

# DOE Bioenergy Technologies Office (BETO) 2019 Project Peer Review

## FCIC Future Plans (FY19 and beyond)

March 7, 2019

Zia Abdullah,	NREL
Paul Bryan,	SNL
Katy Christiansen,	LBNL
Meltem Urgan Demirtas,	ANL
Corinne Drennan,	PNNL
Richard Hess,	INL
Babs Marrone,	LANL
Bill Smith	NETL
Tim Theiss	ORNL



## How are biorefineries engineered today, and what are the limits of current practice?

- Presently biorefineries are designed and built by firms that engineer equipment for **agricultural and pulp & paper industry**
  - These firms use engineering approaches **based on prior experience**
  - This approach is **adequate for mature industries** where changes are incremental, but is **not suitable for new industries**, where the physics and scaleup rules are not well understood
- Bench scale & pilot operations are generally limited because of need to commercialize quickly and therefore **underlying physics is poorly understood**
- Biomass at commercial production scale (~1,000 tons/day) generally has **higher variability** than that of small batches used in bench and pilot scales.



# Goal Statement

## Goals:

1. Develop **First Principles based knowledge and tools for technology development firms** to use when designing, building and operating biorefineries.
2. Develop a **framework** through which technology developers will be able **to assess the quality and value of streams** to make decisions to achieve successful, profitable operations.

## Outcome:

- **Increase chance of successful startup & operation** from 30% to 70%.

**Demonstrable Metric:** Achieve target product quality with variable feed for continuous operation over 500 hours for selected unit operations.

## Relevance and Payoffs:

- . If FCIC is successful we will:
  - be instrumental in aiding the startup of the bioenergy industry by enabling design and operating practices which **allow continuous process flows at nameplate capacity**
  - change the paradigm to **use fundamental knowledge rather than empiricism** to solve technical problems in the bioenergy industry



# Quad Chart Overview

## Timeline

- Project Start Date: February 2019
- Project End Date : September 2021
- Percent Complete: 0% (New Start)

	FY 19 Plan	FY 20 Plan	FY 21 Plan	Total Planned Funding (FY 21 -Project End Date)
<b>DOE Funded</b>	\$14M	\$14M	\$14M	\$42M
<b>Project Cost Share*</b>	N.A.	N.A.	N.A.	N.A.

**Partners:**\$4,927K (INL), \$3,847K (NREL), \$475K (LBNL), \$610K (LANL), \$1,235K (ORNL), \$1,060K (PNNL), \$225K (SNL), \$1,155K (ANL), \$300K (NETL)

**2017 Forward Funded: \$8M for Direct Funding Opportunity**

## Barriers addressed

Ct-A. Feedstock Variability, Ct-B. Reactor Feed Introduction, Ct-C. Efficient Preprocessing, Ct-D. Efficient Pretreatment, Ct-J. Process Integration , Ct-N. Materials Compatibility and Reactor Design and Optimization Integration, Ft-E. Terrestrial Feedstock Quality, Monitoring, Ft-G. Biomass Physical State Alteration and Impact on Conversion Performance Ft-I. Overall Integration and Scale-Up , Im-A. Inadequate Supply Chain Infrastructure, It-B. Risk of First-of-a-Kind Technology, It-C. Technical Risk of Scaling

## Goals & Outcome

- Develop knowledge and tools for biorefinery developers, so that with improved design and process specifications chance of successful startup & operation of a pioneer biorefinery increases from 30% to 70%.
- Develop a framework through which technology developers will be able to assess the quality and value of streams for the purpose of using that valuation to make decisions to achieve successful, profitable operations.

## End of Project Goal

- Deliver First Principles based tools and knowledge which engineers will be able to access and use when designing, building and operating biorefineries.
- Achieve target product quality with variable feed for continuous operation over 500 hours for selected unit operations.



## What's new in our approach and why do we think it will be successful?

- Understand **fundamental mechanisms which** relate system performance to biomass properties
  - biomass composition, micro and macro structure
- Develop **first principles based, mechanistic models** of system performance
  - Validate using bench scale and pilot scale data
- Develop **scaling rules** based on
  - Mechanistic models
  - Experimental data
- Quantify, understand, and manage **variability**
- Develop **TEA/LCA models**
  - Value of variable feedstock as it goes through the value chain.



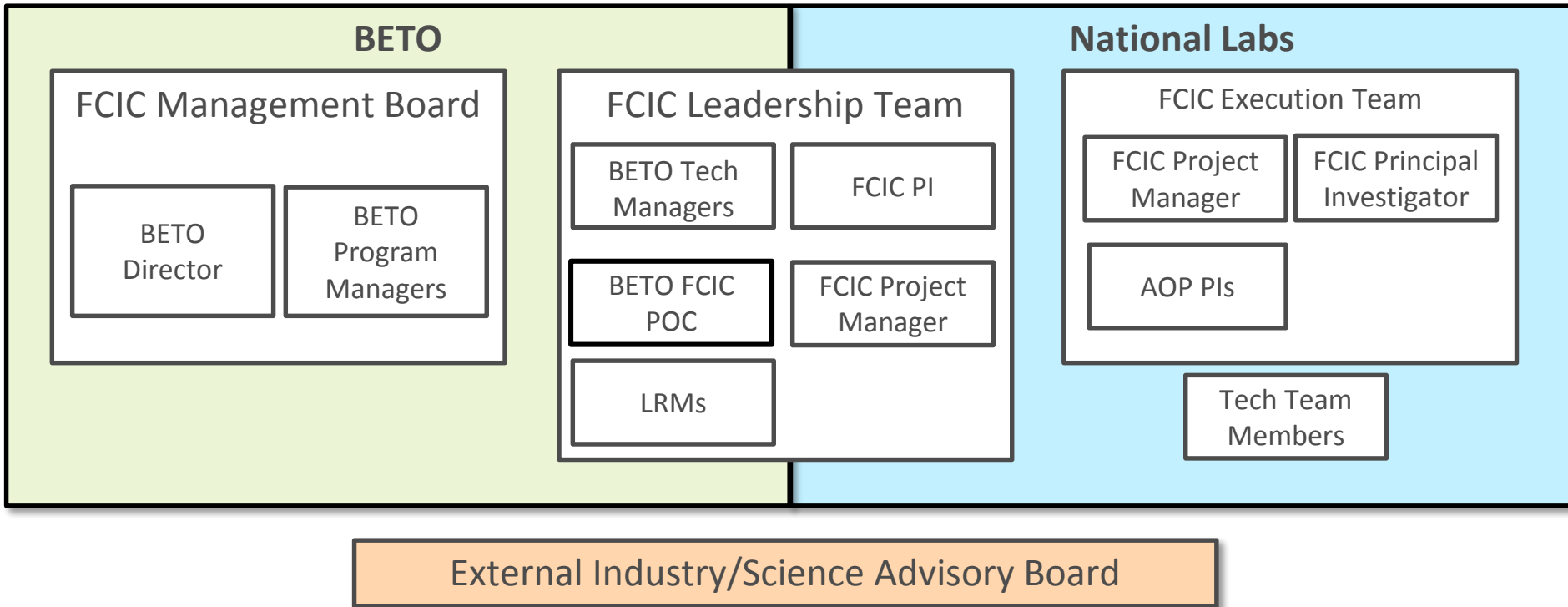
## What tangible value add will we deliver at the end of three years?

- **Knowledge and tools** that will help technology developers
  - Design Principles
  - Design Specifications
  - Materials of Construction specifications
  - Scaling Parameters
  - Models
  - Decision trees
  - Models & software tools
  - Feed material specifications
  - Product specifications
  - New process concepts
- A framework to assess the **quality and value of streams** to make decisions to achieve successful, profitable operations.



# Approach – Management

## FCIC Leadership Structure<sup>1</sup>



1: Additional slides detailing Management Approach are in the Appendix

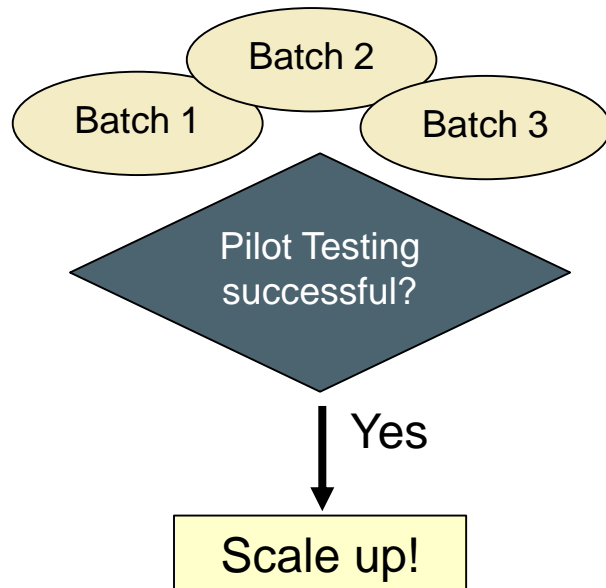


# Approach – Technical

We Will Use First Principles Based ‘Quality by Design’ Approach rather than the conventional ‘Quality by Testing’ Approach

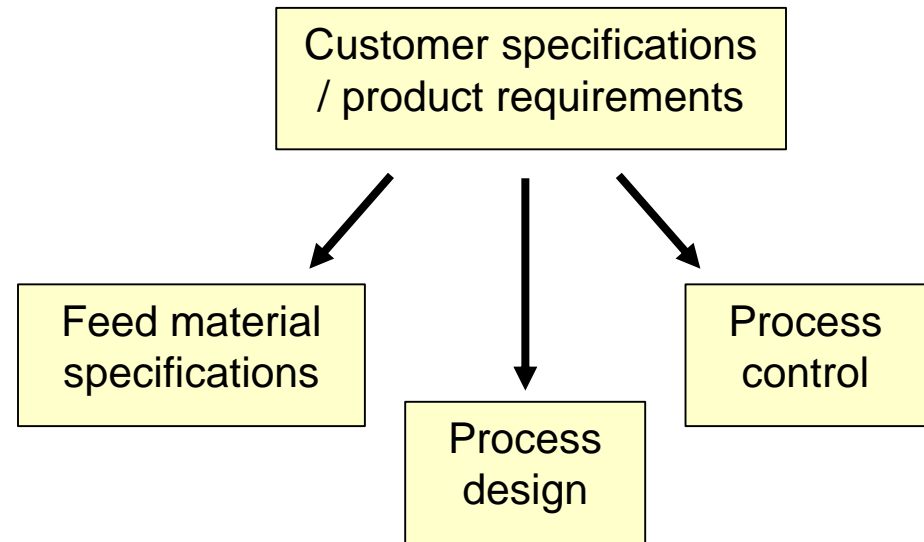
- **Quality by Testing:**

- **Product specification set by data from a small number of batches.** Acceptance criteria that required future batches to be the same.



- **Quality by Design:**

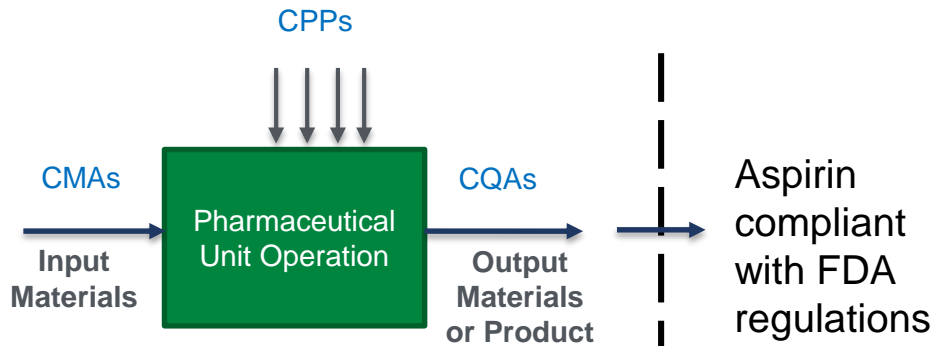
- **Design and control of the manufacturing process** and the product specification pre determined by customer





# Approach – Technical

## Quality by Design Approach as used in the Pharmaceutical Industry



- Based on sound science
- Predefined objectives
- Product and process understanding
- Process design and control
- Risk management

### Example: Blending/Mixing of Aspirin

CMA: Particle Size Distribution

CPP: Mixer load level

CQA: Blend uniformity

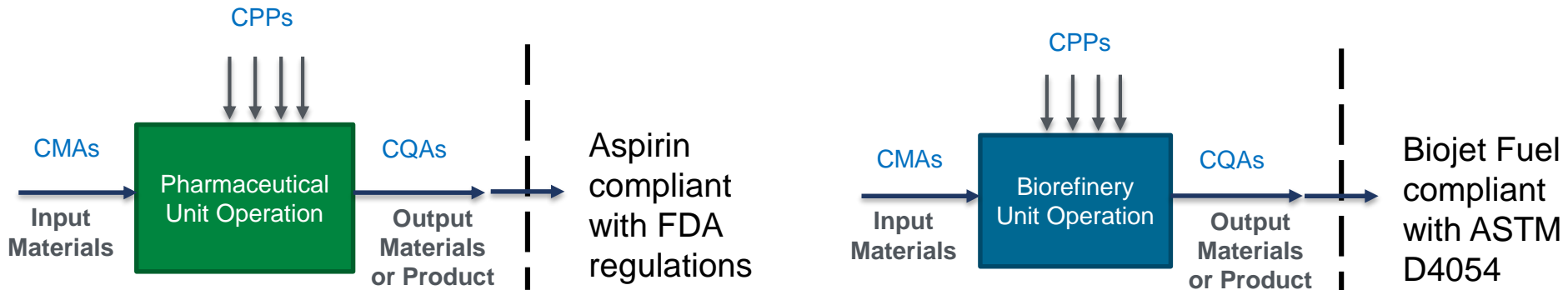
Critical Material Attribute (CMA)  
Critical Process Parameter (CPP)  
Critical Quality Attribute (CQA)

$$\text{CQAs} = f(\text{CMA}_1, \text{CMA}_2, \text{CMA}_3 \dots \text{CPP}_1, \text{CPP}_2, \text{CPP}_3 \dots)$$



# Approach – Technical

## Quality by Design Approach Can Be Analogous for Biorefinery Operations



### Example: Blending/Mixing of Aspirin

CMA: Particle Size Distribution

CPP: Mixer load level

CQA: Blend uniformity

### Example: Jet Fuel Production

CMA: lignin content, H<sub>2</sub> content

CPP: process design & operation

CQA: Aromatic content < 25%

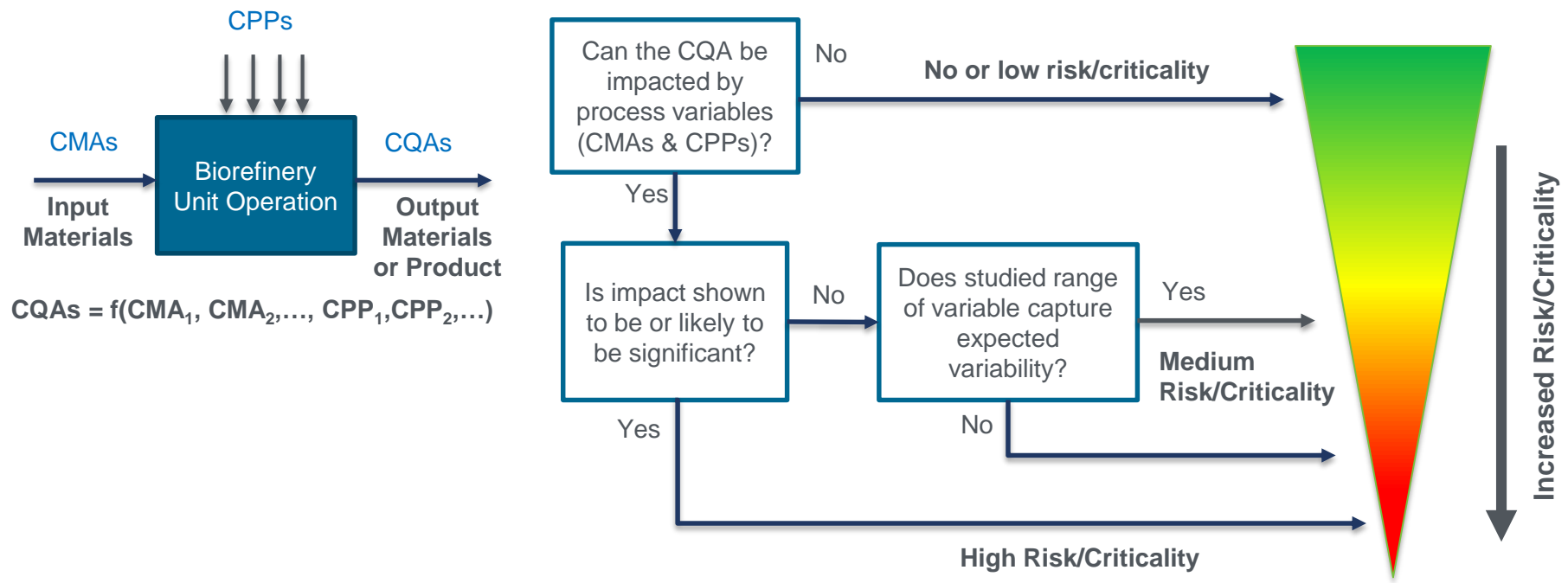
Critical Material Attribute (CMA)  
Critical Process Parameter (CPP)  
Critical Quality Attribute (CQA)

$$\text{CQAs} = f(\text{CMA}_1, \text{CMA}_2, \text{CMA}_3 \dots \text{CPP}_1, \text{CPP}_2, \text{CPP}_3 \dots)$$



# Approach – Technical

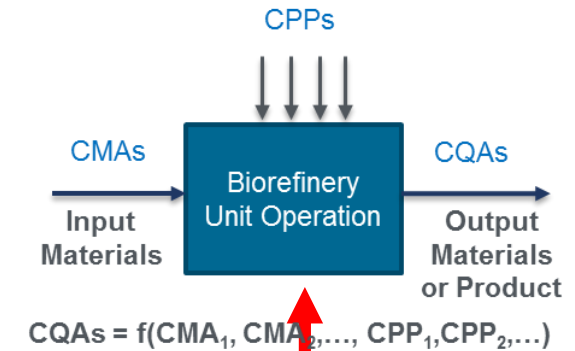
- A material stream may have many attributes
- Not all may play a significant role in the unit operation, *i.e.* “Critical”
- The flowchart below can be used to prioritize the high risk, “Critical” attributes which have a big impact on the unit operation



# Approach – Technical

Research will focus on the unit operation (CPP), which, with given CMAs would allow the process to achieve:

- **Predictable operation:**
  - Process will perform as expected
- **Reliable:**
  - The process will perform as expected over an extended period of time, across the range of variability
- **Scalable:**
  - Perform as expected across bench, pilot, and commercial scales
- CMA, CQA, and CPP should be Specific, and Measurable and Achievable within cost constraints.



**Research Focus**

Goal is fundamental, science-based understanding of the processes



# Approach – Technical

Critical Success Factor	Challenges	Strategy to Address challenges
First principles based representative models developed for all unit operations	Underlying phenomena are too complex to be understood and modeled within available resources	Alternatives to first principles models. Piecewise empirical relationships may have some element of science but will clearly have limits of applicability
Identification of CMAs and CPPs on CQAs	Not feasible to experimentally isolate a particular variable	Use first principles modeling to understand impact of independent variables on unit ops.
Cost effective technical solution to process all types of biomass	Some extremes of variability may be too difficult / expensive to handle	Identify limits to acceptable CMAs This may result in commoditization of biomass and may eliminate some types.
Solutions are scalable and result in successful operation of full scale equipment	Theoretical and lab scale work actually captures the ‘real’ problems faced by full scale equipment	Strive for first principles based, validated scaling parameters. Where this is not possible, recommend large scale piloting and further analysis.
Solutions will be adopted by industry	Industry is risk averse and may not adapt science developed at the National Labs	Employ Energy iCorps, DFOs, FOAs and other industrial engagement venues. Involve industry from the beginning through IAB.



# Approach – Technical

## FCIC Task TOOLS FOR TECHNOLOGY DEVELOPERS, BIOREFINERY DESIGNERS AND OPERATORS

Feedstock

Preprocessing

Conversion

Product QA/QC & Shipment

### Feedstock Variability:

Develop tools that quantify & understand sources of biomass feedstock variability with the objective of reducing sources of variability.

### Preprocessing:

Develop tools to enable technologies that provide well defined, homogeneous, quality controlled feedstock.

### Conversion (High Temperature & Low Temperature):

Develop tools to enable technologies that produce homogeneous, quality controlled intermediates that can be converted into market ready products.

### Materials Handling:

Develop tools that enable continuous, steady, trouble free feed into reactors

## Enabling Tasks

### Materials of Construction:

Develop tools that specify materials that do not corrode, wear, or break at unacceptable rates.

### Crosscutting Analyses TEA/LCA & Merit function Development:

Develops tools that enable valuation and intermediate streams and quantify impact of variability. Merit function develops tools that optimize on selected target globally.

### Data Integration/Data Management & Validation:

Develop tools that can facilitate the transfer of data and information both internally and externally. Verify and vet tools developed in the other tasks via reliability models, iCorps, industrial engagement.



## TOOLS FOR TECHNOLOGY DEVELOPERS, BIOREFINERY DESIGNERS AND OPERATORS

### Task 1: Materials of Construction:

Customers: **Equipment designers, Plant engineers**

Objective: Develop tools that specify materials that do not corrode, wear, or break at unacceptable rates.

### Task 2: Feedstock Variability:

Customers: **Process designers, Plant engineers**

Objective: Develop tools that quantify & understand sources of feedstock variability with the objective of reducing sources of variability.

### Task 3: Materials Handling:

Customers: **Process reactor designers, Plant engineers**

Objective: Develop tools that enable continuous, steady, trouble free feed into reactors

### Task 4: Data Integration/Data Management & Validation:

Customers: **Technology developers, Engineers**

Objective: Develop tools that can facilitate transfer of data and information both internally and externally. Verify and vet tools developed in the other tasks via reliability models, iCorps, industrial engagement..

### Task 5: Preprocessing:

Customers: **Process reactor designers, Plant engineers**

Objective: Develop tools to enable technologies that provide well defined, homogeneous, quality controlled feedstock.

### Task 6, 7: Conversion Tasks (one for High Temperature and one for Low Temperature):

Customers: **Process reactor designers who use conversion intermediates**

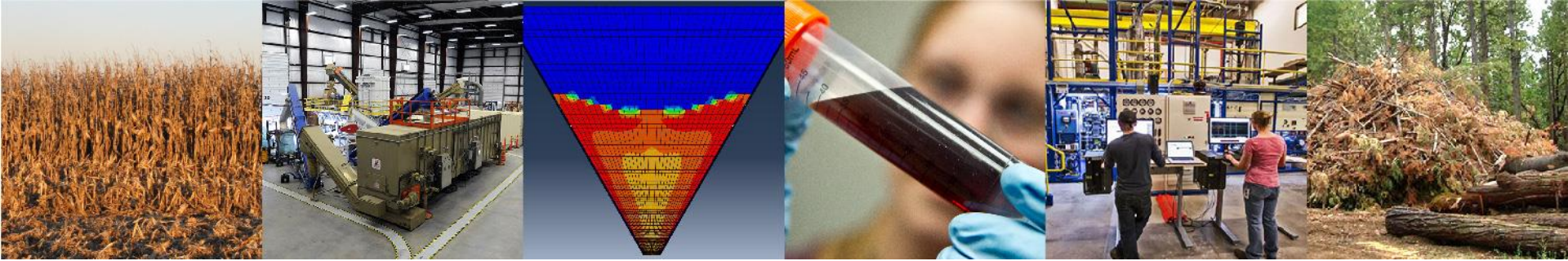
Objective: Develop tools to enable technologies that produce homogeneous, quality controlled intermediates that can be converted into market ready products.

### Task 8: Crosscutting Analyses TEA/LCA & Merit function Development:

Customers: **Investors, Regulatory bodies**

Objective: TEA/LCA develops tools that enable valuation and intermediate streams and quantify impact of variability. Merit function develops tools that optimize on selected target globally.





# Future Work



# Future Work – Task 1

## Materials of Construction

- **Objectives:**
  - Gain fundamental understanding of the **failure modes and wear mechanisms**
  - Develop **analytical tools/models** to predict wear and establish material property specifications
  - Identify and demonstrate **mitigation strategies** that meet specifications.
- **Technical Approach (Subtasks):**
  - 1.1 Understand and mitigation equipment wear in preprocessing (ORNL-INL-ANL)
  - 1.2 Understand and mitigation equipment wear in LT pre-conversion (NREL-ORNL-ANL)
  - 1.3 Mechanics of Wear (ANL)
- **Major Task Outcome(s)**
  - Fundamental understanding of equipment failure mechanisms
  - **Validated models/tools** to predict wear and degradation of materials
  - Identification and demonstration of **mitigation strategies**
- **Relevance:**
  - First principals based tools will enable equipment designs that will have **acceptable wear rates** and will **not fail through fracture** and similar mechanisms.



# Future Work – Task 2

## Feedstock Variability

- **Objectives:**
  - **Reduce feedstock variability** by quantifying & understanding its range and sources
- **Technical Approach (Subtasks):**
  - How **structural and physicochemical attributes** of cell wall architecture impact **flow behavior** & mechanical, biochemical, and thermochemical **deconstruction**.
    - 2.1: Variability, Transport and Synergistic Impacts of **Inorganic Species**
    - 2.2: Quantify and Understand Variability of **Molecular-scale attributes**
    - 2.3, 2.4: Feedstock Variability at the **Micro-scale & Macro scale**
    - 2.5: Data Analytics for Identifying CMAs of Feedstocks
- **Major Task Outcome(s)**
  - Provide information, data, and **tools that facilitate** a better understanding of the range of biomass material attributes and how variability can be modified through pre-processing into a feedstock with **well defined CMAs for conversion**.
- **Relevance:**
  - This task will **enable well defined CMAs** with predictable, and reasonably managed variability through pre-processing operations.



# Future Work – Task 3

## Materials Handling

- **Objectives:**
  - Enable **continuous, steady, trouble-free bulk flow** transport to reactor throat.
- **Technical Approach (Subtasks):**
  - Bulk flow experiments using **industry relevant biomass**
  - **Experimentally validated models:**
    - Discrete element models (DEM)
    - Finite Element Models (FEM)
    - Computational Fluid Dynamics (CFD)
- **Major Task Outcome(s):**
  - **Tools for equipment designers** and **gap identification** (knowledge and technology) **for end users/operators.**
  - **Acceptable CPPs and CMAs** for processing train
- **Relevance:**
  - This task develops **physics-based modeling tools** to enable design and operation of processing train equipment for reliable feeding.



# Future Work – Task 4

## Data Integration and Collaborative Computation

- **Objectives:**
  - Achieve **consistent workflow management, integration of datasets** between subtasks, and a **portal for public access** to results.
- **Technical Approach (Subtasks):**
  - 4.1: LabKey will be deployed at each NL to support FCIC R&D.
  - 4.2: Shared use of workflows, datasets, and software across the FCIC.
  - 4.3: **Harmonize and standardize analytical protocols, methods, and data formats.**
- **Major Task Outcome(s)**
  - **Facilitate collaboration** across eight labs.
  - Parameters uniformly applied.
  - Metadata and documentation to ensure that **experimental work is repeatable.**
- **Relevance:**
  - Ensure that **data will be Findable, Accessible, Interoperable**, and Reusable in accordance with DOE FAIR data principles and provenance requirements.
  - Eight labs will be able to **work effectively in a coordinated manner.**



# Future Work – Task 5

## Preprocessing

- **Objectives:**
  - Enable **predictable, reliable, and scalable performance of preprocessing** unit operations.
- **Technical Approach (Subtasks):**
  - Use a Quality by Design approach to develop models for select unit operations.
  - Relate CQAs to CMAs and CPPs.
- **Major Task Outcome(s)**
  - Science-based understanding of unit operations
  - **Design principles (equations)** that relate unit operation CQAs to CMAs and CPPs
  - Unit operation and **CMA specifications**
  - Process control models to achieve **CQA with lower variability that that in CMA**
- **Relevance:**
  - **Science-based design principles** will replace semi empirical and rule-of-thumb approaches, and will result in **improved performance**, value add, and **lower cost**.



# Future Work – Task 6

## Principles of Direct Biomass Liquefaction (high temperature conversion)

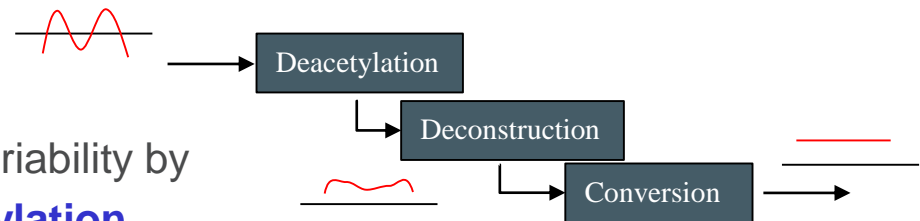
- **Objectives:**
  - Predict the effects of **variable CMA and CPP on pyrolysis** CQA
- **Technical Approach (Subtasks):**
  - Multiscale, state-of-the-art, **coupled experimental and modeling approach** that captures the fundamental physics and chemistry of high-temperature biomass feeding and pyrolysis reactor unit operations.
- **Major Task Outcome(s)**
  - Pyrolysis reactor **process operational map** to optimize productivity by predicting CQA for variable CMA.
- **Relevance:**
  - The **pyrolysis reactor process operational map** will be a first principles based tool which will **enable biorefinery designers to build full scale systems** with predictable performance, and which, for pre-specified CMA will meet product CQA.



# Future Work – Task 7

## Low-Temperature Conversion of Sugars and Lignin

- **Objectives:**
  - Determine impact of CMA **variability** on the low temperature conversion
  - Develop **tools to mitigate the risks posed by this variability**.
- **Technical Approach (Subtasks):**
  - Apply **real-time process monitoring and control** strategies to deacetylation
  - Investigate **impacts of CMA variability** using a experimental and modeling.



- **Major Task Outcome(s):**
  - Mitigate the risks posed by feedstock variability by
    - **minimizing variability after deacetylation**
    - understanding and predicting impacts of **variability** on downstream processes
- **Relevance:**
  - Implementing process monitoring and control will help **minimize CQA variability after deacetylation** and enable predictable and stable deconstruction and conversion processes to achieve **stable CQA and product quality**.



# Future Work – Task 8

## Crosscutting Analyses: TEA/LCA & Merit Function Development

- **Objectives:**
  - Enable valuation of intermediate streams and quantify impact of feedstock variability.
- **Technical Approach (Subtasks):**
  - Provide feedback to help bound research space to **ensure the outcomes are economically relevant**
  - **Trade-off** analyses to evaluate strategies to mitigate variability.
- **Major Task Outcome(s)**
  - **Systems-level understanding** of impacts of variability on economics and sustainability metrics.
- **Relevance:**
  - Tools to enable developers to **quantify the impact of feedstock variability** on their project's **economic and sustainability metrics**.
  - Enable biorefinery operators to make the most **appropriate feedstock choices** for their operations.





# Future Work (Year 3)

## Achieve target CQA with variable CMA for continuous operation over 500 hrs.

- **Objectives:**
  - Achieve **continuous 500 hours ‘time of stream’ at nameplate capacity**, while achieving target CQA with variable CMA.
- **Technical Approach (Subtasks):**
  - Select one or more unit operations
  - Plan & execute 500 hour run.
- **Major Task Outcome(s)**
  - **500 hours of continuous operation**
  - In case there is an interruption of continuous operation before the 500 hour mark, a detailed failure analysis report to demonstrate understanding of the underlying physics.
- **Relevance:**
  - 500 hours of continuous operation at nameplate capacity, while achieving target CQA with variable CMA will demonstrate that sufficient understanding of the fundamentals of that unit operation have been achieved.



## Goals:

1. Develop First Principles based knowledge and tools for technology developers to use when designing, building and operating biorefineries.
2. Develop a framework through which technology developers will be able to assess the quality and value of streams for the purpose of using that valuation to make decisions to achieve successful, profitable operations.

## Relevance to Industry:

- If FCIC is successful we will:
  - enable design and operating practices that can maintain **continuous operation at nameplate capacity**
  - **change the paradigm** to use fundamental knowledge rather than empiricism
  - Increase chance of **successful startup & operation** of pioneer biorefineries



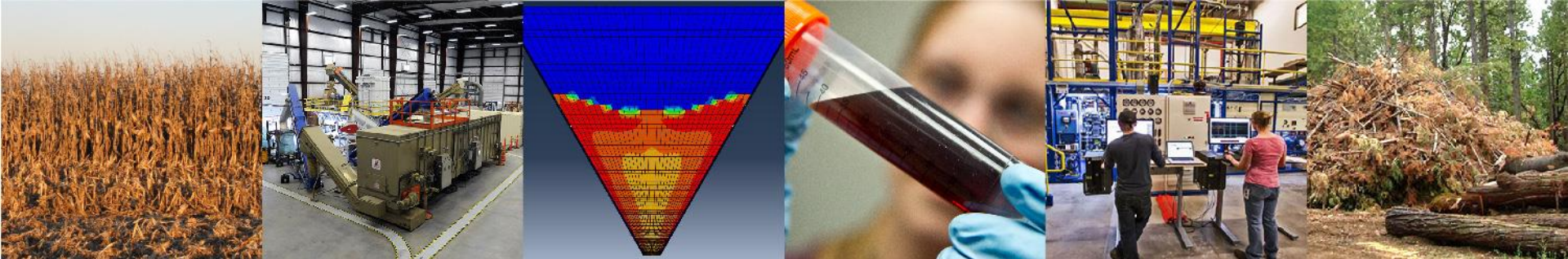
## Relevance to BETO:

- No technology can be successful if biomass cannot be fed consistently and continuously, at nameplate scale to the reactor throat and if the conversion process cannot operate with inherent feedstock variability. This program will specifically address these problems to develop approaches that will enable consistent feed into reactors and ability to manage variability.

## Technology Transfer:

- We plan to employ Energy iCorps, DFOs, FOAs and other industrial engagement venues. We will involve industry from the beginning through advisory board.
- The technology developed under this consortium will be applicable more broadly to thermochemical and biochemical systems.





## Acknowledgements:

### BETO

#### Management Board and Leadership Team

Jonathan Male

Kevin Craig

Mark Elless

Alison Goss Eng

Beau Hoffman

Liz Moore

Jim Spaeth

### National Lab Main Task PIs, Co-PIs

Mary Bidy NREL

Danny Carpenter NREL

Jim Collett PNNL

Bryon Donohoe NREL

Rick Elander NREL

Rachel Emerson INL

George Fenske ANL

Hai Huang INL

Kevin Kenney INL

Jim Parks ORNL

Steven Phillips PNNL

Jun Qu ORNL

Allison Ray INL

Mike Resch NREL

Troy Semelsberger LANL

Deepti Tanjore LBNL

Ed Wolfrum NREL

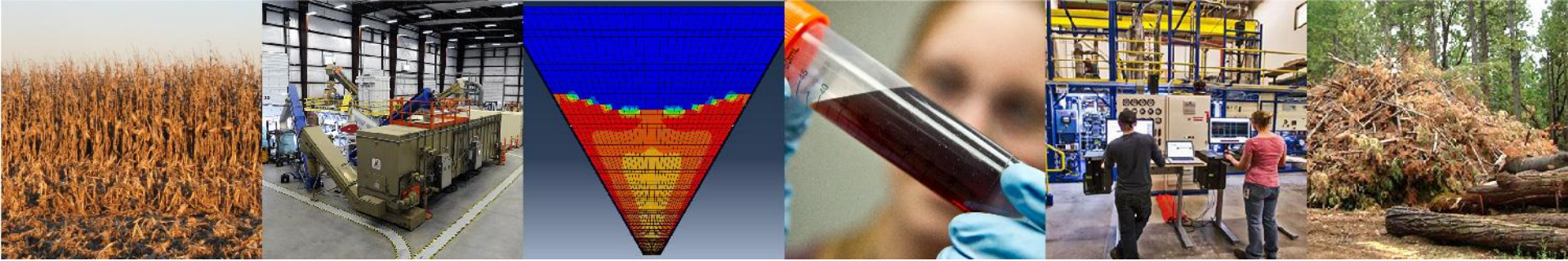


# Summary

- 1. Overview** – We have stood up a Consortium of 9 National Laboratories to work together to solve the very difficult and pervasive problem of pioneer refineries failing to start up and operate in a commercially successful manner. We hypothesize that that this failure rate is because of feedstock variability and biorefinery design is based on empiricism and experience.
- 2. Approach** – We will develop first principles hypotheses based, knowledge and tools for biorefinery developers, so that with improved design and process specifications chance of successful startup & operation of a pioneer biorefinery increases from 30% to 70%. We will also develop a framework through which technology developers will be able to assess the quality and value of streams for the purpose of using that valuation to make decisions to achieve successful, profitable operations.
- 3. Relevance** - If FCIC is successful we will 1) be instrumental in aiding the startup of the bioenergy industry by enabling design and operating practices that can maintain continuous process flows at nameplate capacity, and 2) change the paradigm to use fundamental knowledge rather than empiricism to solve technical problems in the bioenergy industry.
- 4. Future Work** – We have planned future work along 8 tasks which will address materials of construction, feedstock variability, materials handling, data integration, preprocessing, conversion, crosscutting analysis and 500 hour demonstration. Each of these tasks is focused on developing and demonstrating tools for technology developers and biorefinery designers / operators, so that with improved design and process specifications chance of successful startup & operation of a pioneer biorefinery increases from 30% to 70%.

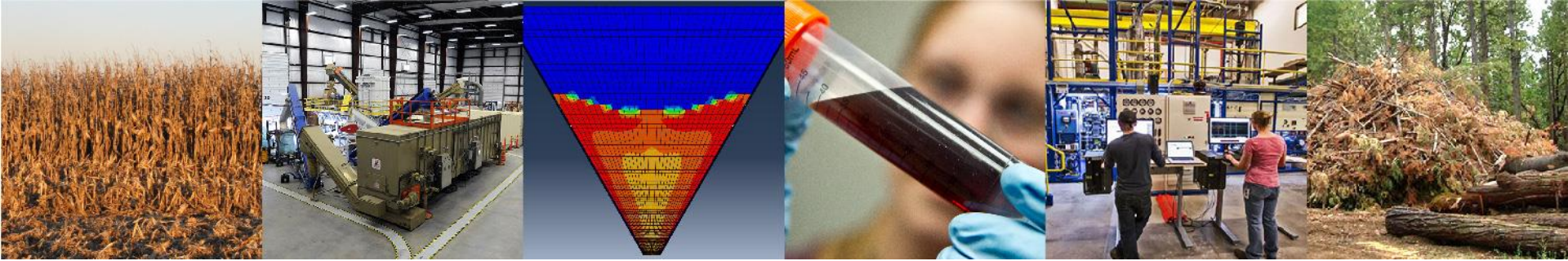






# *Discussion*





## Appendix

### Additional Slides on Management Approach



# Approach – Management

## FCIC Leadership Structure

### BETO

#### FCIC Management Board

BETO  
Director

BETO  
Program  
Managers

Exter

#### FCIC Management Board

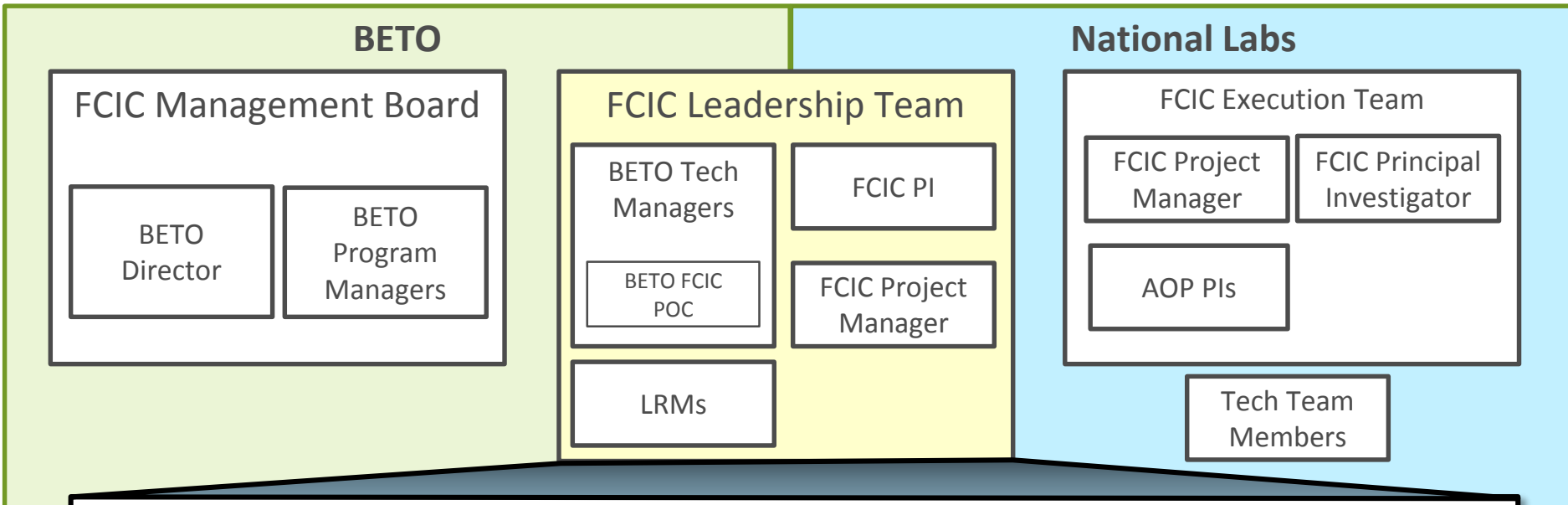
- Members
  - BETO Director and Program Managers
- Responsibilities
  - Meet twice yearly, or as needed
  - Advise Leadership Team on issues related to strategy and engaging w/ stakeholders
  - Approve changes in focus and direction or other major issues
  - Final approval of annual objectives for each FCIC task
  - Final approval of any DFO topics and subsequent awardees
  - Approve additions of members or other major changes in external advisory board
  - Oversee the handling of internal issues, as needed
  - Ensure strategic vision of FCIC is aligned with BETO goals and strategy (MYP, etc.)





# Approach – Management

## FCIC Leadership Structure



### FCIC Leadership Team

- Members
  - BETO Technology Managers LRM, FCIC PI, and FCIC PM
- Responsibilities
  - Set vision for FCIC and maintain focus on vision throughout the consortium's membership
  - Assess performance against goals at least annually, w/ input from External Advisory Board
  - Celebrate team successes and recognize contributions
  - Provide frequent feedback to team
  - Make decisions on funded tasks and budget breakdown

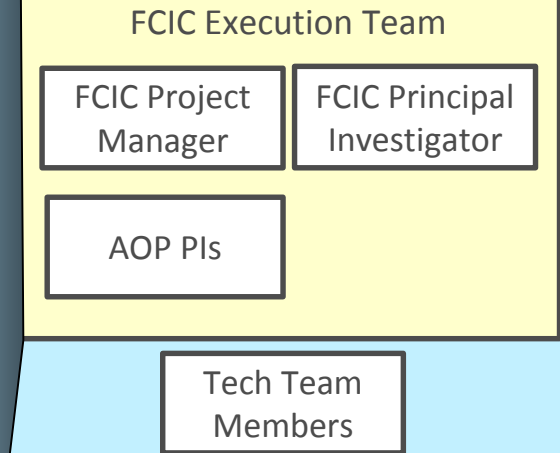
# Approach – Management

## FCIC Leadership Structure

### FCIC Execution Team

- Members
  - FCIC PI, PM, task and sub-task AOP PI's, Co-PIs
  - At least one member per lab
- Selected Responsibilities
  - Lead research execution under AOP
  - Identify gaps / overlaps and recommend mitigation
  - Look for cross collaboration opportunities and minimize 'silos'
  - Update changes in FCIC priorities, strategies, and operations with lab staff and management
  - Take responsibility for resolving personnel issues
  - Communicate staffing and personnel changes/concerns to the FCIC Leadership Team in a timely manner
  - Manage AOP development and responses to lab calls (if necessary)
  - Establish and work with External Advisory Board
  - Mentor team leads and PIs; arbitrate and resolve disagreements between PIs

### National Labs



board

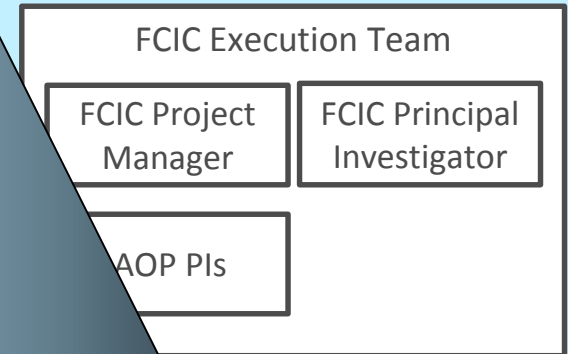
# Approach – Management

## FCIC Team Skill Sets

### FCIC Team Skills

- Technical
  - Chemical Engineering
  - Mechanical Engineering
  - Materials and Metallurgical Engineering
  - Tribology (friction& wear)
  - Microbiology, Synthetic Biology
  - Chemistry
  - Physics
  - Thermodynamics
  - Analytical (Physical, chemical, biological)
  - Modeling (CFM, FEM, DEA, NN, AI, Process)
  - Data management / data analysis
  - Statistical analysis.
  - Techno economic analysis
  - Life Cycle Analysis

### National Labs



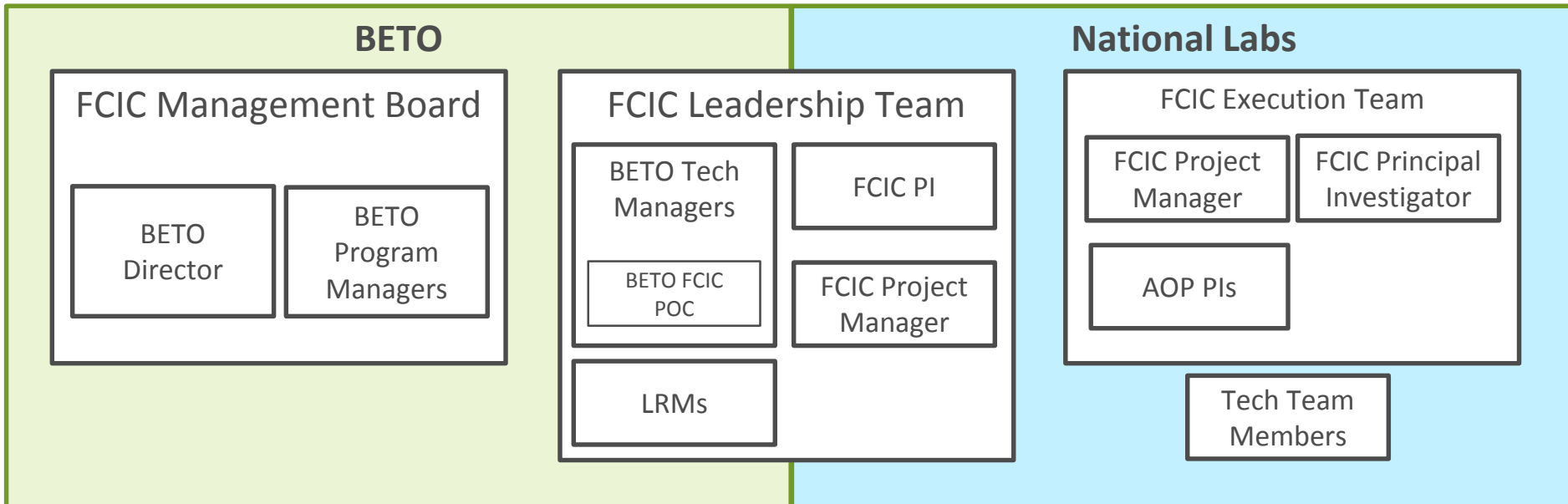
Tech Team Members

rd



# Approach – Management

## FCIC Leadership Structure



External Industry/Science Advisory Board

- External Industry/Science Advisory Board**
- Members
    - Biomass industry experience
    - Adjacent industry experience
    - Science background

