U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Catalyst Cost Model Development

WBS: 2.5.4.301/302

U.S. Department of Energy (DOE)
Bioenergy Technologies Office (BETO)
2017 Project Peer Review

Thermochemical Conversion

March 7th, 2017

Project Leads:

Frederick Baddour – NREL

Lesley Snowden-Swan – PNNL

ChemCatBio Structure

Core Catalysis Projects

Catalytic Upgrading of Biochemical Intermediates
(NREL, PNNL, ORNL, LANL)

Liquid Fuels via Upgrading of Indirect Liquefaction Intermediates
(NREL, PNNL)

Fast Pyrolysis and Upgrading
(PNNL, ORNL)

Catalytic Fast Pyrolysis
(NREL, PNNL)

Recovering and Upgrading Biogenic Carbon in Aqueous Waste Streams
(PNNL, NREL)

Zeolites and Metal Oxide Catalysts

Supported Metal Catalysts

Cross-cutting Discussion Groups

Enabling Projects

Advanced Catalyst Synthesis and Characterization
(NREL, ANL, ORNL)

Catalyst Cost Model Development
(NREL, PNNL)

Consortium for Computational Physics and Chemistry
(ORNL, NREL, PNNL, ANL, NETL)

Consortium Integration

- Core catalysis projects focused on specific *applications*
- *Collaborative* projects leveraging core capabilities across DOE laboratories
- *Cross-fertilization* through discussion groups

Goal Statement and Outcomes

Project Goal – Develop a **catalyst cost estimation tool** to enable rapid and informed cost-based decisions in research and commercialization of catalysts

Project Outputs and Outcomes

- ***An industrially validated*** and ***publicly-available*** catalyst cost estimation tool
- A ***first-of-its-kind*** tool for considering costs of ***novel and pre-commercial catalysts*** and paves the way for ***faster commercialization*** catalytic materials
- ***Catalyst R&D is accelerated*** by focusing efforts on cost and scaling challenges
- More informed decisions can be made on the basis of ***both cost and performance metrics***

Relevance to Biofuels

- **Nearly all biomass conversion processes rely on catalysis as do many biochemical processes**
  - Catalytic technology development is leveraged by a major portion of conversion pathways across BETO's portfolio
  - Design and optimization of novel catalysts to improve selectivity, efficiency, and durability to enhance yields spans multiple R&D areas
- **An absence of available tools**
  - ***The need for tools*** to guide catalyst development towards economical and commercially viable targets has been identified as a key research challenge

Quad Chart Overview

Timeline

- Project start date: 10/1/2015
- Project end date: 9/30/2018
- Percent complete: 42%

Budget

	FY15 Costs	FY16 Costs	Total Planned Funding (FY17-FY18)
DOE Funded	$0	$228	$250k*

*FY17 operating budget reduced to $125k

Barriers addressed & Actions

- **Ct-H** – Efficient Catalytic Upgrading of Sugars/Aromatics, Gaseous and Bio-Oil Intermediates to Fuels and Chemicals
  - ***Guiding R&D efforts towards developing cost-effective and scalable catalysts***

Partners

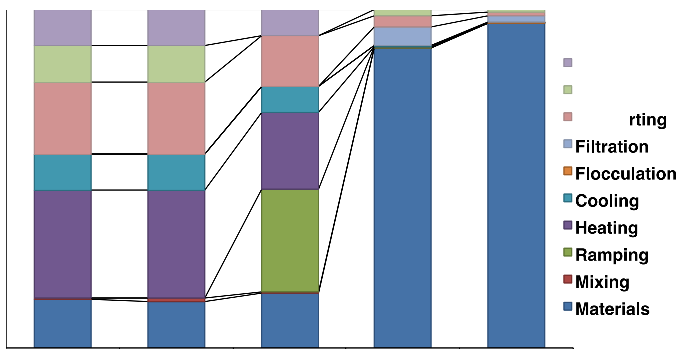
- **National Labs**
  – NREL (75%)
  – PNNL (25%)
- **Industry**
  – Forge Nano

Overview: The Catalyst Cost Model (CCM)

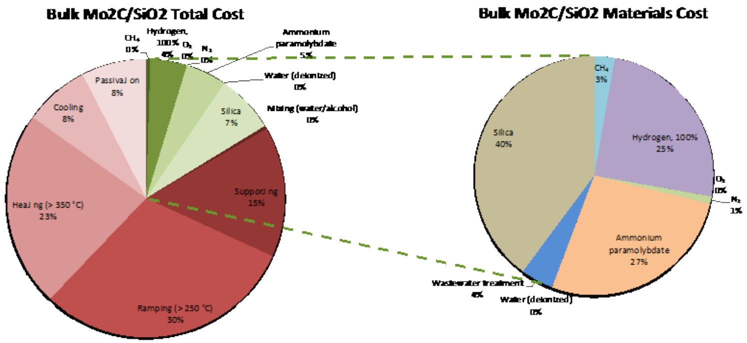
What information does the CCM provide to researchers?

- ***Estimated costs*** of manufacture for pre-commercial catalysts
- Identification of ***areas of greatest cost***
- ***Identification of roadblocks*** to scaling and suggested mitigation strategies
- ***A standard metric*** for comparing catalyst synthesis methods and materials

Comparison of Multiple Catalysts
(purchasing, deployment testing)



Component Cost Analysis
(directing R&D to areas of need)



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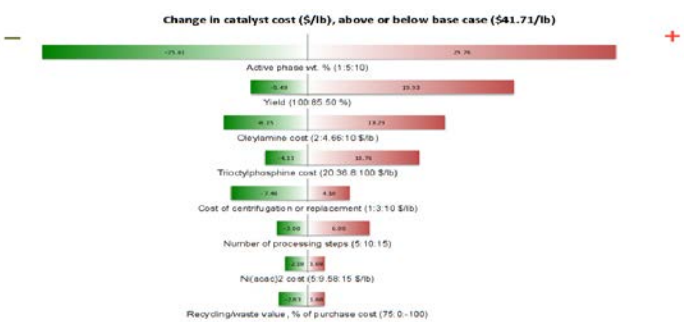
Overview: The Catalyst Cost Model (CCM)

What does this information enable researchers to *do*?

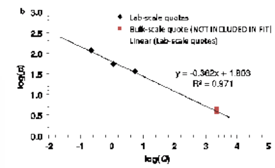
- ***Focus efforts*** on areas with greatest potential for cost reduction
- ***Make decisions*** based on performance and cost
- ***Guide catalyst development*** at early stages
- ***Improve the accuracy*** of TEA involving pre-commercial catalysts

Cost Sensitivity Analysis
(assessing commercialization potential and risks)



Cost Analysis Framework
(incorporation into TEA studies; LCA-compatible outputs, etc.)

$$m_{AP} = {m_{LR}}/{MW_{LR}} \times \left(\frac{mol_{AP}}{mol_{LR}}\right) \times MW_{AP} \times yield$$



$$(Per\text{-}Unit\ Labor\ Cost)_i = \frac{\left(\frac{Operator\ Hours}{Equipment\ Hours}\right)_i}{(Productivity)} \times (Local\ Labor\ Rate)$$

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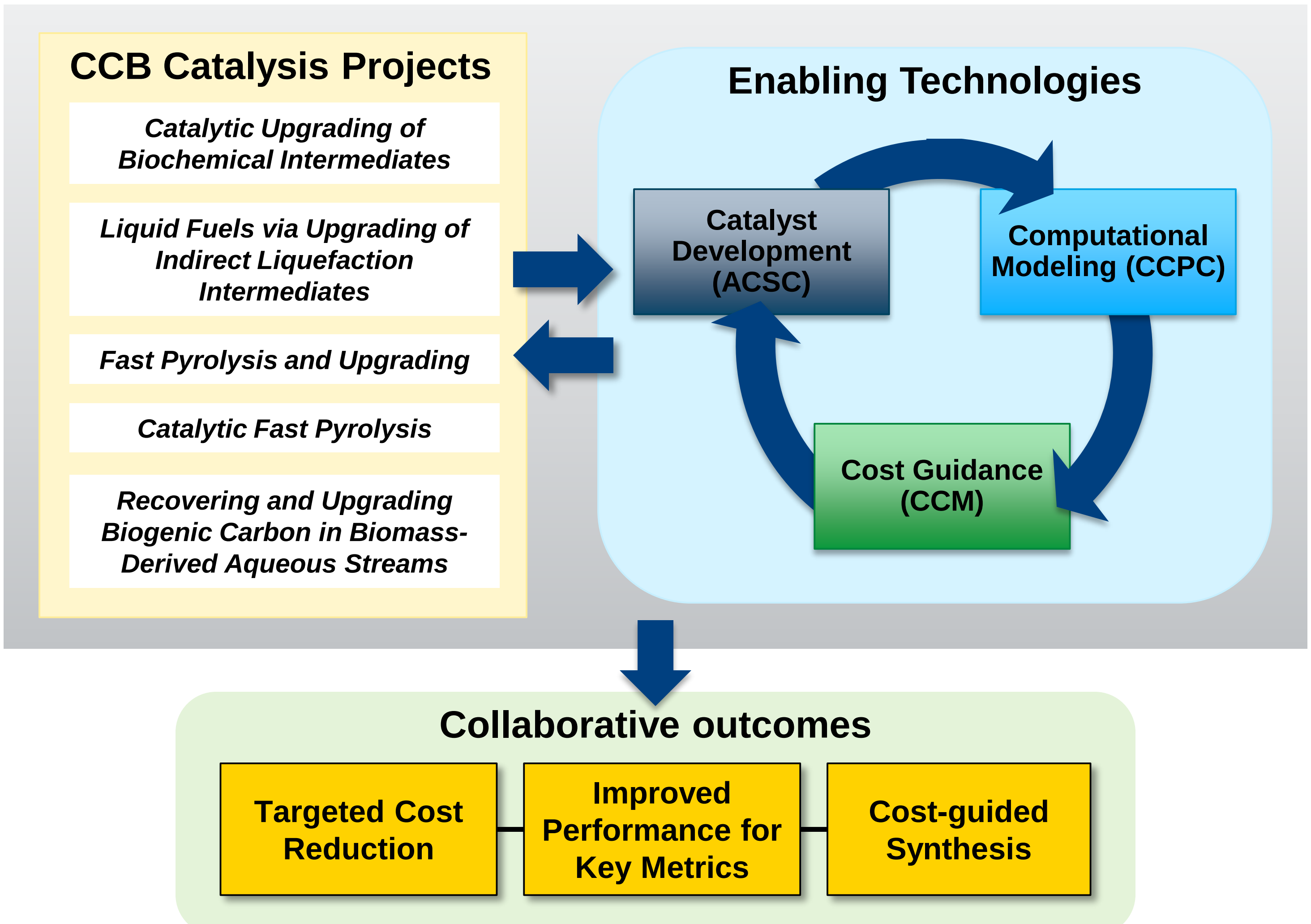
Project overview – Integrated approach

Establish an integrated and collaborative portfolio of catalytic and enabling technologies



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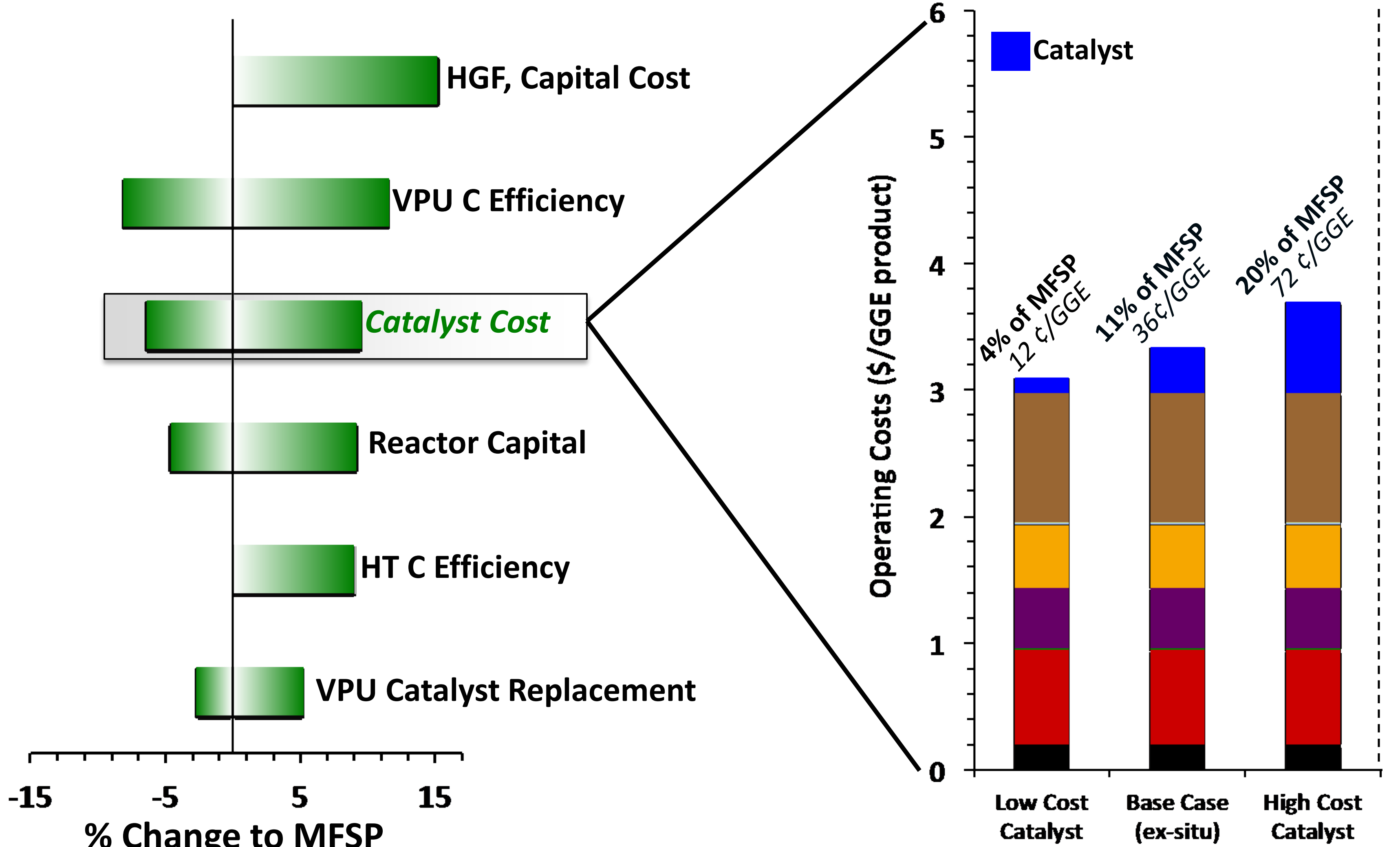
Overview: Impact of Uncertain Catalyst Cost

Objective**: To **reduce uncertainty** associated with pre-commercial catalyst cost in techno-economic analysis and **guide cost driven catalyst development



Management Approach

Closely integrated with industry to guide development of functional and relevant tool

NREL
Frederick Baddour

Primary tool development, interface design, methodology testing

PNNL
Lesley Snowden-Swan

Decision making logic development, recycling incorporation

Assessment of SOT / Data Gathering

Implementation of Best Practices

Industrial Expert Review

Refinement

Industrial Expert Review

Finalized Module

Industrial Expert Review

Biannual methodology review

Annual user-interface review

Data gaps

Immediate changes to design, assumptions, minor omissions

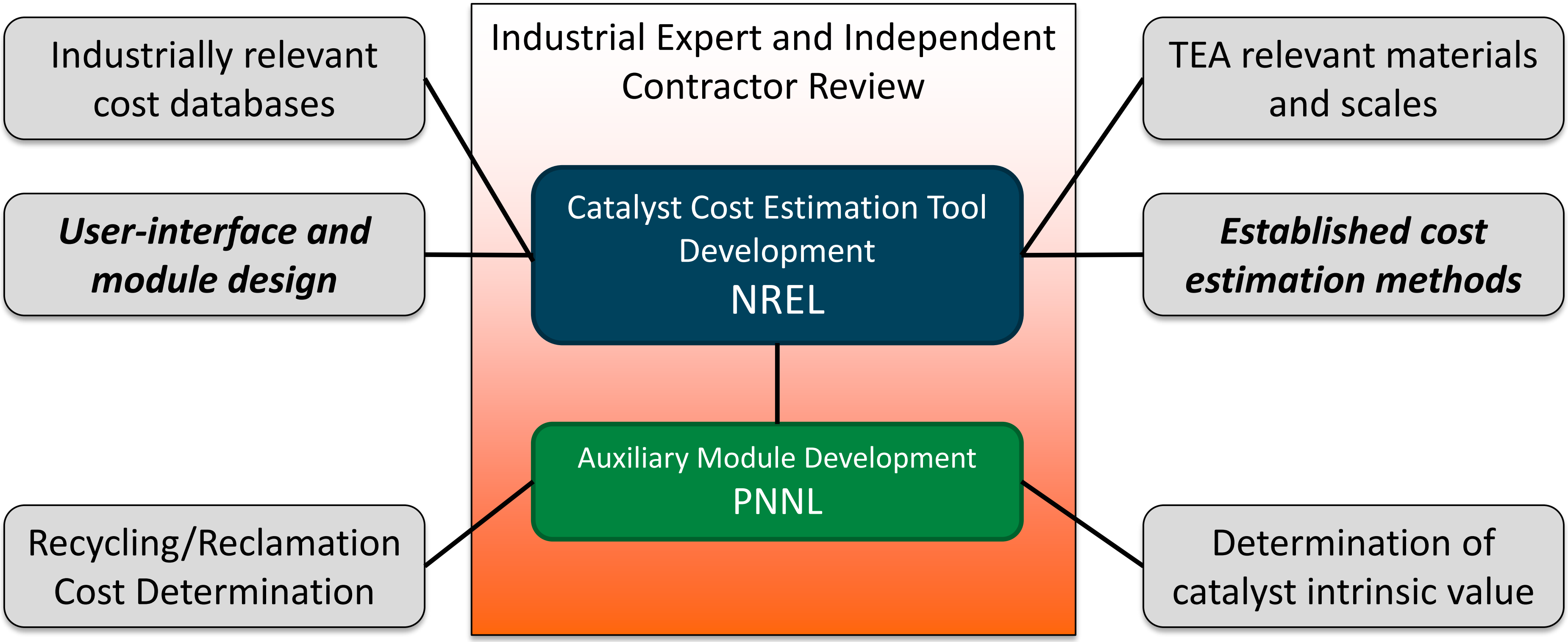
ID of Critical Components

Incorporation into AOP, go/no-go, planned milestone efforts

FY17 Go/No-go decision based on accuracy and implementation

FY18 Target: Tool Deployment

Technical Approach



Success Factors

- Production of an ***accurate*** and ***industrial validated*** tool with ***broad applicability***
- ***Flexibility*** to handle multiple catalyst scale-up technologies
- ***Informative visualization*** and comparative tools
- ***Public release*** and consumption
- ***Internal deployment*** throughout BETO's core catalysis projects
- ***Integration*** with well-established analysis tools (GREET)

Research Progress Roadmap

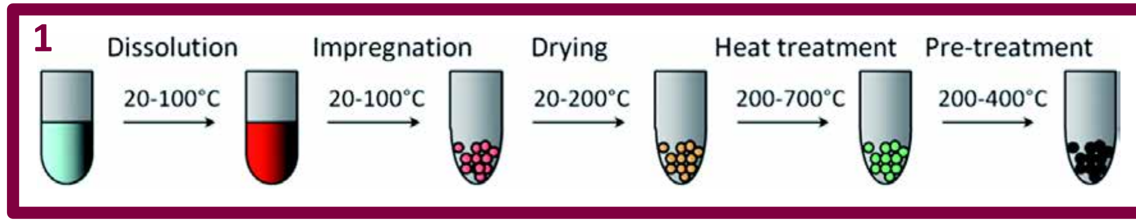
Method Development: Building the Catalyst Cost Estimation Tool

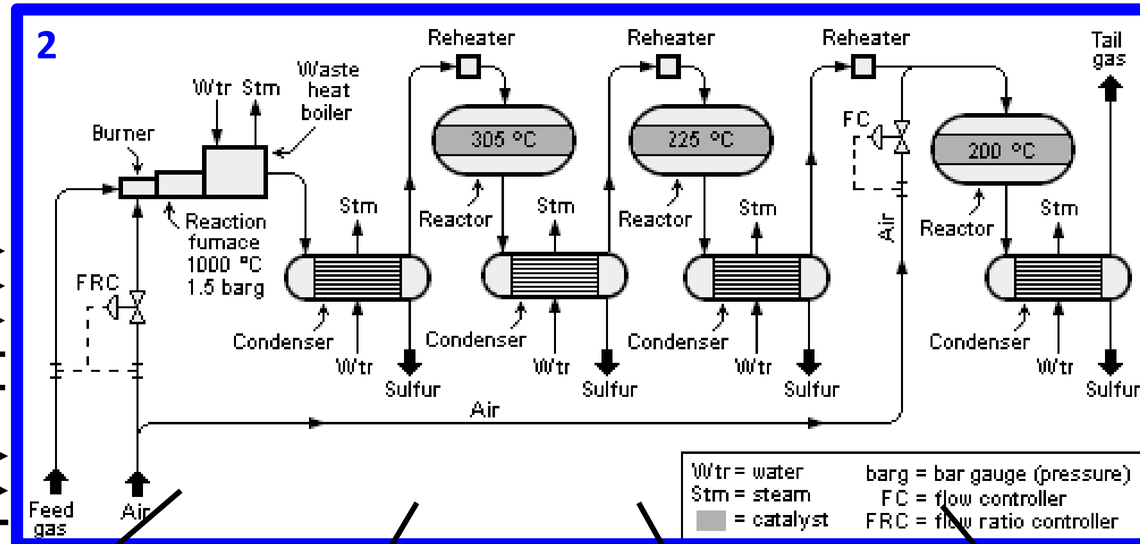
Implementation: Utilization of the Tool

Technical Approach: Determining Cost Contributors

Challenge – Identify and incorporate major cost drivers involved in translating from bench to industrial scales

1. Lab-scale process
2. Industrial process (PFD)
3. Design parameters
4. Cost components





3

Materials Flows (FY16)
Raw material supply
Byproducts
Waste/Salvage

4
Materials Costs

Utility Flows
Electricity
Steam
Cooling water
Wastewater

Utility Costs

Operating Labor
Direct
Supervisory
Lab/QA

Labor Costs

Maintenance
Supplies
Labor
Site Services

Maint. Costs

Equipment Capital
Installation
Piping
Instrumentation

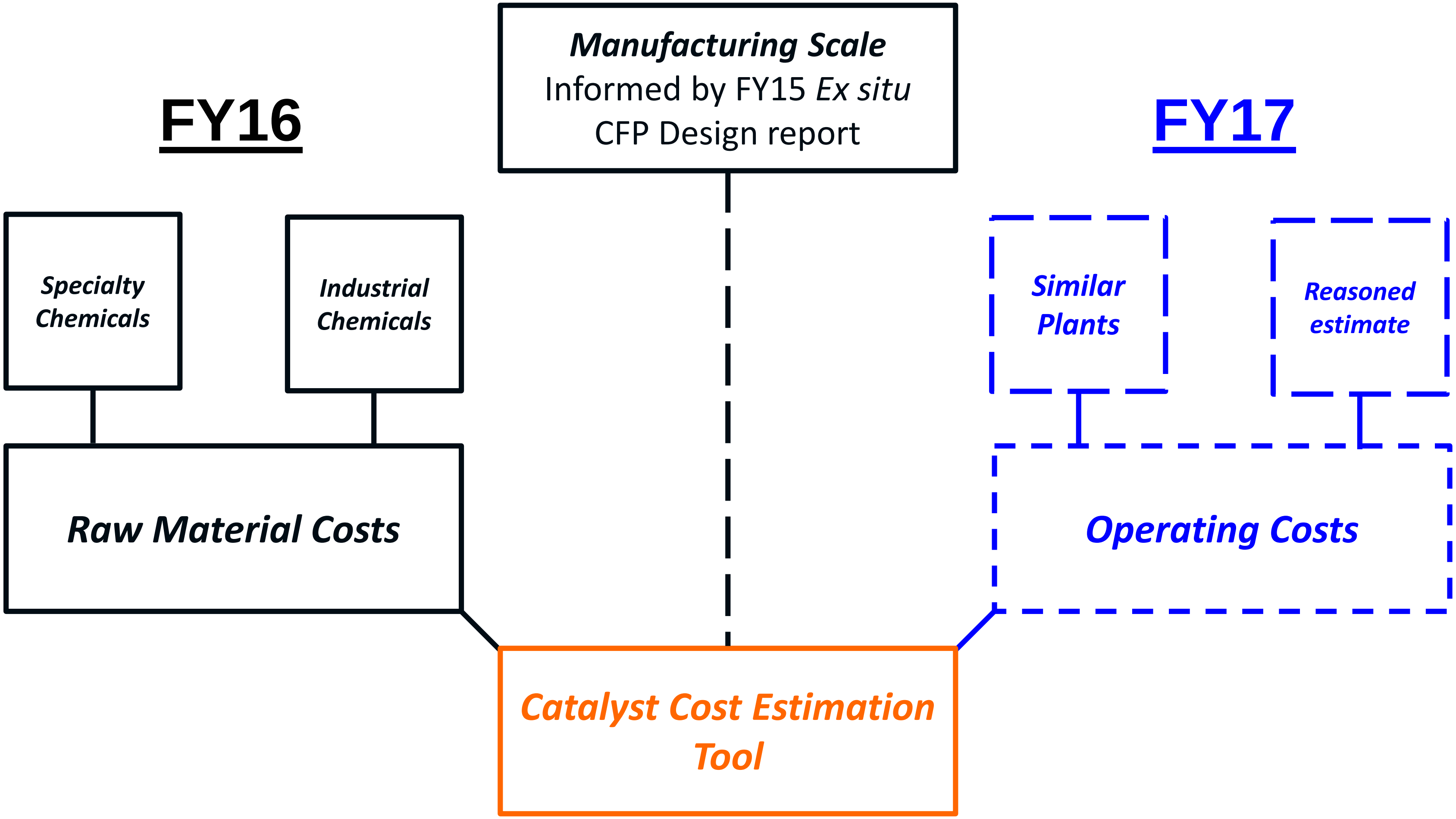
Equipment Costs

Production Site
Buildings
Land
Design & Constr.

Site Costs

Factored Costs
Contingencies
Working Capital
Administrative

Research Progress: Building a Framework



3 modes of raw material cost entry incorporated into the CCM tool: bulk quote, Integrated open-source database, lab-to-pilot extrapolation

Research Progress: Building a Framework

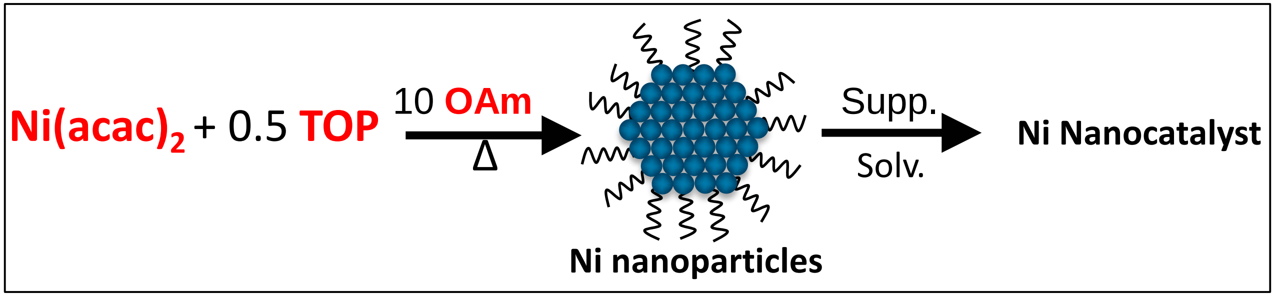
Manufacturing Scale
Informed by FY15 *Ex situ*
CFP Design report

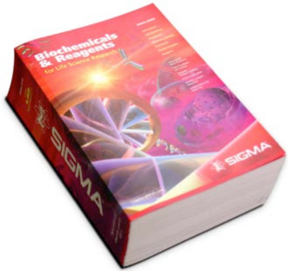
Ex situ CFP Biorefinery
Biomass Handling: 2000 dry tonnes/day
Catalyst Inventory: 77 tons
Replenishment Rate: 2% of inventory
Attrition Rate: 1.6% of inventory
Operating Uptime: 90%

Catalyst Consumption
2.78 tons/day
17.5 tons/week
911 tons/year
~ 1.8 million lbs/year

Research Progress: Laboratory to Plant Material Pricing

Challenge – Many chemicals required for synthesis of pre-commercial catalyst require raw materials that lack industrial market data



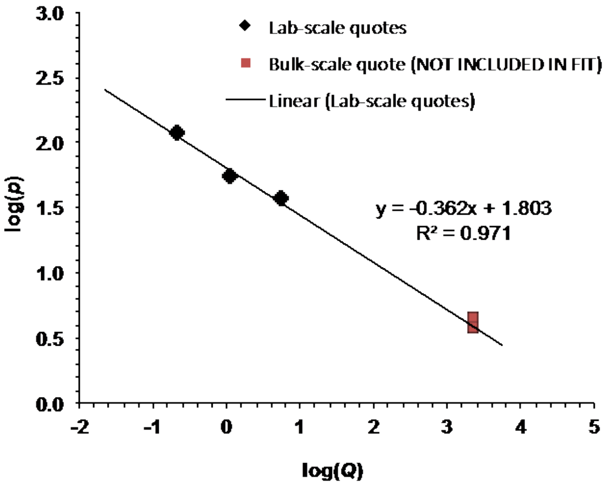


Quote Information (Inputs)		
Quantity, *Q*	Units	Total Price, *P* ($)
100	g	25.72
500	g	60.20
2.5	kg	200.09

c Nickel(II) Acetate Tetrahydrate Lab-Scale Log-Log Fit Details

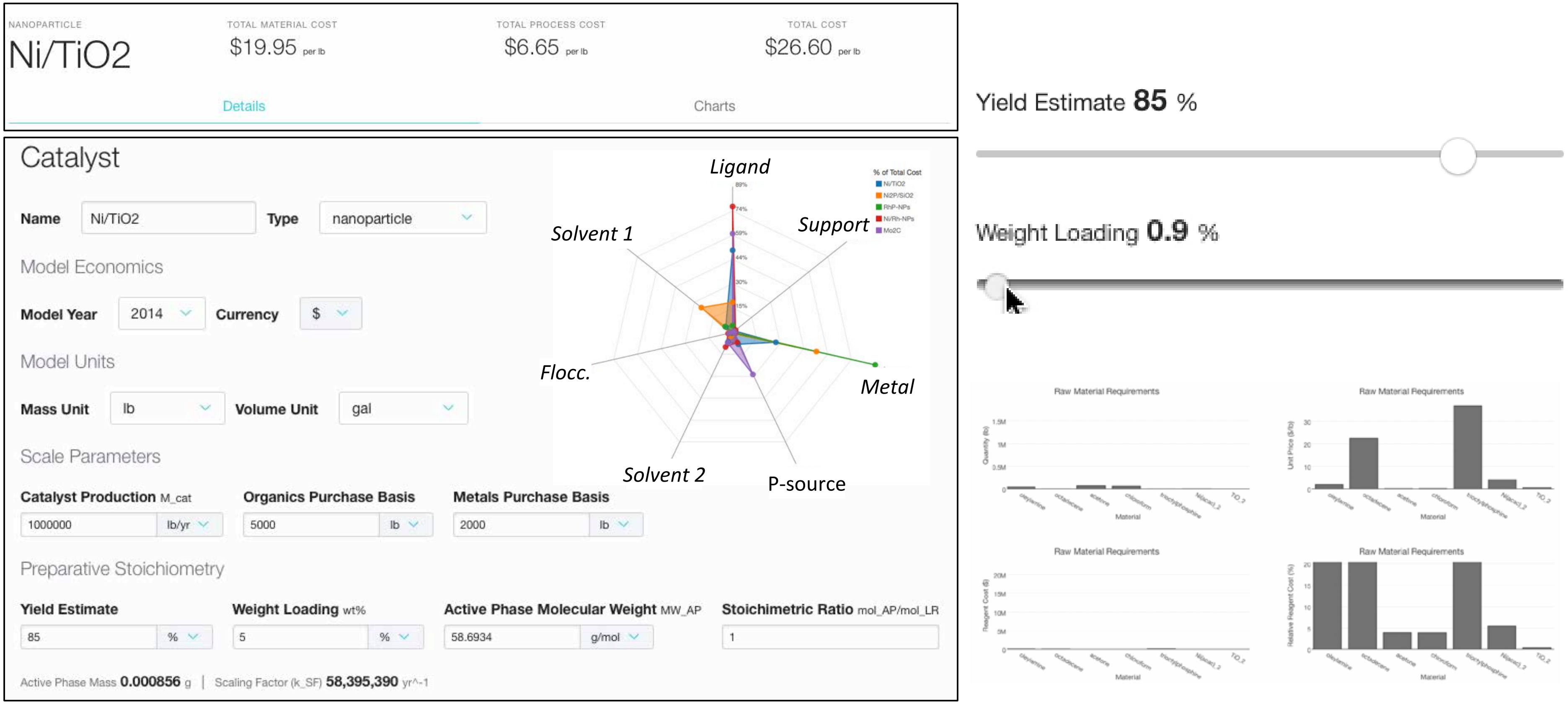
Quote Information (Inputs)			*Calculated Values*			
Quantity, *Q*	Units	Total Price, *P* ($)	Quantity, *Q*, in lb	Unit Price, *p*, ($/lb)	Log(*Q*)	Log(*p*)
100	g	25.72	0.22	116.66	-0.66	2.07
500	g	60.20	1.10	54.61	0.04	1.74
2.5	kg	200.09	5.51	36.30	0.74	1.56

Data Fit		*Calculated Bulk Pricing*		
Slope:	-0.363	*Bulk Quantity =*	2,000	lb
Intercept:	1.803	*Bulk Price =*	4.04	$/lb



- Determination of ***price as a function of scale***
- Provides reasonable estimation of ***unconventional materials***
- ***Expanded the scope*** of the CCM tool to include pre-commercial catalysts requiring specialty chemicals

Research Progress: UI Design



Our Web UI Offers:

- ***Seamless user experience*** with the same spread-sheet core functionality
- ***Powerful visualization*** tools for cost comparison between catalysts
- ***Real-time*** variable adjustment
- ***Up-to-date*** pricing information from public databases
- ***Exportable*** cost data

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Research Progress: A Complete Scaffold

$Ni(NO_3)_2 \cdot 6\,H_2O$ + $(NH_4)_2HPO_4$ —[HNO_3/H_2O; mix, support, dry]→ IW-Ni_2P/SiO_2 precursor —[heat, cool; passivate]→ IW-Ni_2P/SiO_2 catalyst

Processing Steps

Cost ($/lb)	Step
0.05	mix
2	support
1	dry
3	heat
1	cool
1	passiv.

Catalyst	Material	Function	density	MW of precursor	amount	unit
IW-Ni_2P/SiO_2	water	solvent	1		35	mL
	ammonium phosphate dibasic	P-source			0.89	g
	Conc. Nitric Acid	additive	1.51		1	mL
	$Ni(NO_3)_2$ - 6 H_2O	metal source		290.79	1.96	g
	Sipernat-22	support			9.50	g
	Final Catalyst				**10.00**	**g**

Scaled by basis for purchase

Materials	Quantity (Lb)
water	135830
ammonium phosphate dibasic	3454
Conc. Nitric Acid	5860
$Ni(NO_3)_2$ - 6 H_2O	7606
Sipernat-22	36868

Price ($/Lb material)	Price ($)	Source
0.005	677	IHS PEP
0.462	1597	IHS PEP
0.089	522	IHS PEP
1.984	15089	Alfa
0.874	32227	IHS CEH

Σ costs

Comprehensive approach to estimating novel catalyst costs

$10/lb IW-$Ni_2P/SiO_2$

Research Progress Roadmap

Method Development: Building the Catalyst Cost Estimation Tool

Implementation: Utilization of the Tool

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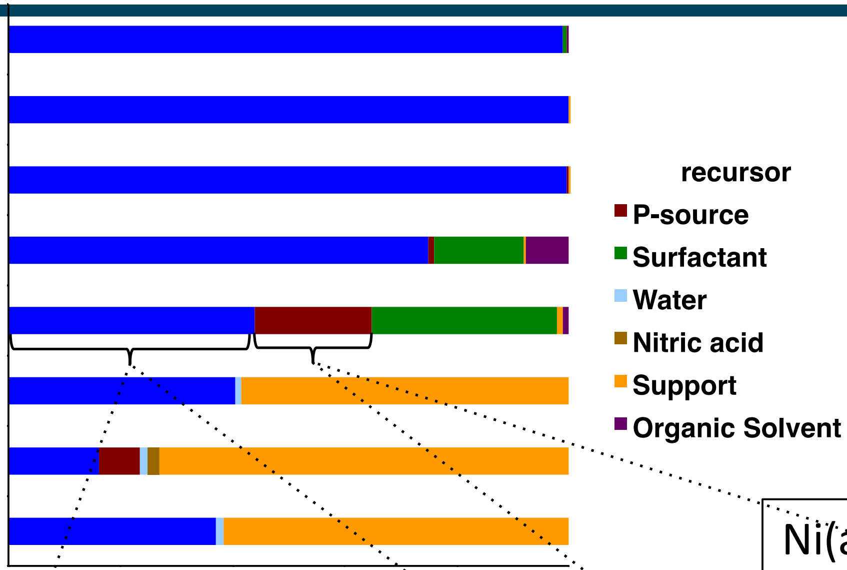
Research Progress: *Ex-situ* CFP Case Study

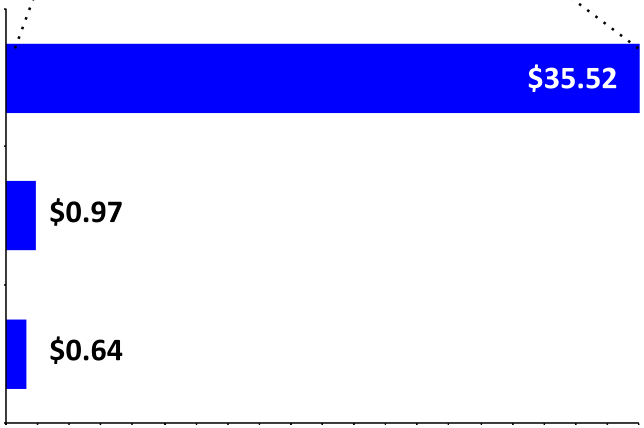


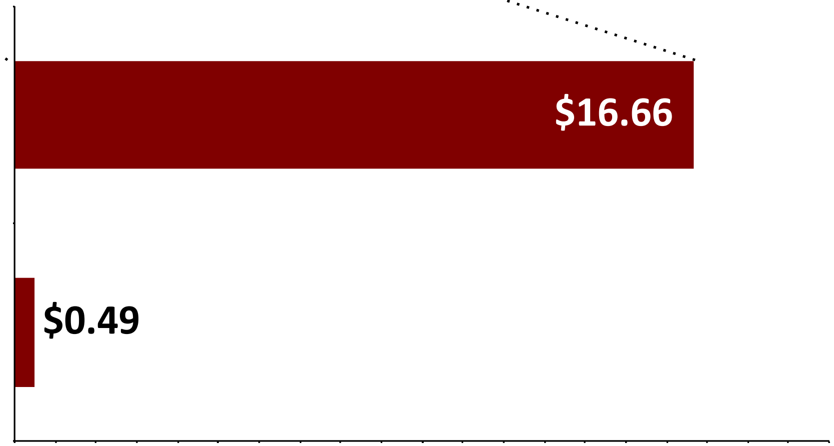
The CCM tool successfully assessed the areas of greatest cost for CFP catalysts

Ni(acac)$_2$ → Ni(OAc)$_2$: ***38% mat. cost red.***

TOP → PPh$_3$: ***18% mat. cost red.***

Materials Cost Allocation





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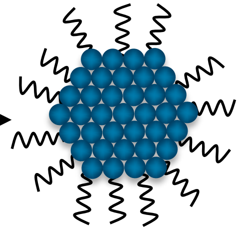
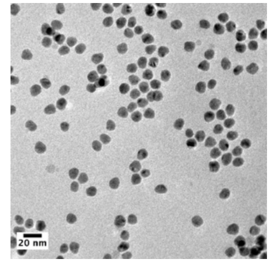
Relevance: Cost-effective Synthesis with the ACSC

Utilizing the CCM to directing synthesis towards lower cost targets

$Ni(acac)_2$ + 0.5 TOP $\xrightarrow[\Delta]{10\ OAm}$

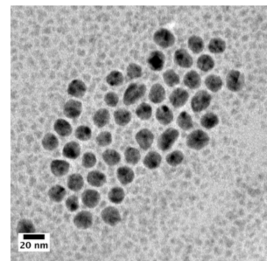


Ni nanoparticles



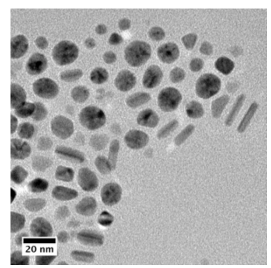
Base Case
11.1 ± 1.0 nm
85% Yield
$95/lb catalyst

$Ni(OAc)_2(OH_2)_4$ + 0.5 TOP $\xrightarrow[\Delta]{10\ OAm}$



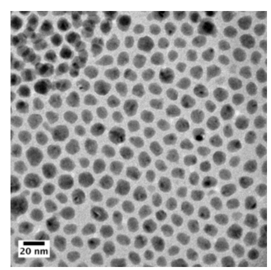
19 nm
75% Yield
$65/lb catalyst

$Ni(OAc)_2(OH_2)_4$ + 1 PPh_3 $\xrightarrow[\Delta]{10\ OAm}$



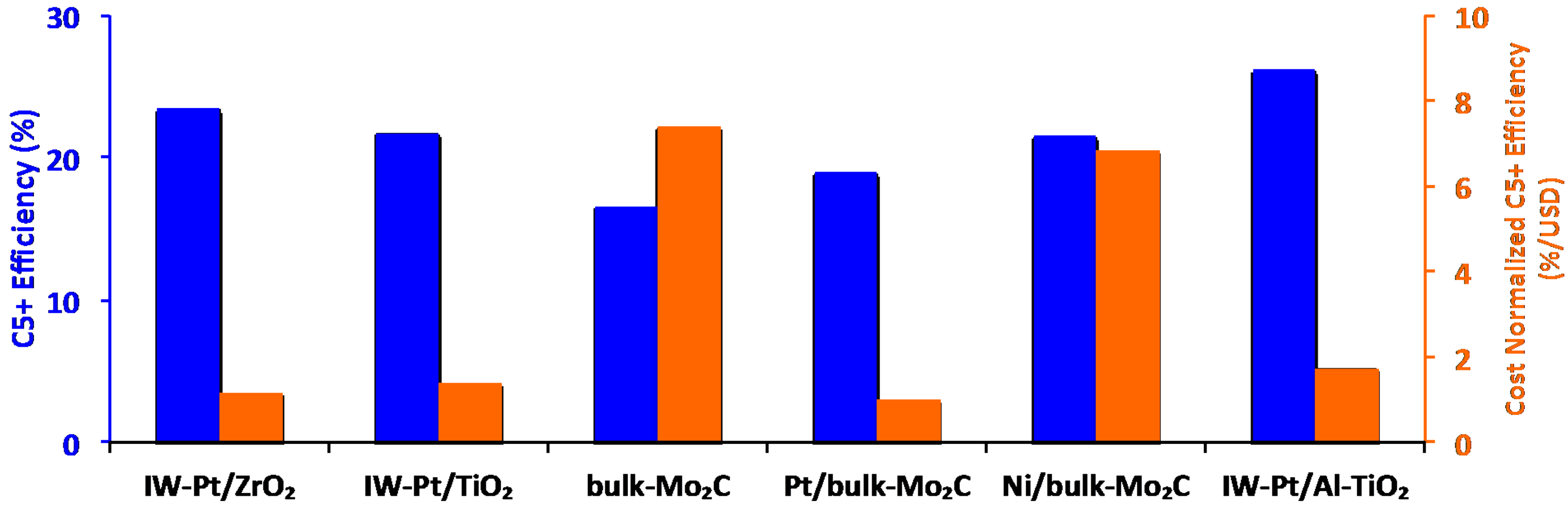
22 nm
50% Yield
$64/lb catalyst

$Ni(OAc)_2(OH_2)_4$ + 4 PPh_3 $\xrightarrow[\Delta]{10\ OAm}$



12.0 nm ± 1.8
85% Yield
$46/lb catalyst

Relevance: Assessing the Value Proposition



- Analysis with the CCM tool enables an early assessment of the ***value proposition of a catalyst***
- Catalyst performance metrics (e.g. lifetime, yields, regenerability) can be ***normalized by cost***

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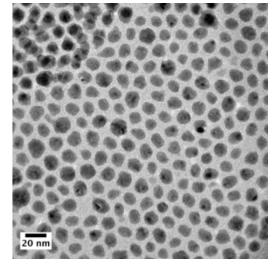
Relevance

Pre-commercial catalyst development and usage is heavily-leveraged within BETOs conversion portfolio

The CCM tool enables a detailed assessment of the ***value proposition*** of advanced catalysts early in development

Catalyst cost contributes significantly to biofuels commercialization risk

Sensitivity analyses show catalyst cost as one of the top factors driving uncertainty in MFSP

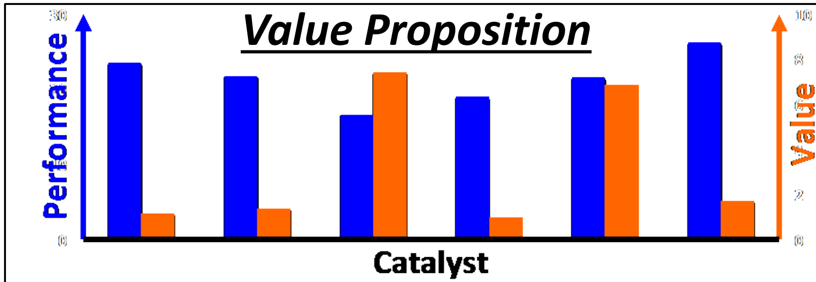


Targeted Synthesis

Identical Catalyst

Identical Yield

52% Cost Reduction



CCM-generated cost metrics offer guidance for catalyst development

The CCM can be used to ***guide materials development*** much like TEA guides research through performance targets

External R&D groups have demonstrated interest in the CCM tool and its capabilities

University professors, national laboratory staff, and companies have expressed interest in collaborating on both tool development and testing

FORGE NANO

Established new collaboration with a small manufacturing business

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Future Work: Recycling and Decision Making

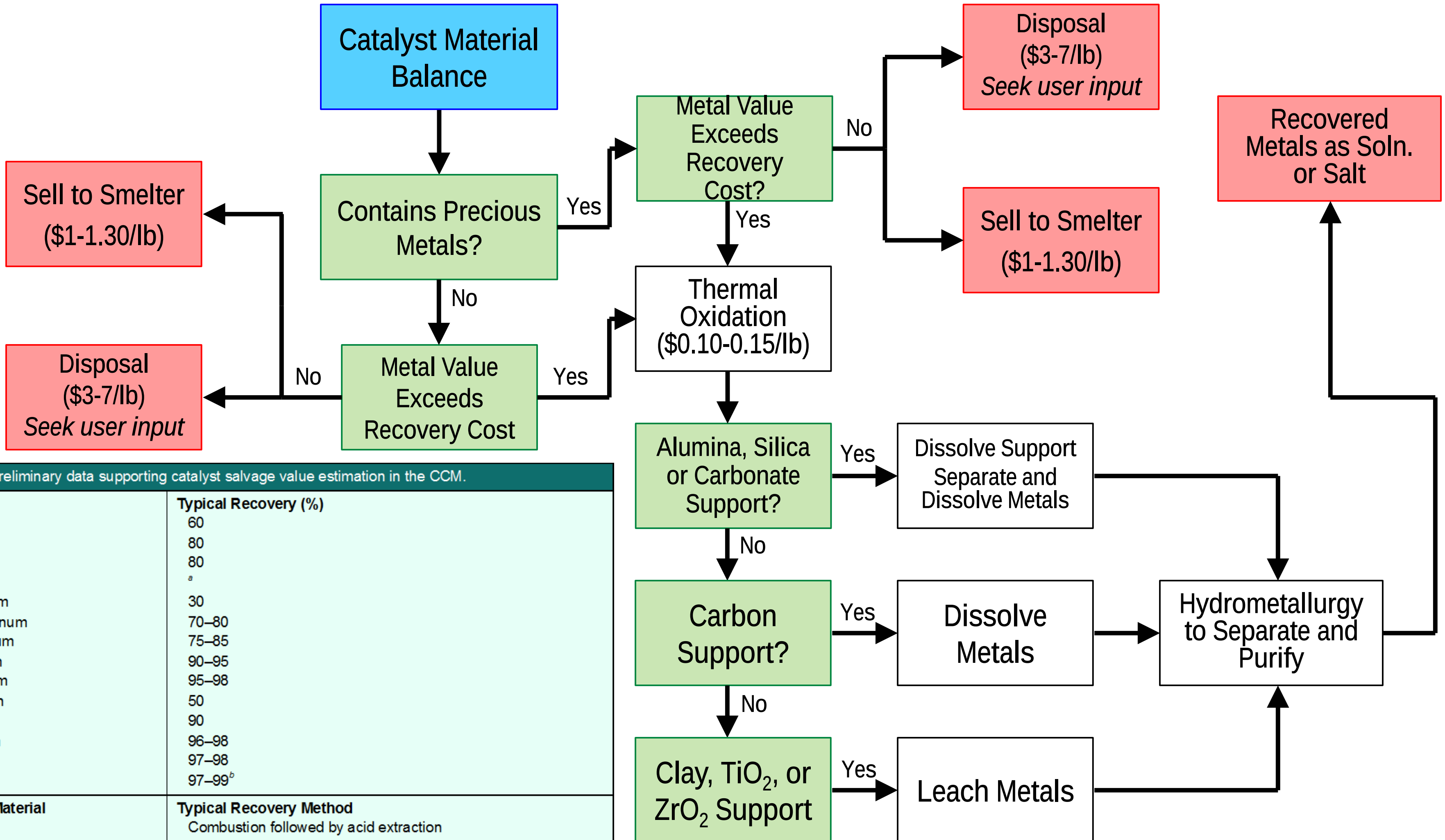
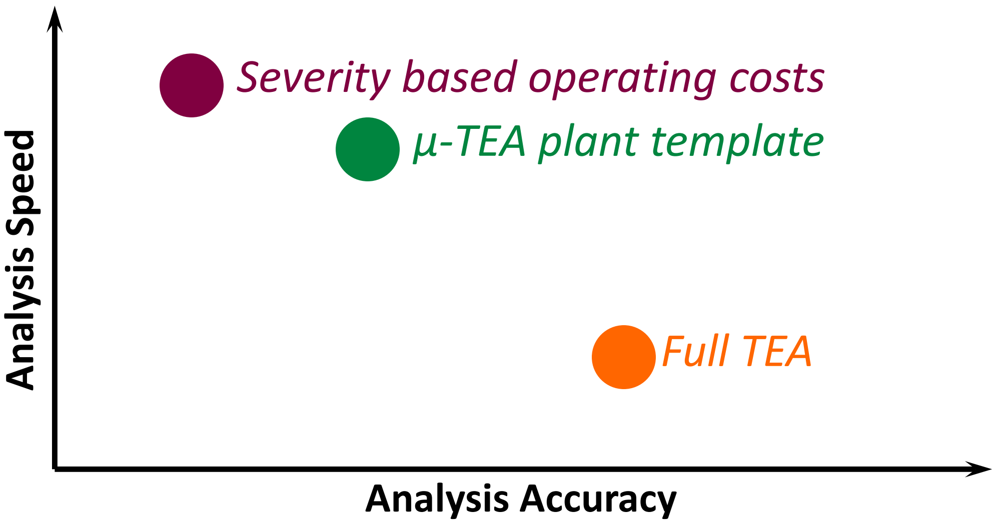


Table 1. Preliminary data supporting catalyst salvage value estimation in the CCM.

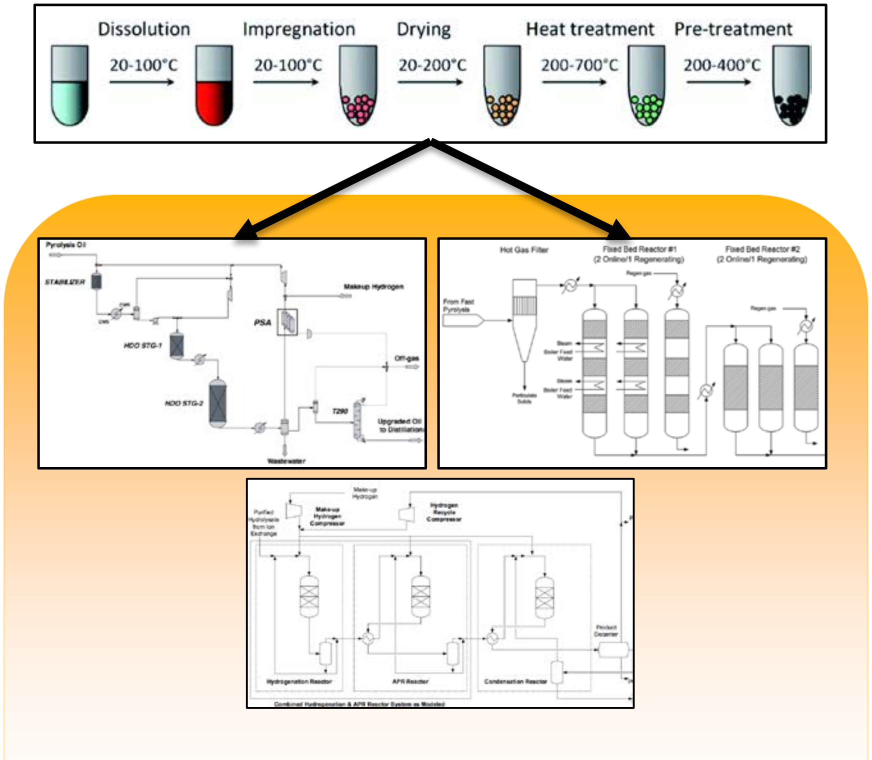
Metal	Typical Recovery (%)
Iron	60
Cobalt	80
Nickel	80
Copper	[a]
Aluminum	30
Molybdenum	70–80
Ruthenium	75–85
Rhodium	90–95
Palladium	95–98
Tungsten	50
Iridium	90
Platinum	96–98
Silver	97–98
Gold	97–99[b]
Support Material	**Typical Recovery Method**
Carbon	Combustion followed by acid extraction
Silica	De-coking and dissolution of silica
Titania	De-coking and extraction of metals
Alumina	De-coking and dissolution of alumina
No support (e.g. zeolite catalyst)	Dissolution of framework, extractions

Paraphrased comments from CCM reviewers: [a]Copper is difficult to separate from precious metals during recovery. [b]Few smelters will accept Au-containing catalysts, and none will accept Ru, Re, or Os-containing catalysts. Catalysts containing these elements in their active phase would require hydrometallurgical processing, after decoking, to recover the metals.

Future Work: A Tiered-complexity Approach to Operating Costs



Laboratory Procedure



Parameterized scale-up templates

Rapid and accurate processing cost estimation

Tiered Complexity of Operating Costs

- ***Severity based***
  - Order-of-magnitude estimate
- ***Templated full-plant analysis***
  - ***TEA templates*** to include traditional means of catalyst production
  - Informed by TEA from industrial databases
  - ***Rapid analysis*** of processing costs
  - All fields ***user-adjustable***

Future Work: Linking Cost and Environmental Impact

The CCM Tool generates data that can be incorporated into existing LCA tools (GREET)

CCM Tool Inputs

- Catalyst composition
- Raw material usage
- Energy consumption to produce catalyst
- Water consumption
- Solvent consumption

Greenhouse gases
Regulated
Emissions
Energy use in
Transportation

Argonne NATIONAL LABORATORY

GREET Outputs

- Cradle-to-gate impacts of catalyst production
- GHG emissions (kg CO_2e/kg catalyst)
- Air pollutant emissions (kg/kg catalyst)
- Water consumption (L/kg catalyst)
- Fossil fuel energy consumption (MJ/kg catalyst)

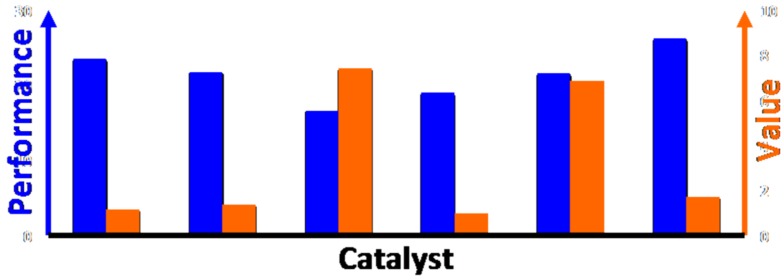
Combined CCM/GREET Analysis enables:

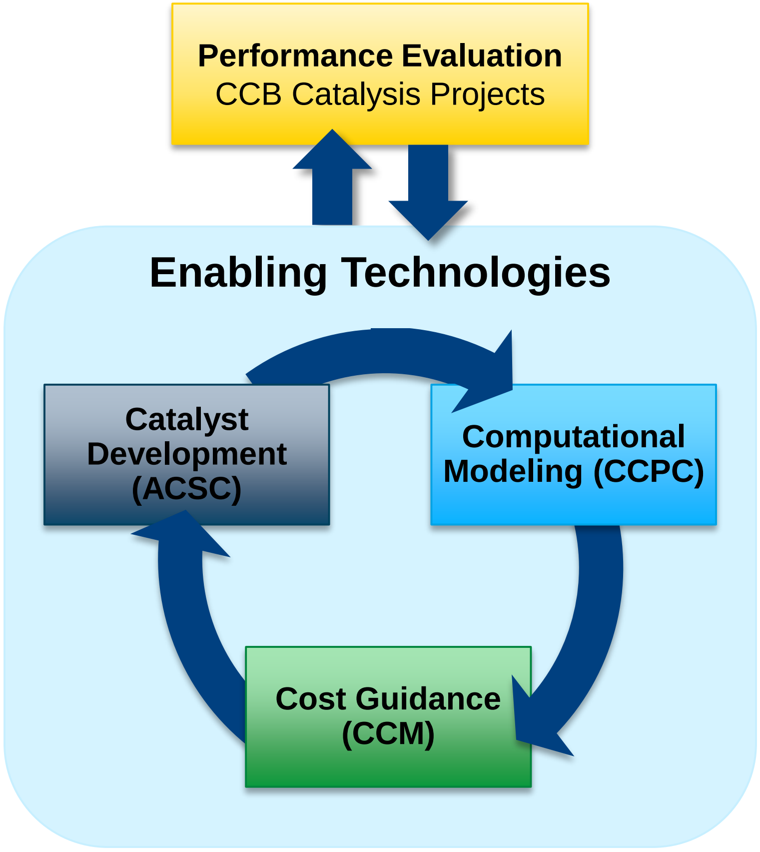
– Determination of the ***relationship between cost and environmental impact*** for catalyst manufacture

– Identification of the major ***environmental and cost drivers*** of catalyst production and mitigation measures

Summary

- A catalyst cost estimation tool has been developed ***versatile materials pricing***, initial ***processing cost estimation*** methods, and ***salvage value*** of recycling.
- The CCM project enables an ***assessment the value proposition*** of pre-commercial catalysts developed within BETO's conversion portfolio
- ***Rigorous industrial expert review*** of the CCM tool has been conducted throughout development to ensure the relevance and veracity of the tool
- Future efforts aim to increase detail of existing modules, ***interface with LCA frameworks***, and expand user-operability





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Model Design

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Recycling, Reclamation & Lifecycle Analysis

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John Frye
Eric Tan
Jennifer Dunn
Thathiana Pahola

NREL NATIONAL RENEWABLE ENERGY LABORATORY

Pacific Northwest NATIONAL LABORATORY

Argonne NATIONAL LABORATORY

ChemCatBio Chemical Catalysis for Bioenergy

Energy Materials Network U.S. Department of Energy

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Questions

Additional Slides

Publications and Presentations

- Presentations
  - <u>Frederick Baddour</u>, Kurt Van Allsburg, Joshua Schaidle, “From Lab to Market: Designing a Cost Estimation Tool for Catalyst Scaling” *Frontiers in Biorefining*, **November 2016**, St. Simons Island, GA.
  - <u>Kurt Van Allsburg</u>, Joshua Schaidle, Frederick Baddour, “Development of a Catalyst Cost Estimation Tool to Reduce Information Barriers to Commercialization” *Invited talk at UC Berkeley*, **December 2016** Berkeley, CA.
- Publications
  - A. Dutta, J. A. Schaidle, D. Humbird, F. G. Baddour, A. Sahir; “Conceptual Process Design and Techno-Economic Assessment of Ex Situ Catalytic Fast Pyrolysis of Biomass: A Fixed Bed Reactor Implementation Scenario for Future Feasibility” *Top. Catal.* **2015**, 59, 1, 2-18.
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Acronyms and abbreviations

ACSC	Advanced Synthesis and Characterization project
ANL	Argonne National Laboratory
AOP	Annual operating plan
BETO	Bioenergy Technologies Office
CCB	Chemical Catalysis for Bioenergy Consortium; ChemCatBio consortium
CCM	Catalyst Cost Model Development project
CCPC	Consortium for Computational Physics and Chemistry
CFP	Catalytic fast pyrolysis
DOE	U.S. Department of Energy
EMN	Energy Materials Network
FY	Fiscal year
GGE	Gallon gasoline equivalent
HGF	Hot gas filter
HT	Hydrotreating
LANL	Los Alamos National Laboratory
LCA	Life-cycle analysis

Acronyms and abbreviations (cont.)

MFSP	Minimum fuel selling price
MYPP	Multi-Year Program Plan
NETL	National Energy Technology Laboratory
NREL	National Renewable Energy Laboratory
$Ni(acac)_2$	Nickel acetylacetonate
$Ni(OAc)_2$	Nickel acetate hydrate
OAm	Oleylamine
ORNL	Oak Ridge National Laboratory
PFD	Process flow diagram
PNNL	Pacific Northwest National Laboratory
PPh_3	Triphenylphosphine
SOT	State of technology
TEA	Techno-economic analysis
TOP	Trioctylphosphine
VPU	Vapor phase upgrading
wt%	Percentage by weight