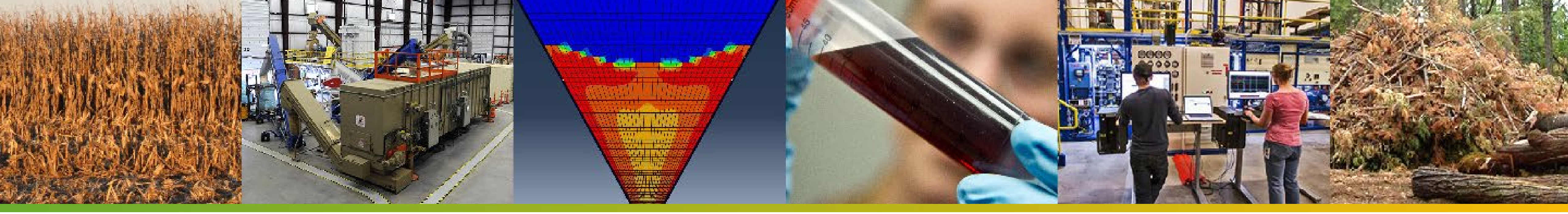


DOE Bioenergy Technologies Office (BETO) 2023 Project Peer Review

FCIC Task 6 – High Temperature Conversion

April 6, 2023
Feedstock-Conversion Interface Consortium (FCIC)

Presenter: Jim Parks (Oak Ridge National Laboratory)

FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM
U.S. DEPARTMENT OF ENERGY

Our Team

FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM
U.S. DEPARTMENT OF ENERGY

Sub-Task 6.10. Liquid Intermediate CQAs


Huamin Wang (PNNL)


Jennifer Jocz (PNNL)


Miki Santosa (PNNL)


Ben Davis (LANL)


Ricardo Navar (LANL)


Steven Rowland (NREL)

Sub-Task 6.11. High Throughput Conversion Screening

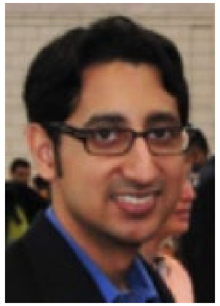

Anne Starace (NREL) [Task Co-Lead]


Jordan Klinger (INL)

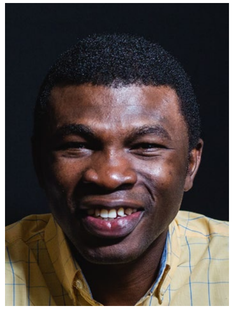
Sub-Task 6.12. Hierarchical Conversion Modeling Development


Mehrdad Shahnam (NETL)


Yupeng Xu (NETL)


Subhodeep Banerjee (NETL)


Jim Parks (ORNL) [Task Lead]


Femi Oyedeji (ORNL)

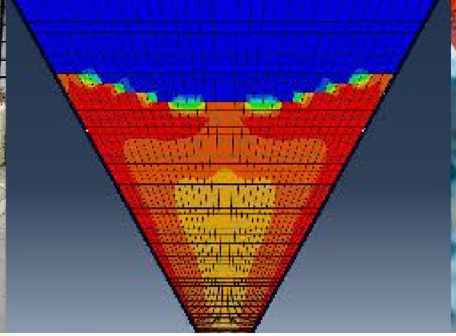
Sub-Task 6.13. Experimental Validation of Hierarchical Models


Reinhard Seiser (NREL)


Peter Ciesielski (NREL)

We gratefully acknowledge former team contributors: Gavin Wiggins, Danny Carpenter, Brennan Pecha, Bill Rogers

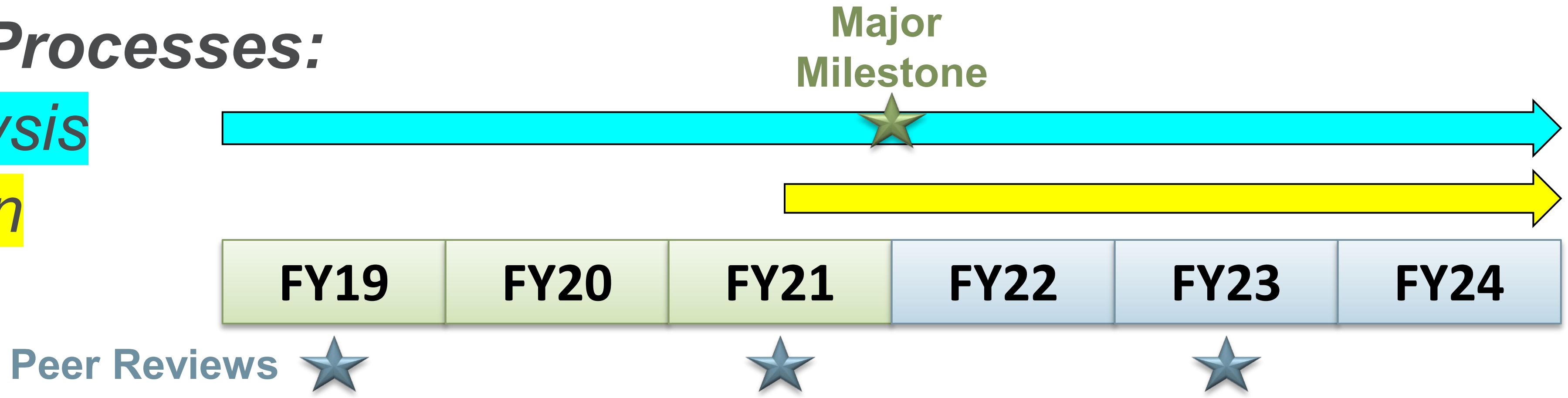





Project Overview

Project Overview: High Temperature Conversion

- ***Objective:*** *Provide a fundamental science-based understanding of the high-temperature conversion of low-cost, complex mixtures of biomass and waste feedstocks for Sustainable Aviation Fuels (SAF) and related co-products*
- ***Conversion Processes:***
  - *Fast Pyrolysis*
  - *Gasification*



- ***Targeted Outcomes:*** *Knowledge and tools to enable low-cost feedstocks utilization, increased process reliability, and optimized reactor design to achieve BETO 2030 and 2050 Performance Goals*

FCIC Task Organization

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Feedstock → **Preprocessing** → **Conversion**

Task 2: Feedstock Variability

Task 5: Preprocessing

Task 6: High-Temperature Conversion

Task 1: Materials of Construction

Task 7: Low-Temperature Conversion

Task 3: Materials Handling

Enabling Tasks

Task X: Project Management

Task 4: Data Integration

Task 8: TEA/LCA
Task 9: FMEA

Task X: Project Management: Provide scientific leadership and organizational project management

Task 1: Materials of Construction: Specify materials that do not wear, or break at unacceptable rates

Task 2: Feedstock Variability: Quantify & understand the sources of biomass resource and feedstock variability

Task 3: Materials Handling: Develop tools that enable continuous, steady, trouble free feed into reactors

Task 4: Data Integration: Ensure the data generated in the FCIC are curated and stored – FAIR guidelines

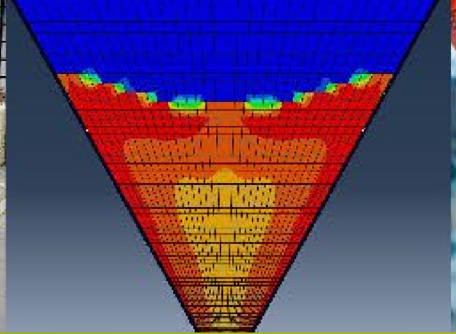
Task 5: Preprocessing: Enable well-defined and homogeneous feedstock from variable biomass resources

Task 6 & 7: Conversion (High- & Low-Temp Pathways): Produce intermediates for further processing

Task 8:Crosscutting Analyses TEA/LCA: Valuation of intermediate streams & quantify variability impact

Task 9:Failure Mode & Effects Analysis (FMEA): Standardized approach for assessing attribute criticality






1 – Approach

Thermo-Chemical Conversion to Sustainable Aviation Fuel

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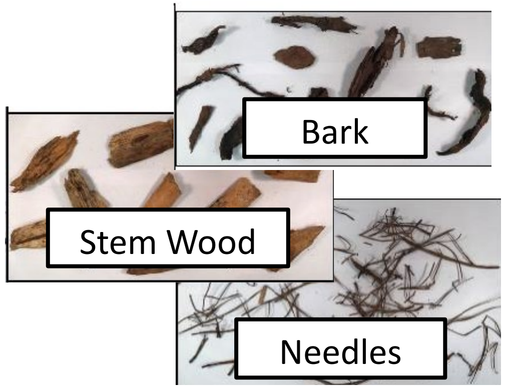
ChemCatBio Chemical Catalysis for Bioenergy

Low-Cost, Complex Feedstocks | **Thermo-Chemical Conversion** | **Downstream Unit Operations**

Biomass [various species & anatomical fractions]



Fast Pyrolysis

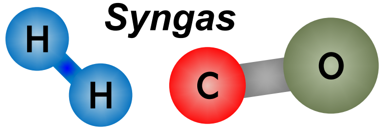
Catalytic Upgrading

Co-Processing

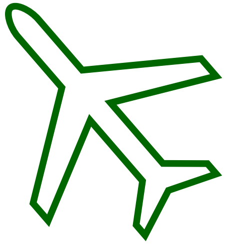
Municipal Solid Waste (MSW)

Gasification

Fischer-Tropsch



Microbial Conversion

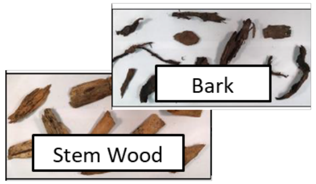


Sustainable Aviation Fuel (SAF)

Technical Approaches to Achieve Impact

Low-Cost, Complex Feedstocks | Thermo-Chemical Conversion | Downstream Unit Operations

Biomass [various species & anatomical fractions]



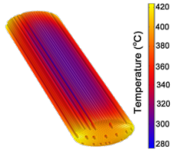
→ **Fast Pyrolysis** →

Catalytic Upgrading

Co-Processing

Technical Approaches

Quality by Design (QbD)	*Critical Material Attributes (CMAs)*	**Process** →	*Critical Quality Attributes (CQAs)*
Multi-Scale Model-Experiment Coupling	*Meso Scale [Feedstock Particles]*	**Science-to-Application** →	*Reactor Scale*
Industry Input-Output	*Industry Interviews on Needs & Challenges*	**Impact** →	*Tech Transfer of Outcomes to Bioenergy Industry*

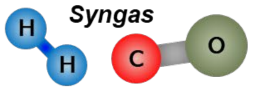


CCPC
Consortium for Computational Physics and Chemistry
U.S. DEPARTMENT OF ENERGY
BIOENERGY TECHNOLOGIES OFFICE

Municipal Solid Waste (MSW)

→ **Gasification** →

Fischer-Tropsch



Microbial Conversion

Task Structure

Sub-Task 6.10.
Liquid Intermediate CQAs

Sub-Task 6.11.
High Throughput Conversion Screening

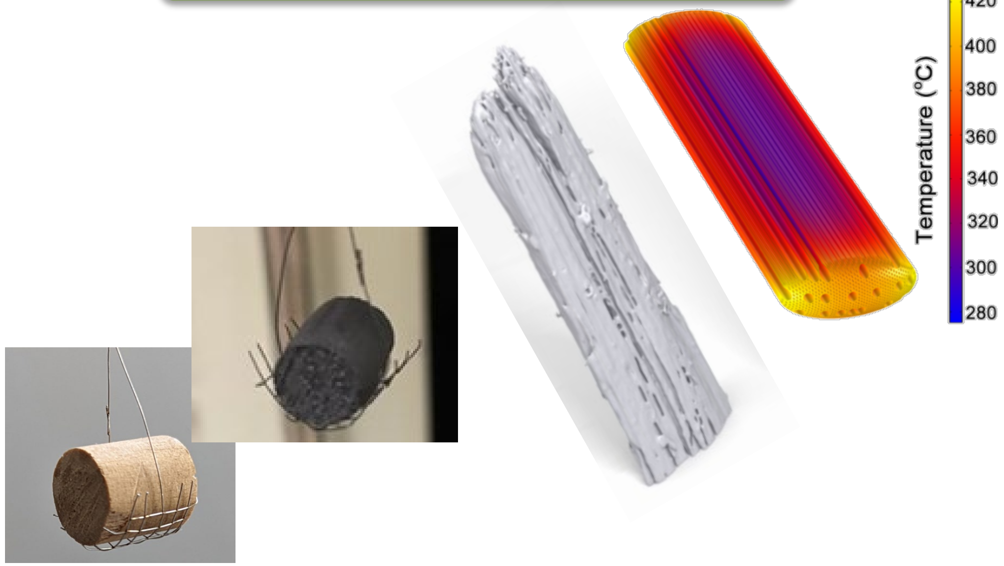
Sub-Task 6.12.
Hierarchical Conversion Modeling Development

Sub-Task 6.13.
Experimental Validation of Hierarchical Models

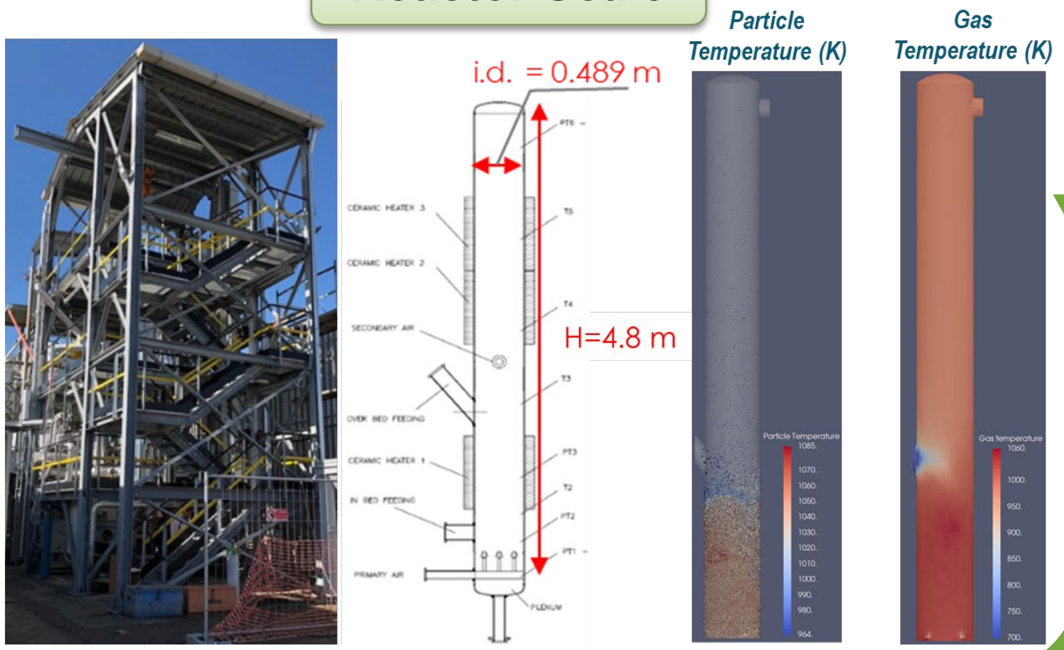
Validation is Critical to Success

- Our primary goal is to mitigate risks with conversions of highly complex and diverse feedstocks
- Risk mitigation for our approach is … ***VALIDATION AT MULTIPLE SCALES***
- Experimental-modeling coupling strengthens with every iteration

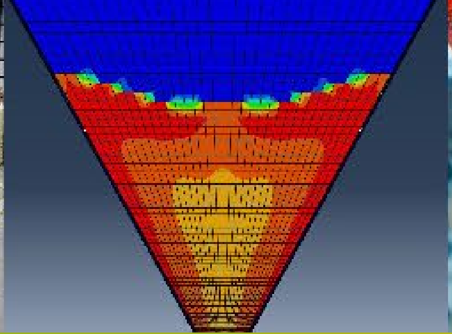
Feedstock Particle Scale



Reactor Scale



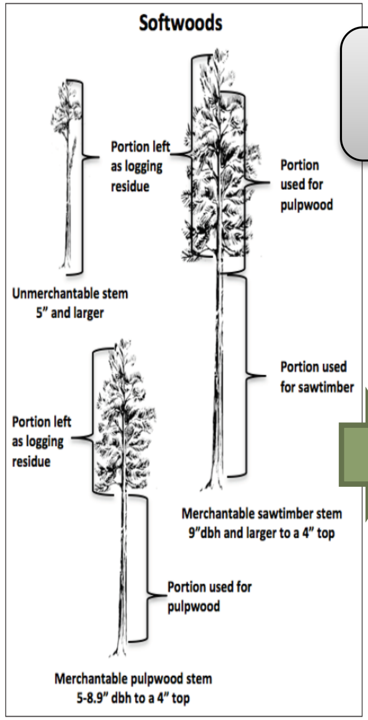





2 – Progress and Outcomes

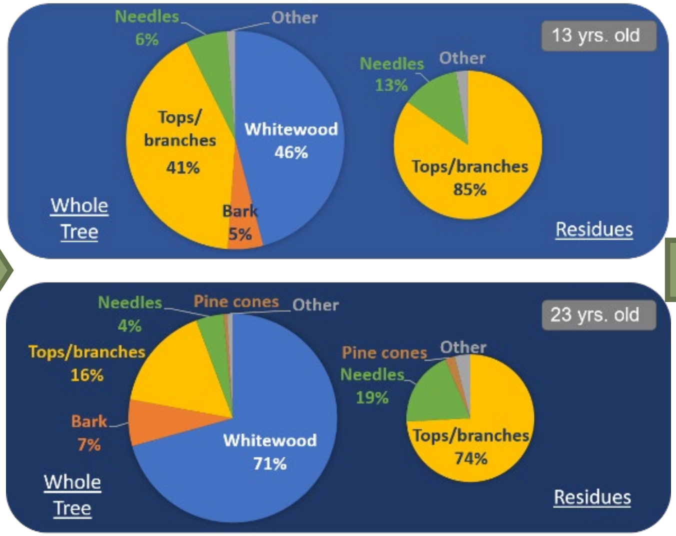
Fast Pyrolysis

Challenges in Fast Pyrolysis of Biomass



(Bardon and Hazel, 2014)

Case Study in Feedstock Variability: 13-yr vs. 23-yr old tree*



Pre-Processing

Physical Characteristics

Chemical Speciation

Aerodynamic Properties

Other Properties

Critical Material Attributes (CMAs) → **Approach: Quality by Design (QbD)** → Critical Quality Attributes (CQAs)

Critical Process Parameters

Fast Pyrolysis → **Downstream Upgrading**

Challenges toward goal of sustainable low life-cycle C renewable fuels from biomass:

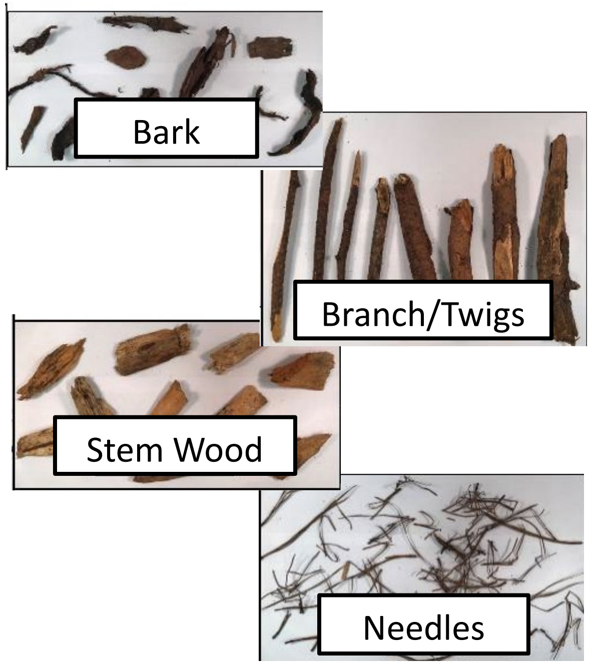
- **Feedstock Variability:** Biomass has inherent variability as function of source, geography, climate, species, etc.
- **Optimal Thermo-Chemical Conversion Efficiency:** Ideally, yield of fast pyrolysis oil is high & energy input is low
- **Lowest Costs:** “Waste” or “scrap” feedstock lowest cost (but often highest variability); reactors & processes must be robust to variable feedstocks to operate most cost effectively (and with maximum up time)

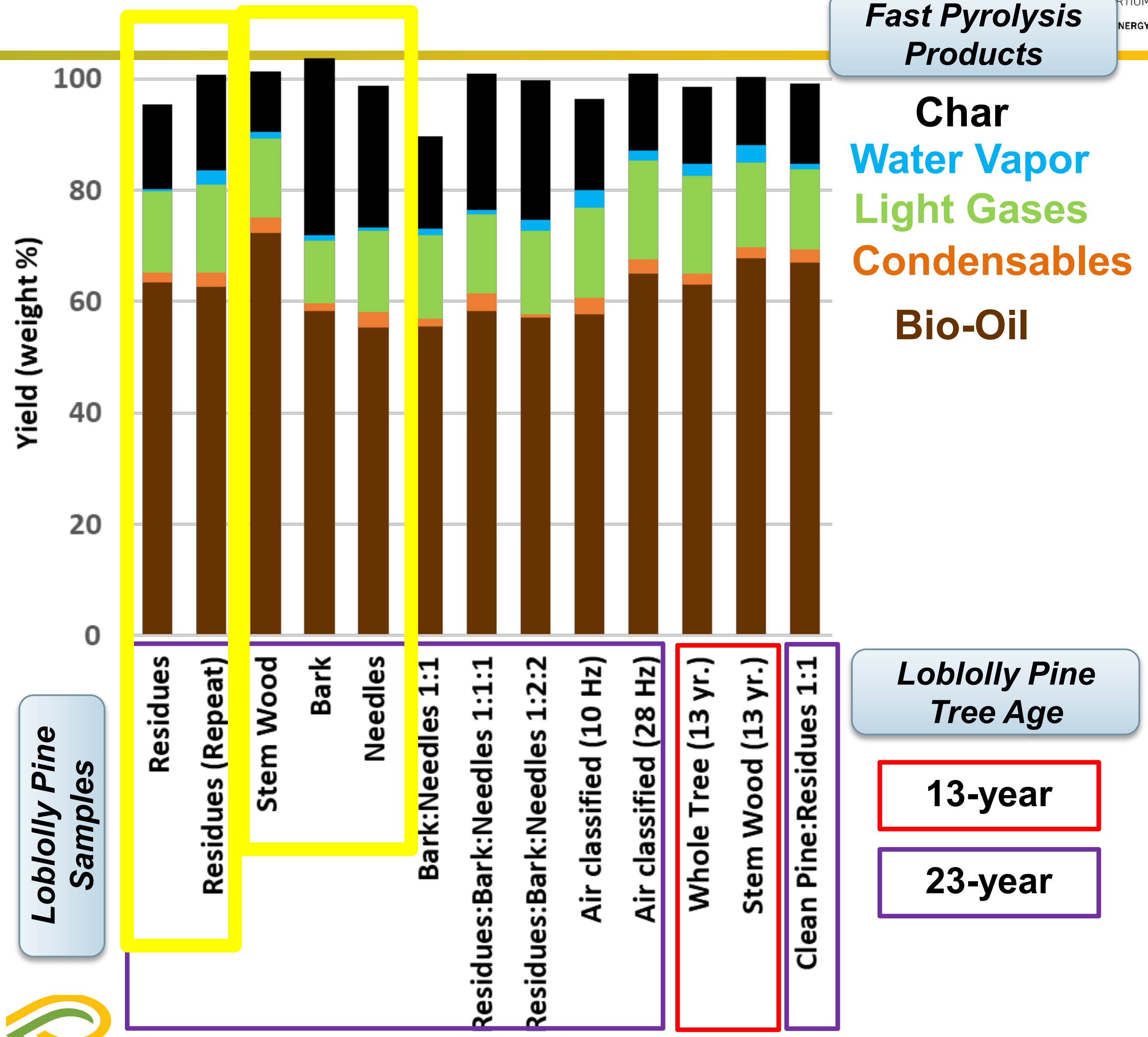
*bioenergy.labworks.org/labkey/FCIC/T.08.00 Cross-Cutting Analysis Overview

Product Mass Yields from Fast Pyrolysis Experiments

Fast Pyrolysis of Loblolly Pine Forest Residues
in 2" Fluidized Bed Reactor (2FBR) at NREL
23-year-old and 13-year-old trees

Anatomical Fractions of Forest Residues

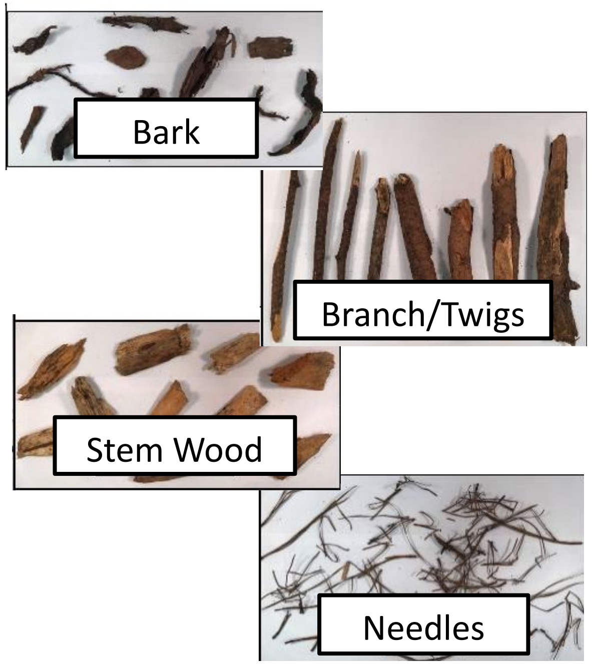




Note: **bio-oil** measured gravimetrically; **condensable** products measured by GC; **water vapor** as measured by a dew point analyzer; **char** collected by cyclone and hot filter.

Critical Material Attributes (CMAs) of Forest Residues

Anatomical Fractions of Forest Residues



Feedstock Particle

Characteristics (CMAs)

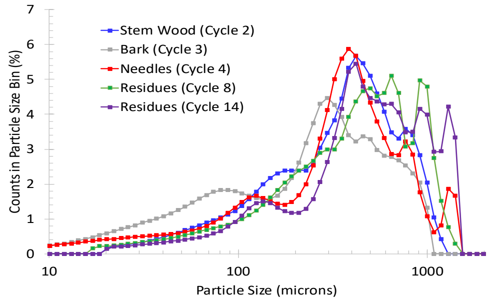
Physical Characteristics
Particle shape/size, density, structure, porosity

Aerodynamic Properties
Density and aerodynamic properties (fluidization)

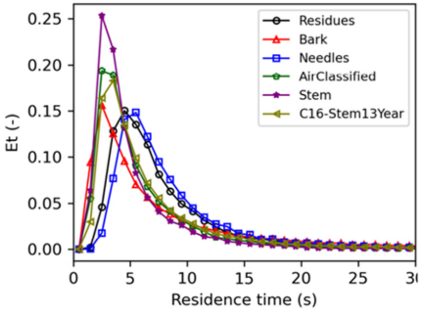
Chemical Speciation
Lignin, hemicellulose, cellulose, moisture, ash, etc.

Other Properties
Surface properties (stickiness), attrition susceptibility

Particle Size Distributions



Residence Time Distributions



Debiagi *et al.* Kinetics
(+ a lot of analysis)

Complex Chemistry Necessary: Model Based on Kinetics by Debiagi et al.*

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25 Reactants and Intermediates → **31 Products**

CELL	$C_6H_{10}O_5$
CELLA	$C_6H_{10}O_5$

Cellulose (4 reactions, 2 species)

GMSW	$C_5H_8O_4$
HCE1	$C_5H_8O_4$
HCE2	$C_5H_8O_4$

Hemicellulose (6 reactions, 3 species)

LIG	$C_{11}H_{12}O_4$
LIGC	$C_{15}H_{14}O_4$
LIGCC	$C_{15}H_{14}O_4$
LIGH	$C_{22}H_{28}O_9$
LIGO	$C_{20}H_{22}O_{10}$
LIGOH	$C_{19}H_{22}O_8$

Lignins (8 reactions, 6 species)

TGL	$C_{57}H_{100}O_7$
TANN	$C_{15}H_{12}O_7$
ITANN	$C_8H_4O_4$

Extractives (3 reactions, 3 species)

G{COH2} loose	CH_2O
G{CO2}	CO_2
G{CO}	CO
G{CH3OH}	CH_4O
G{CH4}	CH_4
G{C2H4}	C_2H_4
G{C6H5OH}	C_6H_6O
G{COH2} stiff	CH_2O
G{H2}	H_2
G{C2H6}	C_2H_6

"Metaplastic" (10 reactions, 10 species)

ACQUA	H_2O

H_2O (1 reaction, 1 species)

Fast Pyrolysis

Ash Factor *adjusts for 0-5% ash content*

Char (1 species - Carbon)

CHAR	C

"Tar" (Oil) (22 species)

C2H3CHO	C_3H_4O
C2H5CHO	C_3H_6O
C2H5OH	C_2H_6O
C5H8O4	$C_5H_8O_4$
C6H10O5	$C_6H_{10}O_5$
C6H5OCH3	C_7H_8O
C6H5OH	C_6H_6O
C6H6O3	$C_6H_6O_3$
C24H28O4	$C_{24}H_{28}O_4$
CH2OHCH2CHO	$C_3H_6O_2$
CH2OHCHO	$C_2H_4O_2$
CH3CHO	C_2H_4O
CH3CO2H	$C_2H_4O_2$
CH3OH	CH_4O
CHOCHO	$C_2H_2O_2$
CRESOL	C_7H_8O
FURFURAL	$C_5H_4O_2$
H2O	H_2O
HCOOH	CH_2O_2
MLINO	$C_{19}H_{34}O_2$
U2ME12	$C_{13}H_{22}O_2$
VANILLIN	$C_8H_8O_3$

Light Gases (7 species)

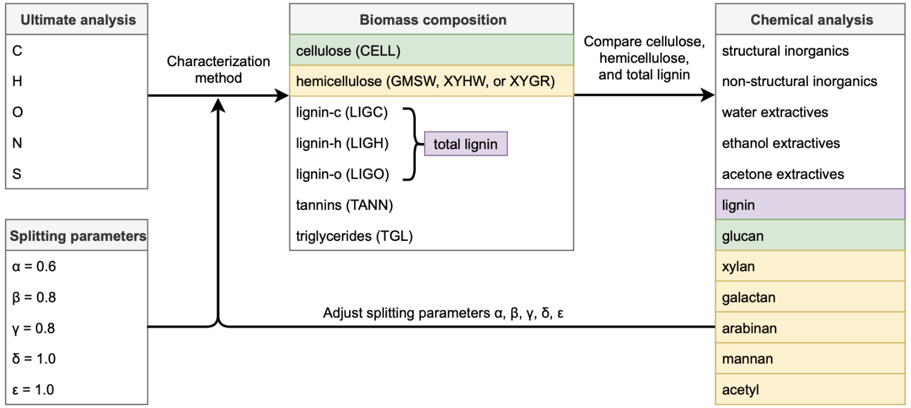
C2H4	C_2H_4
C2H6	C_2H_6
CH2O	CH_2O
CH4	CH_4
CO	CO
CO2	CO_2
H2	H_2

*Paulo Debiagi, et al., "A predictive model of biochar formation and characterization." *Journal of Analytical and Applied Pyrolysis*, **vol. 134**, pp. 326-335, 2018.

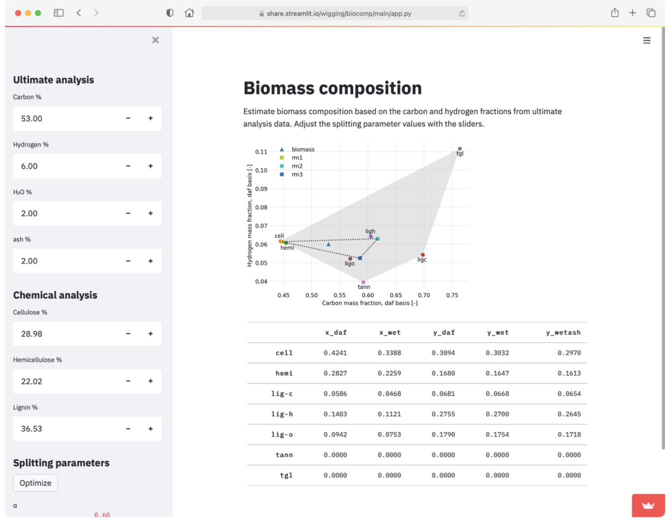
*Also see CRECK Modeling Group at Politecnico di Milano (creckmodeling.chem.polimi.it)

Methodology Developed to Link Biomass Analyses to Debiagi Reactants: LIG-C vs. LIG-H vs. LIG-O Critical

Experimental biomass composition from ultimate and chemical analysis data utilized to determine critical apportionment into Debiagi reactants



An online tool was developed to determine the Debiagi reactants for biomass from ultimate and chemical analysis data.



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TANN	$C_{15}H_{12}O_7$
ITANN	$C_8H_4O_4$
G{COH2} loose	CH_2O
G{CO2}	CO_2
G{CO}	CO
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G{C2H4}	C_2H_4
G{C6H5OH}	C_6H_6O
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G{H2}	H_2
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ACQUA	H_2O

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Lignins
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Extractives
(3 reactions, 3 species)

"Metaplastic"
(10 reactions, 10 species)

H_2O
(1 reaction, 1 species)

Fast Pyrolysis

Ash Factor *adjusts for 0-5% ash content*

*Reference: Gavin Wiggins. BioComp: A web tool for estimating biomass composition. Version 22.02. Available at https://github.com/wigging/biocomp

Comparison of Model Predicted Oil Chemistry to Experimental Oil Analysis is Challenging – Efforts Ongoing

31 Products

Fast Pyrolysis

Ash Factor *adjusts for 0-5% ash content*

Char (1 species - Carbon)

CHAR	C

"Tar" (Oil) (22 species)

C2H3CHO	C_3H_4O
C2H5CHO	C_3H_6O
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C6H10O5	$C_6H_{10}O_5$
C6H5OCH3	C_7H_8O
C6H5OH	C_6H_6O
C6H6O3	$C_6H_6O_3$
C24H28O4	$C_{24}H_{28}O_4$
CH2OHCH2CHO	$C_3H_6O_2$
CH2OHCHO	$C_2H_4O_2$
CH3CHO	C_2H_4O
CH3CO2H	$C_2H_4O_2$
CH3OH	CH_4O
CHOCHO	$C_2H_2O_2$
CRESOL	C_7H_8O
FURFURAL	$C_5H_4O_2$
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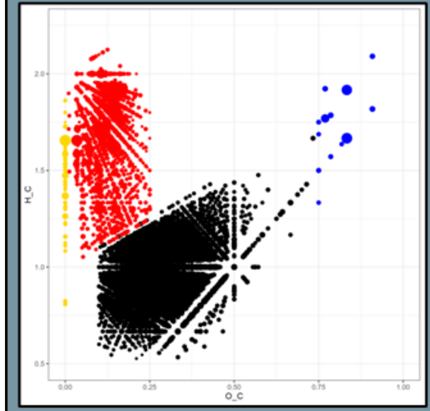
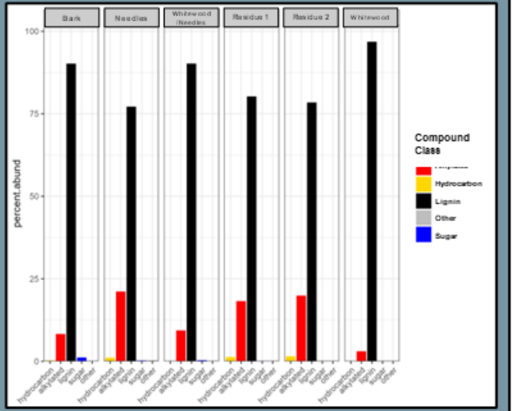
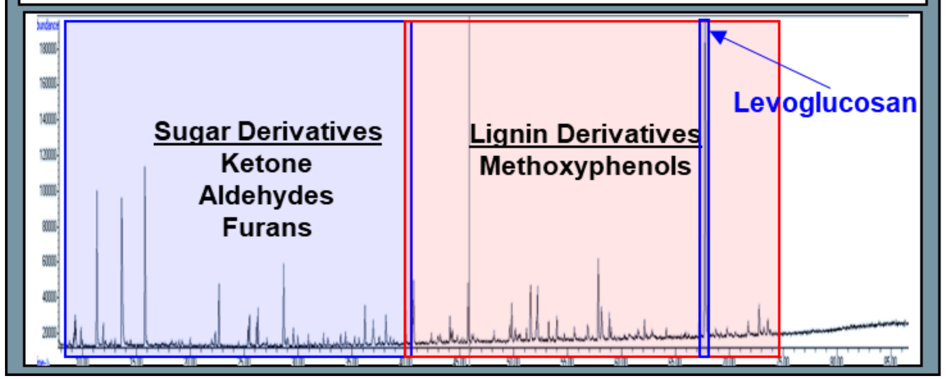
C2H4	C_2H_4
C2H6	C_2H_6
CH2O	CH_2O
CH4	CH_4
CO	CO
CO2	CO_2
H2	H_2

Comparison of Classes by Ultrahigh Resolution Mass Spectrometry





Compound Identification by GC-MS



Critical Quality Attributes (CQAs)

Acidity

Stability

O Content

C Number

Outcome: Validated Multi-Scale Framework

Includes Three Levels of Complexity & Capability for Range of Users

A validated, multiscale experimental & computational framework that allows biorefinery design engineers & operators to optimize productivity & control critical product quality attributes with variable incoming feedstock attributes.

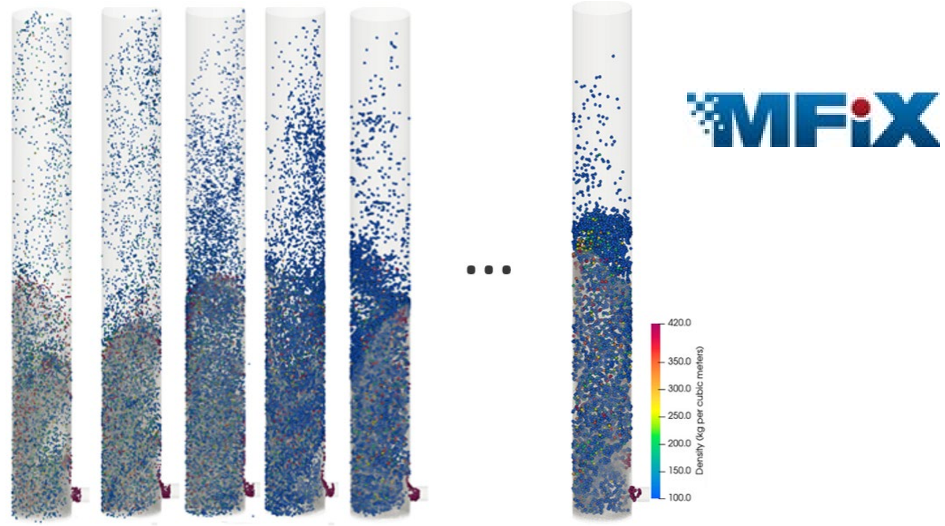
Consistent Kinetics and Approach

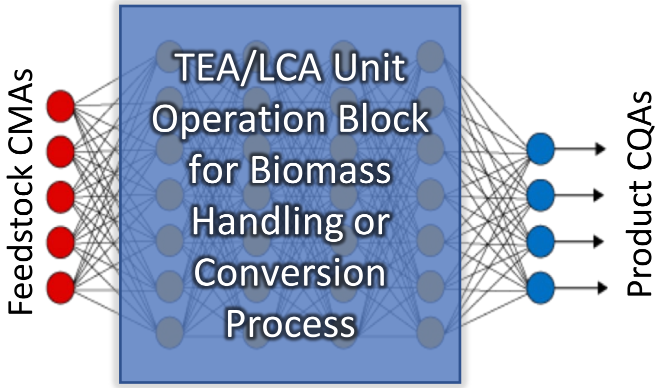
FCIC Multiscale Computational Framework

Hi-Fidelity Framework
CFD Model with Full Capture of Physics and Chemistry

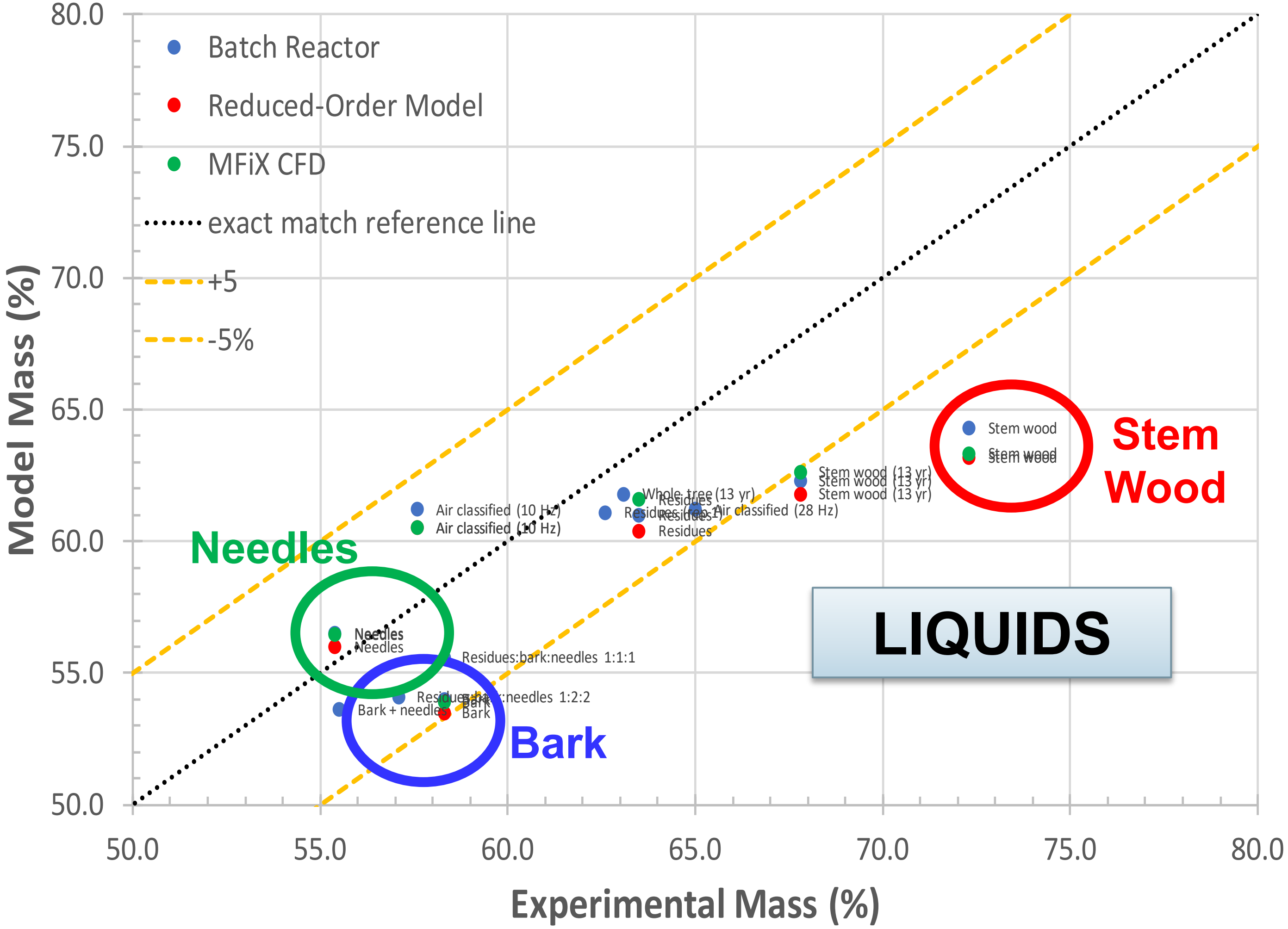
Reduced-Order Framework
Rapid Execution on Typical Desktop/Laptop

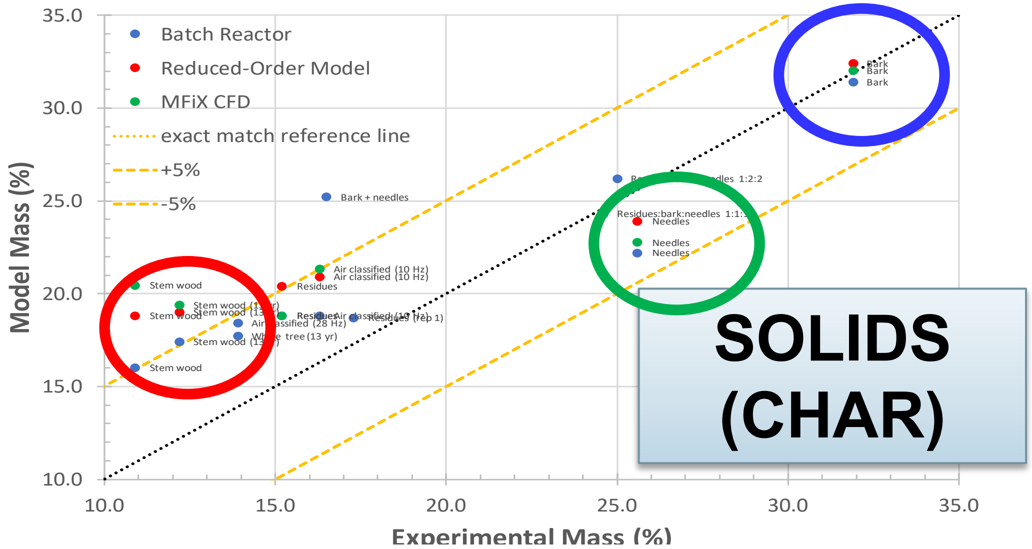
Techno-Economic Analysis Module (e.g. ASPEN)
User-Friendly Toolset and/or Module Input

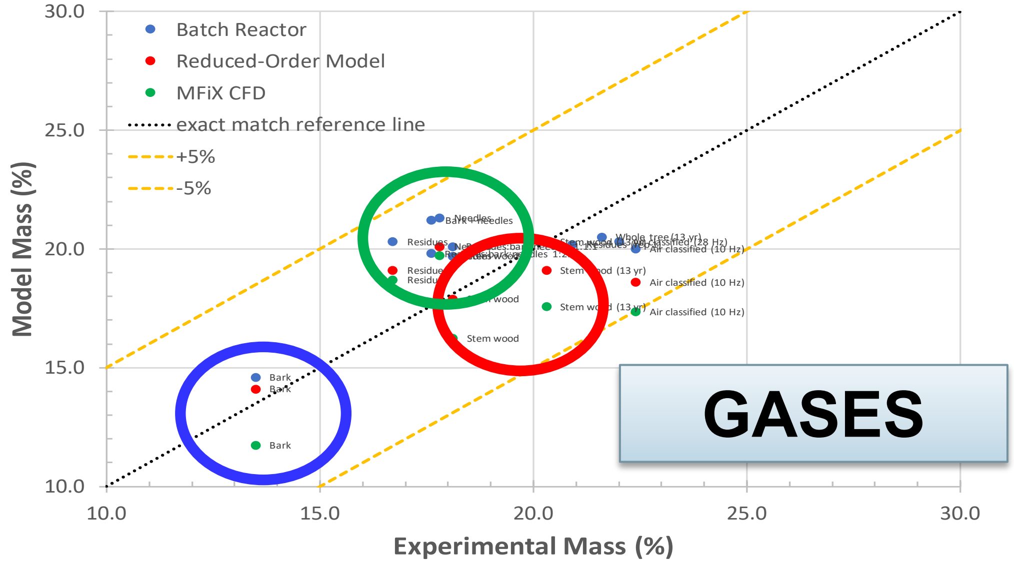




Validation Results Show Generally Good Agreement and Utility for Model Predictions of Complex Biomass Feedstocks





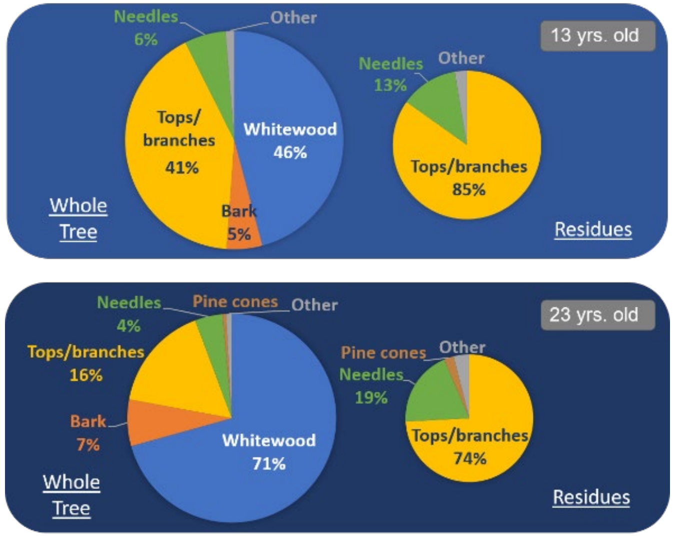


Note: gases include light gases as well as condensables and water vapor which were not included in the experimentally reported oil yield mass.

Outcome: Utility for Techno-Economic Analysis

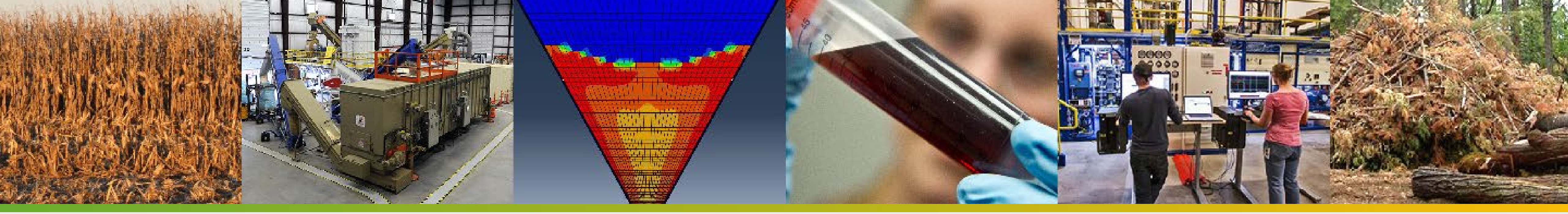
Techno-Economic Analysis results for the conversion of 13-year-old whole thinnings, 23-year-old residues, and combined thinnings + residues.

Case Study in Feedstock Variability: 13-yr vs. 23-yr old tree*



	Thinnings	Residues	Thinnings + Residues
Feedstock supply cost ($/MT)	$105.59	$117.85	$96.84
Feedstock preprocessing cost ($/MT)	$26.90	$28.54	$27.72
Delivered feedstock cost ($/MT)	$132.49	$146.39	$124.56
Biorefinery Fuel C Yield	26.4%	25.3%	25.9%
MFSP ($/GGE)	**$5.23**	**$5.43**	**$5.08**

*bioenergy.labworks.org/labkey/FCIC/T.08.00 Cross-Cutting Analysis Overview



2 – Progress and Outcomes

Gasification

FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

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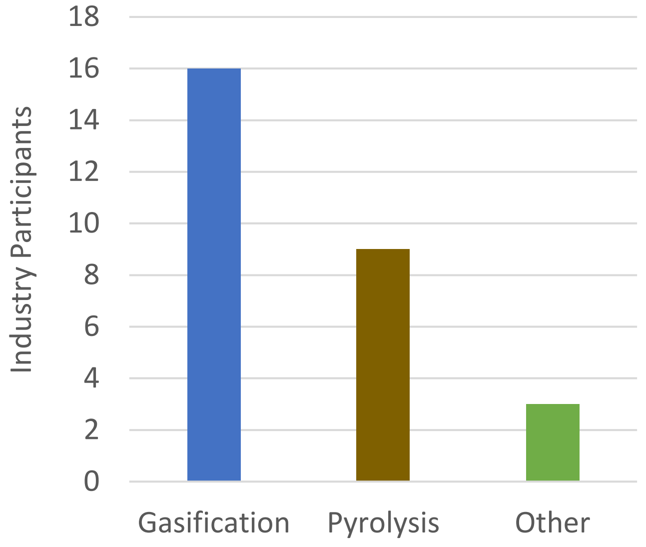
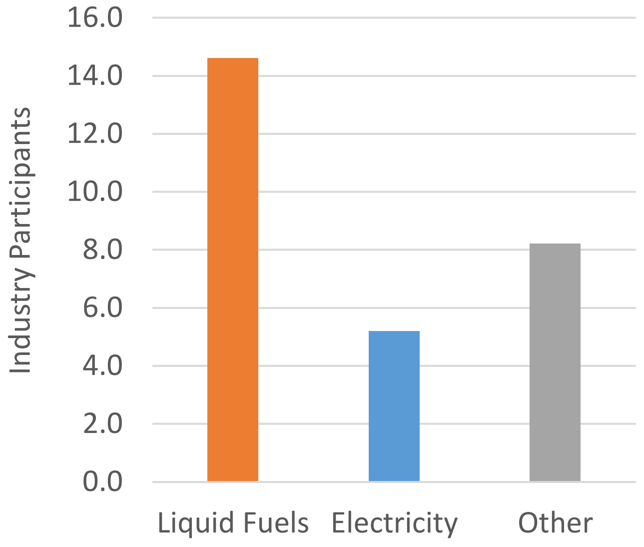
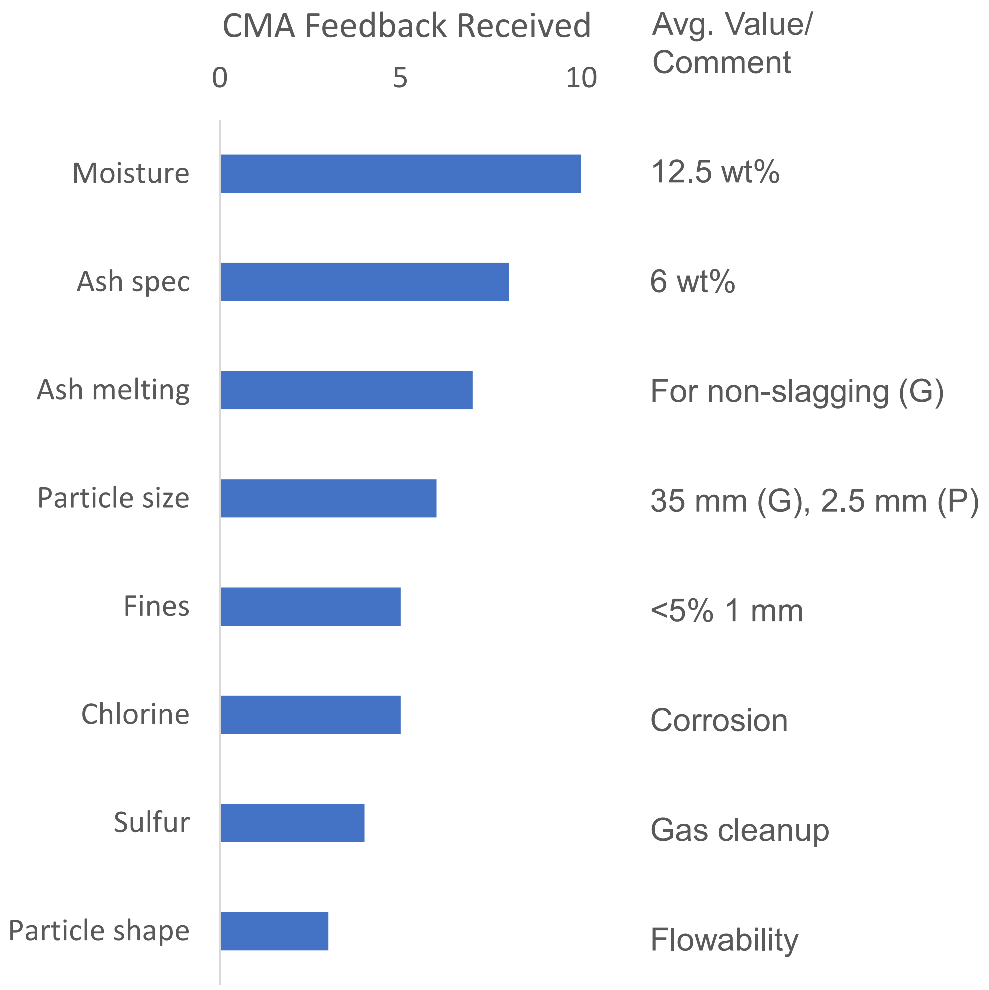
Industry Input from 28 Companies Collected via Survey to Guide R&D

- 28 Industry technology providers provided feedback. They included gasification (G), pyrolysis (P), and other conversion technologies.
- The final products considered are liquid fuels, electricity, and other products (biochar, chemicals, gases).
- Feedback on CMAs was received and summarized.







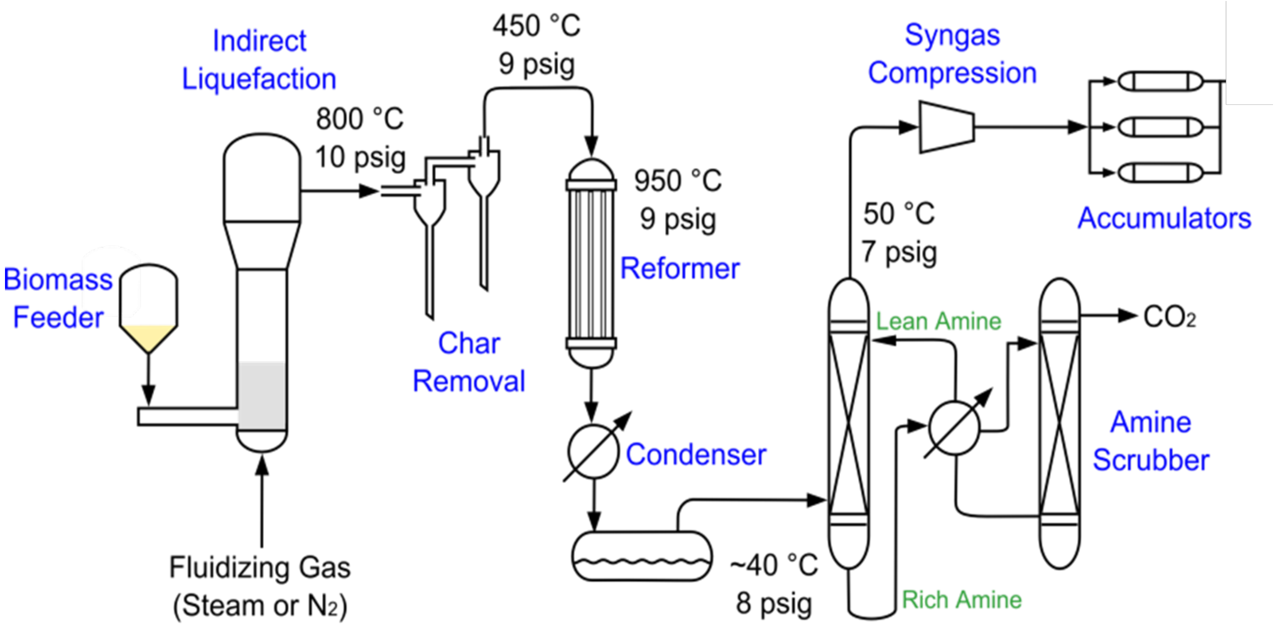
Gasification Capabilities Building with Multi-Scale Experimental and Modeling Approach Continuing

Fast Pyrolysis vs. Gasification: New Challenges

Fast Pyrolysis of Forest Residues	Gasification of MSW
• Complex size and shaped particles • Chemistry varies • Particle shrinks to char • Particle maintains structure • Aerodynamics (fluidization) varies • End product goal: oil • C objective: maximize oil, minimize gases	• Complex size and shaped particles • Chemistry varies drastically • Particles are consumed • Particle morphology changes • Aerodynamics (fluidization) varies • End product goal: syngas • C objective: maximize H2 (#1), CO (#2), minimize CO2 & tar

MSW Feedstocks

- Plastic-Rich
- As-received
- Paper-Rich



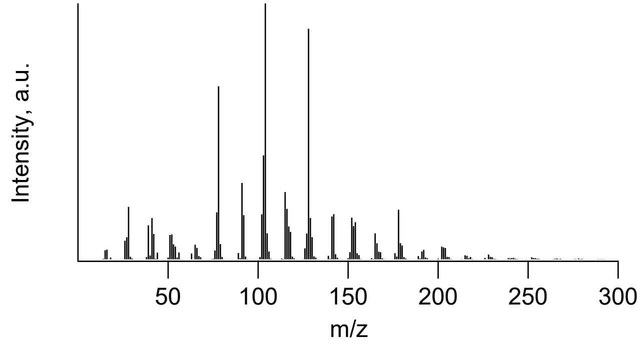
NREL Research Gasifier

New Micro- and Macro-Scale Instruments Enable High-Throughput Studies of Individual Particles

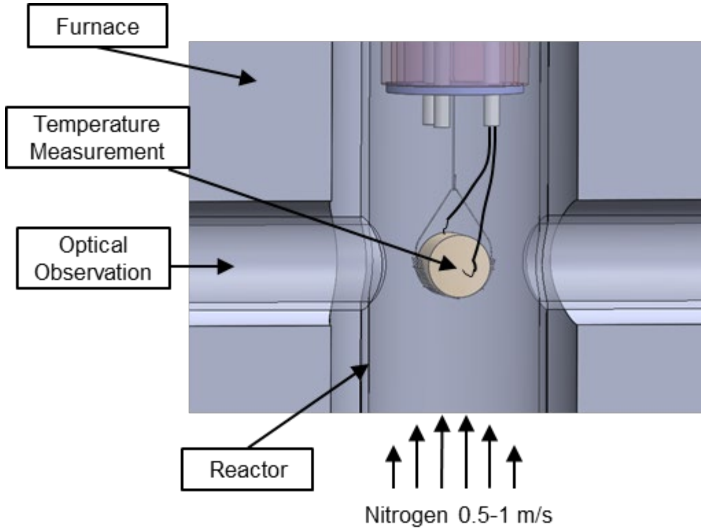
Micro-Scale Reactor

- Plastic-Rich
- Plastic Components
- As-received
- Paper Components
- Paper-Rich
- Mixtures

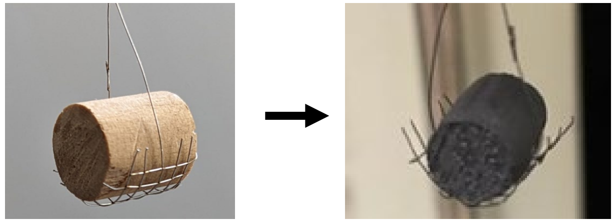
Particle mass: 10-30 mg
Temperatures up to 1000ºC
Real-time online mass spectral analysis



Macro-Scale Thermo-Gravimetric Analyzer (TGA)



Particle mass up to 2 g (resolution +/- 1 mg)
Temperatures up to 800ºC
Heating rates of 50ºC/sec.
Real-time online mass spectral analysis

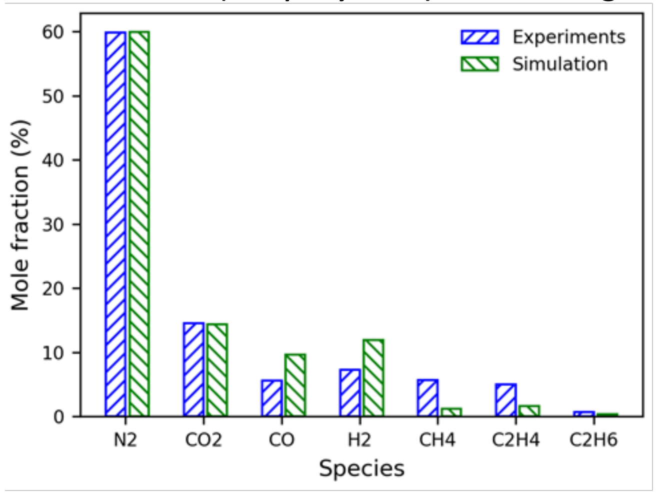


Reactor-Scale Computational Fluid Dynamics Model Developed for Gasification of Biomass & Plastic Feedstocks

- A computational fluid dynamics (CFD) model of a gasification reactor predicts conversion to gas products for biomass and plastic feedstocks; the model has been validated with experimental results from a pilot scale reactor.
- The model has been validated with data from the Fluidized Air Blown Experimental Gasifier Reactor (FABER) in collaboration with Sotacarbo SpA - Sustainable Energy Research Centre in Italy

Validation of Co-Gasification of:

- *Biomass (Eucalyptus) @24.9 kg/hr*
- *Plastic (Blupolymer) @ 34.9 kg/hr*



Photo, Schematic, and MFiX CFD Model of FABER Gasification Reactor

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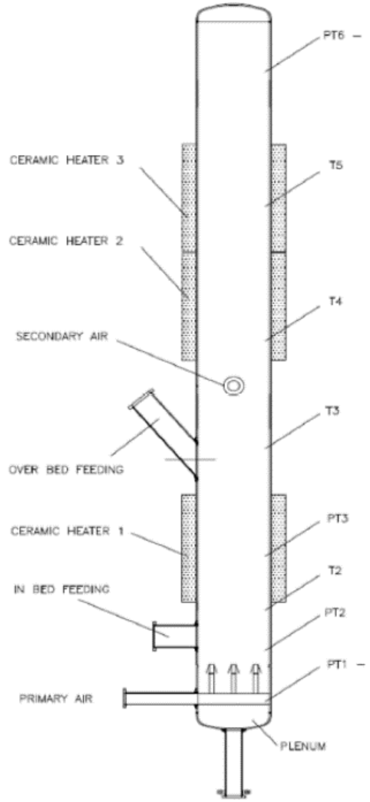
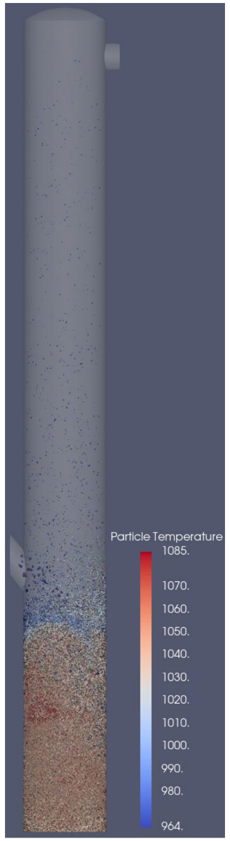
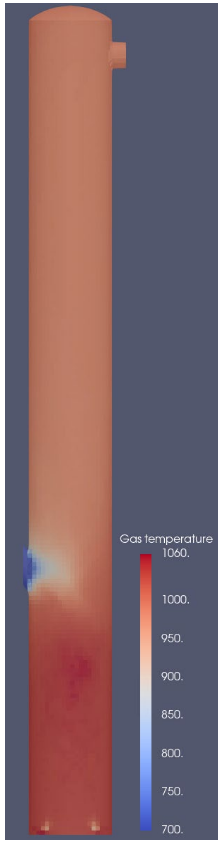
SUSTAINABLE ENERGY RESEARCH CENTRE



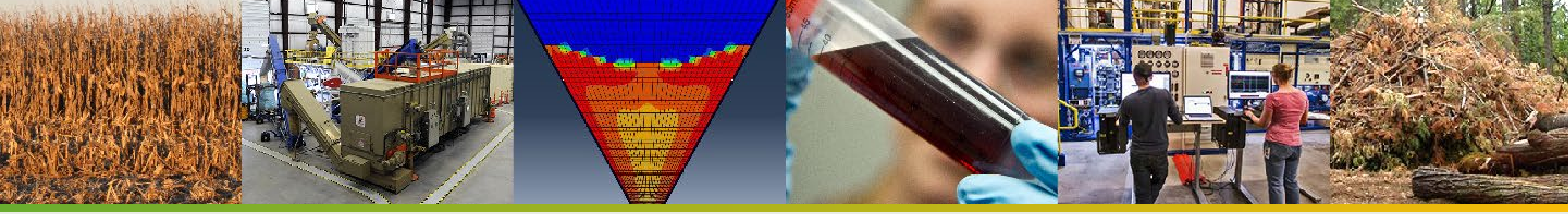
Particle Temperature (K)



Gas Temperature (K)



MFiX
mfix.netl.doe.gov



3 – Impact

Impact

Fast Pyrolysis

- Comprehensive multiscale experimental & computational framework validated with forest residues
  - Computational Fluid Dynamics (CFD) code (MFiX)
  - Reduced-order code
  - On-line (GitHub) tool for translating feedstock analysis to reactant inputs
  - Techno-Economic Analysis (TEA) level code
  - Detailed bio-oil chemistry products
- Tech Transfer of framework ongoing: 23 publications and 5 presentations including:
  - TCBiomass, Denver, CO, April 19-21, 2022
  - American Institute of Chemical Engineers (AIChE) Annual Meeting, Phoenix, AZ, Nov. 13-18, 2022
  - 16th International Biomass Conference & Expo, Atlanta, GA, Feb. 28-March 2, 2023
  - BETO Webinar: "Cost-Effectively Optimize and Scale Bioenergy Technologies with the Consortium for Computational Physics and Chemistry", October 20, 2022
    [available to watch at www.youtube.com/watch?v=6IpMGfcAi8U]
- Industry stakeholders engaged on tech transfer of toolsets

Gasification

- Reactor-scale validation of gasification of plastic-biomass mixtures shows promise for capabilities to model complex low-cost feedstocks

Summary: High Temperature Conversion

Objective: *Provide a fundamental science-based understanding of the high-temperature conversion of low-cost, complex mixtures of biomass and waste feedstocks for Sustainable Aviation Fuels (SAF) and related co-products*

Approach: *Quality by Design (QbD), Multi-Scale Model-Experiment Coupling, Industry Input-Output*

Fast Pyrolysis

- ***Outcomes***
  - A validated, multiscale experimental & computational framework for fast pyrolysis of forest residues feedstock blends
  - *Complex chemistry enabled via Debiagi kinetics and associated translational toolsets*
- ***Impact***
  - Demonstrated utility in range of models: techno-economic analysis modules to full reactor computational fluid dynamic models

Gasification

- ***Progress***
  - Industry survey guiding R&D direction
  - New tools enable high-throughput studies of conversion at micro- and macro-scales for validation at particle scales
  - Recommissioning of national lab-based gasifier for experiments in process
- ***Impact***
  - Initial reactor-scale model validated with Sotacarbo shows promise for accounting for complex feedstock blends

Quad Chart Overview

Timeline (current AOP cycle)

- *October 1, 2021*
- *September 30, 2024*

	FY22 Costed	Total Award
DOE Funding	*~$1,750k*	*$1,750k/yr across 6 NLs in Task 6*
Project Cost Share *	NA	NA

TRL at Project Start: 3
TRL at Project End: 5

Project Goal

Provide a fundamental science-based understanding of the high-temperature conversion of low-cost, complex mixtures of biomass and waste feedstocks for Sustainable Aviation Fuels (SAF) and related co-products

End of Project Milestone

(1) *Validated, high-throughput conversion screening pipeline covering broad conversion options;*

(2) *Critical Quality Attritibutes (CQAs) and ranges for Catalytic Fast Pyrolysis (CFP) and gasification intermediates from forest residues and MSW, respectively, related to Critical Material Attributes (CMAs) for co-processing and fuel synthesis;*

(3) *Validated, multi-scale computational framework to predict intermediate yields and chemistry for CFP and gasification vs. feedstock and air-to-fuel ratio.*

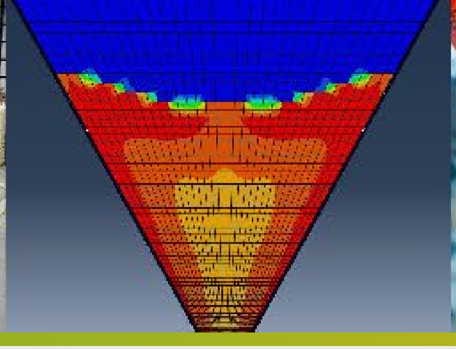
Funding Mechanism

2021 Lab Call – FCIC Merit Review

Project Partners

- 28 Industry partners participated in survey
- Debiagi/CRECK Group
- Sustainable Energy Research Centre (Italy)






Additional Slides

fcic
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Responses to Previous Reviewers' Comments

- **Feedback from FY21 BETO Peer Review:**
  – The primary feedback from the FY21 BETO Peer Review was to include gasification as a pathway for thermochemical conversion.
- **Response:**
  – Per feedback, Task 6 added gasification as a pathway.

Publications (1 of 2)

1. Lu, L. Q. G., X.; Dietiker, J. F.; Shahnam, M.; Rogers, W. A. "MFiX based multi-scale CFD simulations of biomass fast pyrolysis: A review," *Chemical Engineering Science* Vol. 248, 2022, p. 26.
2. Lu, L. Q. L., C.; Rowan, S.; Hughes, B.; Gao, X.; Shahnam, M.; Rogers, W. A. "Experiment and computational fluid dynamics investigation of biochar elutriation in fluidized bed," *AIChe Journal* Vol. 68, No. 2, 2022, p. 11.
3. Lu, L. Brennan Pecha, M.; Wiggins, Gavin M.; Xu, Yupeng; Gao, Xi; Hughes, Bryan; Shahnam, Mehrdad; Rogers, William A.; Carpenter, Daniel; Parks, James E. "Multiscale CFD simulation of biomass fast pyrolysis with a machine learning derived intra-particle model and detailed pyrolysis kinetics," *Chemical Engineering Journal* Vol. 431, 2022, p. 133853.
4. Gao, X. Y., J.; Portal, R. J. F.; Dietiker, J. F.; Shahnam, M.; Rogers, W. A. "Development and validation of SuperDEM for non-spherical particulate systems using a superquadric particle method," *Particuology* Vol. 61, 2022, pp. 74-90.
5. Xu, Y.; Shahnam, M.; Rogers, W. A. CFD Simulation of Biomass Pyrolysis Vapor Upgrading over a Pt/TiO2 Catalyst in Fixed and Moving Beds; DOE.NETL-2022.3734; NETL Technical Report Series; U.S. Department of Energy, National Energy Technology Laboratory: Morgantown, WV, 2022; p 40. https://edx.netl.doe.gov/dataset/cfd-simulation-of-biomass-pyrolysis-vapor-upgrading-over-a-pt-tio2-catalyst-in-fixed-and-moving-beds.
6. Li, C, Gao, X, Rowan, SL, Hughes, B, Rogers, WA. Measuring binary fluidization of nonspherical and spherical particles using machine learning aided image processing. *AIChE J.* 2022; 68(7):e17693.
7. Cheng Li, Rupendranath Panday, Xi Gao, Jiarong Hong, William A. Rogers, Measuring particle dynamics in a fluidized bed using digital in-line holography, *Chemical Engineering Journal*, Volume 405, 1 February 2021, 126824, https://doi.org/10.1016/j.cej.2020.126824
8. Lu, L. G., Xi; Gel, Aytekin; Wiggins, Gavin M.; Crowley, Meagan; Pecha, Brennan; Shahnam, Mehrdad; Rogers, William A.; Parks, James; Ciesielski, Peter N. "Investigating biomass composition and size effects on fast pyrolysis using global sensitivity analysis and CFD simulations," *Chemical Engineering Journal* Vol. 421, 2021, p. 127789.
9. Gao, X. Y., Jia; Lu, Liqiang; Li, Cheng; Rogers, William A. "Development and validation of SuperDEM-CFD coupled model for simulating non-spherical particles hydrodynamics in fluidized beds," *Chemical Engineering Journal* Vol. 420, 2021, p. 127654. https://doi.org/10.1016/j.cej.2020.127654. (https://www.sciencedirect.com/science/article/pii/S1385894720337761)
10. Gao, X. Y., J.; Lu, L. Q.; Rogers, W. A. "Coupling particle scale model and SuperDEM-CFD for multiscale simulation of biomass pyrolysis in a packed bed pyrolyzer," *AIChe Journal* Vol. 67, No. 4, 2021, p. 15. https://doi.org/10.1002/aic.17139.
11. Li, C., Gao, X., Rowan, S., Hughes, B., Jeremy S. Harris, and Rogers, W. A. Experimental investigation on the binary/ternary fluidization behavior of Geldart D type spherical LDPE, Geldart D type cylindrical wood and Geldart B type sand particles; NETL-TRS-2725-2021; NETL Technical Report Series; U.S. Department of Energy, National Energy Technology Laboratory: Morgantown, WV, 2021.

12. Lu, L. Q. G., X.; Shahnam, M.; Rogers, W. A. "Open source implementation of glued sphere discrete element method and nonspherical biomass fast pyrolysis simulation," *AIChe Journal* Vol. 67, No. 6, 2021, p. 14. https://doi.org/10.1002/aic.17211.
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14. Gao, X. L., L. Q.; Shahnam, M.; Rogers, W. A.; Smith, K.; Gaston, K.; Robichaud, D.; Pecha, M. B.; Crowley, M.; Ciesielski, P. N.; Debiagi, P.; Faravelli, T.; Wiggins, G.; Finney, C. E. A.; Parks, J. E. "Assessment of a detailed biomass pyrolysis kinetic scheme in multiscale simulations of a single-particle pyrolyzer and a pilot-scale entrained flow pyrolyzer," *Chemical Engineering Journal* Vol. 418, 2021, p. 12.
15. Yu, J. G., X.; Lu, L. Q.; Xu, Y. P.; Li, C.; Li, T. W.; Rogers, W. A. "Validation of a filtered drag model for solid residence time distribution (RTD) prediction in a pilot-scale FCC riser," *Powder Technology* Vol. 378, 2021, pp. 339-347.
16. Starace, Anne K., et al. "Predicting Catalytic Pyrolysis Aromatic Selectivity from Pyrolysis Vapor Composition Using Mass Spectra Coupled with Statistical Analysis." *ACS Sustainable Chemistry & Engineering* 10.1 (2021): 234-244. (joint effort with Process Monitoring and Predictions Project (WBS 3.1.1.011, part of SDI))
17. Peter N Ciesielski, M Brennan Pecha, Nicholas E Thornburg, Meagan F Crowley, Xi Gao, Oluwafemi Oyedeji, Hariswaran Sitaraman, Nicholas Brunhart-Lupo, “Bridging scales in bioenergy and catalysis: a review of mesoscale modeling applications, methods, and future directions”, *Energy & Fuels* **35** (18), 14382-14499 (2021).
18. M Brennan Pecha, Nicholas E Thornburg, Chad A Peterson, Meagan F Crowley, Xi Gao, Liqiang Lu, Gavin Wiggins, Robert C Brown, Peter N Ciesielski, “Impacts of anisotropic porosity on heat transfer and off-gassing during biomass pyrolysis”, *Energy & Fuels* **35**(24), 20131-20141 (2021).
19. Jordan Klinger, Nepu Saha, Steven M. Rowland, Tim Dunning, Daniel Carpenter, Zach Mills, James Parks, “Impact of forest residue variability on feeding into a high-temperature reactor”, accepted to *Fuel Processing Technology* (Manuscript Number: FUPROC-D-22-01594) (2023).
20. Mario Sánchez, Juan C Maya, Brennan Pecha, Farid Chejne, Adriana M Quinchía-Figueroa, “Effect of particle characteristics, kinetics and transport phenomena on the prediction of particle mass loss and products yields during biomass fast pyrolysis”, Journal of Analytical and Applied Pyrolysis **168**, 105786 (2022).
21. Matthew R Wiatrowski, Abhijit Dutta, M Brennan Pecha, Meagan Crowley, Peter N Ciesielski, Daniel Carpenter, “A simplified integrated framework for predicting the economic impacts of feedstock variations in a catalytic fast pyrolysis conversion process”, *Biofuels, Bioproducts and Biorefining” 16(2), 403-412 (2022).*
22. Meagan F Crowley, Hariswaran Sitaraman, Jordan Klinger, Francois Usseglio-Viretta, Nicholas E Thornburg, Nicholas Brunhart-Lupo, M Brennan Pecha, James H Dooley, Yidong Xia, Peter N Ciesielski, “Measurement of Transport Properties of Woody Biomass Feedstock Particles Before and After Pyrolysis by Numerical Analysis of X-Ray Tomographic Reconstructions”, *Frontiers in Energy Research* **10** (1997).
23. Oluwafemi A Oyedeji, M Brennan Pecha, Charles EA Finney, Chad A Peterson, Ryan G Smith, Zachary G Mills, Xi Gao, Mehrdad Shahnam, William A Rogers, Peter N Ciesielski, Robert C Brown, James E Parks II, “CFD–DEM modeling of autothermal pyrolysis of corn stover with a coupled particle-and reactor-scale framework”, *Chemical Engineering Journal* **446**, 136920 (2022).

Presentations

1. James Parks, Danny Carpenter, Liqiang Lu, William Rogers, M. Brennan Pecha, Gavin Wiggins, Peter Ciesielski, Meagan Crowley, Kristina Iisa, Matthew Wiatrowski, Yupeng Xu, Mehrdad Shahnam, Jordan Klinger, Damon Hartley, Huamin Wang, Erin Webb, “A Multi-Scale Framework for Simulation of the Impact of Feedstock Variability on Fast Pyrolysis Products”, 16th Annual International Biomass Conference & Expo, Atlanta, GA, February 28-March 2, 2023.
2. James Parks, Danny Carpenter, Liqiang Lu, William Rogers, M. Brennan Pecha, Gavin Wiggins, Peter Ciesielski, Meagan Crowley, Kristina Iisa, Matthew Wiatrowski, Yupeng Xu, Mehrdad Shahnam, Jordan Klinger, Damon Hartley, Huamin Wang, Erin Webb, “A Multi-Scale Framework for Simulation of the Impact of Feedstock Variability on Fast Pyrolysis Products”, Feedstock Conversion Interface Consortium – Understanding Feedstock Variability to Enable Next Generation Biorefineries (Invited Talks) at the American Institute of Chemical Engineers Annual Meeting, Phoenix, AZ, November 14, 2022.
3. Jim Parks, Jim Dooley, Kevin Barnett, and Joaquin Alarcon, “Cost-Effectively Optimize and Scale Bioenergy Technologies with the Consortium for Computational Physics and Chemistry (CCPC), Webinar hosted by the U.S. Department of Energy Bioenergy Technologies Office, October 20, 2022.
4. James Parks, Danny Carpenter, Liqiang Lu, Bill Rogers, Brennan Pecha, Gavin Wiggins, Peter Ciesielski, Meagan Crowley, Kristiina Iisa, Matthew Wiatrowski, Yupeng Xu, Mehrdad Shahnam, Jordan Klinger, Damon Hartley, Huamin Wang, Erin Webb, “A Multi-Scale Framework for Simulation of the Impact of Feedstock Variability on Fast Pyrolysis Products”, TCBiomass: Achieving Net Zero Carbon Goals – the Role for Biomass, April 19–21, 2022, Denver, Colorado.
5. Huamin Wang, Miki Santosa, Suh-Jane Lee, Igor Kutnyakov, “Biomass Fast Pyrolysis Vapor and Bio-oil Upgrading: Catalyst Deactivation and its Correlation with Feedstock Properties”, (invited oral presentation) 2021 AIChE Annual Meeting, November 7-9, 2021, Boston, MA.

Abstract

The High-Temperature Conversion Task (Task 6) of the Feedstock-Conversion Interface Consortium (FCIC) addresses challenges with thermochemical conversion of diverse feedstocks. Conversion unit operations include fast pyrolysis and gasification. Feedstocks range from complex mixtures of woody biomass (forest residues) to municipal solid waste (MSW). The research identifies and quantifies the feedstock Critical Material Attributes (CMAs) and product Critical Quality Attributes (CMAs) consistent with the FCIC's overarching approach embracing the Quality by Design methodology. A primary outcome targeted by the research is experimentally-validated computational modeling toolsets that can be utilized by the bioenergy industry to efficiently scale up and operated bioenergy technologies.