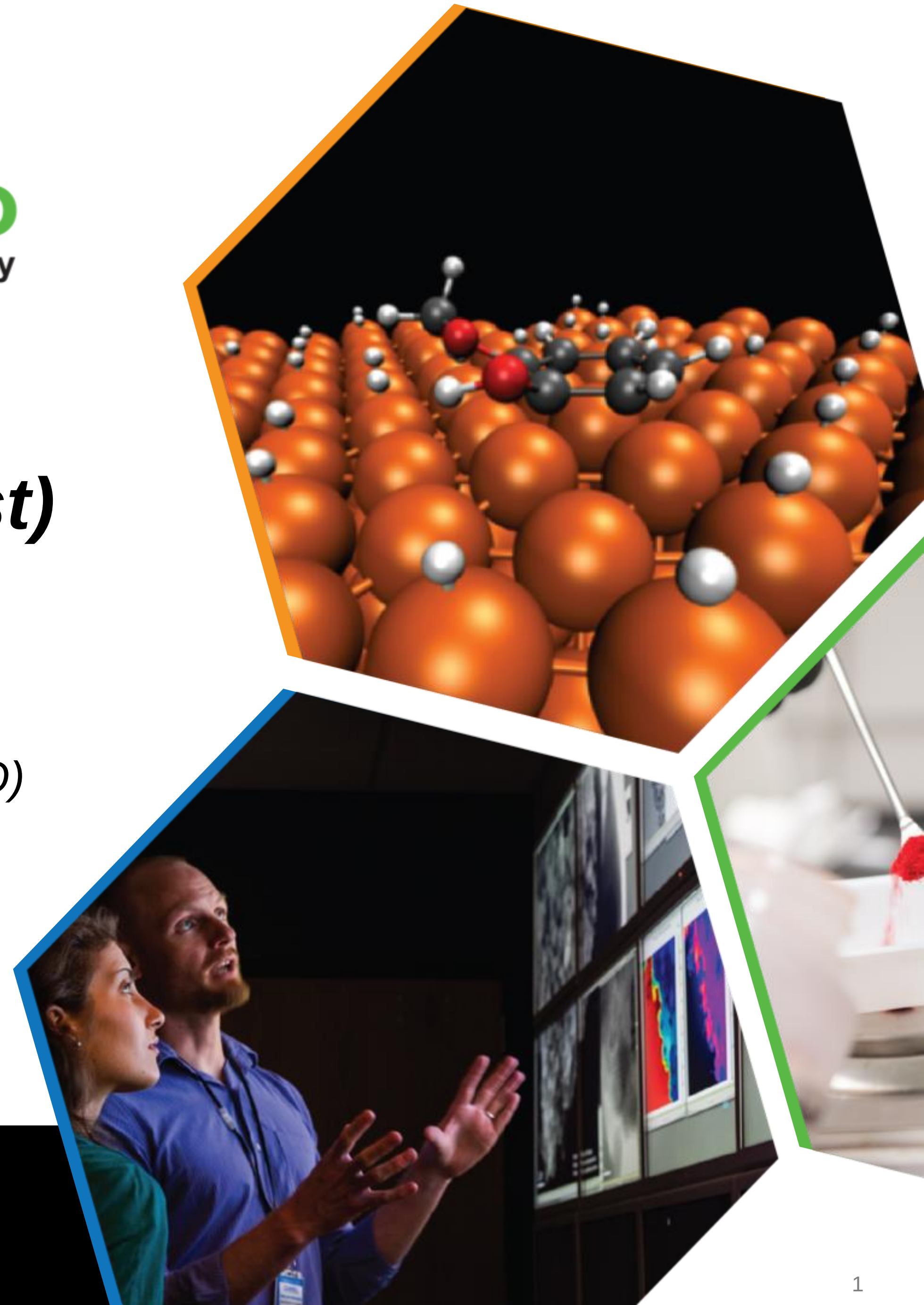
ChemCatBio
Chemical Catalysis for Bioenergy

Catalyst Cost Model Development (CatCost)

WBS # 2.5.4.301/302

U.S. Department of Energy (DOE)
Bioenergy Technologies Office (BETO)
2019 Project Peer Review

Frederick Baddour – NREL
Lesley Snowden-Swan – PNNL



Quad Chart Overview

Timeline

- Project Start: October 1, 2015
- Project End: September 30, 2018
- Percent Complete: 100%

	Total Costs Pre FY17	FY17 Costs	FY18 Costs	Total Planned Funding (FY19)
DOE Funded	$225k	$125k	$300k	$20k
Project Cost Share	N/A	N/A	N/A	N/A

Partners (FY16–FY18):

NREL: $650k (65%)
PNNL: $225k (35%)

Barriers addressed

At-E. *Quantifying economics of bioenergy to reduce risk and clarify value proposition*
Ct-G. *Decreasing the Time and cost to developing novel industrially relevant catalysts*

Objective

The objective of this project is to develop a modular and flexible tool for accurately estimating the cost of pre-commercial catalyst manufacture to be distributed to the public free-of-charge as a web-based interface together with a downloadable spreadsheet-based model. This publicly-available model and the methodologies employed will be published online and a corresponding peer-reviewed article will be published demonstrating the ability of the tool to accurately estimate the costs of existing commercial catalysts to within 20%. This excel- and web-based tool will be the first of its kind to enable rapid assessment of the economics and environmental impacts of pre-commercial catalysts at industrially relevant scales.

End of Project Goal

Develop an online and free-of-charge ***catalyst cost estimation tool*** to enable rapid and informed cost-based decisions in research and commercialization of catalysts

ChemCatBio Foundation

Integrated and collaborative portfolio of catalytic technologies and enabling capabilities

Catalytic Technologies	*Enabling Capabilities*	*Industry Partnerships (Directed Funding)*
Catalytic Upgrading of Biochemical Intermediates (NREL, PNNL, ORNL, LANL, NREL*)	**Advanced Catalyst Synthesis and Characterization** (NREL, ANL, ORNL, SNL)	**Gevo** (NREL) **ALD Nano/JM** (NREL) **Vertimass** (ORNL)
Catalytic Upgrading of Indirect Liquefaction Intermediates (NREL, PNNL, ORNL)	**Catalyst Cost Model Development** (NREL, PNNL)	**Opus12**(NREL) **Visolis** (PNNL)
Catalytic Fast Pyrolysis (NREL, PNNL)	**Consortium for Computational Physics and Chemistry** (ORNL, NREL, PNNL, ANL, NETL)	**Lanzatech** (PNNL) - Fuel **Gevo** (LANL)
Electrocatalytic and Thermocatalytic CO_2 Utilization (NREL, ORNL*)	**Catalyst Deactivation Mitigation for Biomass Conversion** (PNNL)	**Lanzatech** (PNNL) - TPA **Sironix** (LANL)

*FY19 Seed Project

Cross-Cutting Support

ChemCatBio Lead Team Support (NREL)

ChemCatBio DataHUB (NREL)

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

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- ***Cat*** … nges
- Mor … ***rmance*** ***me***

CatCost is available free-of-charge at
https://catcost.chemcatbio.org

Releva…

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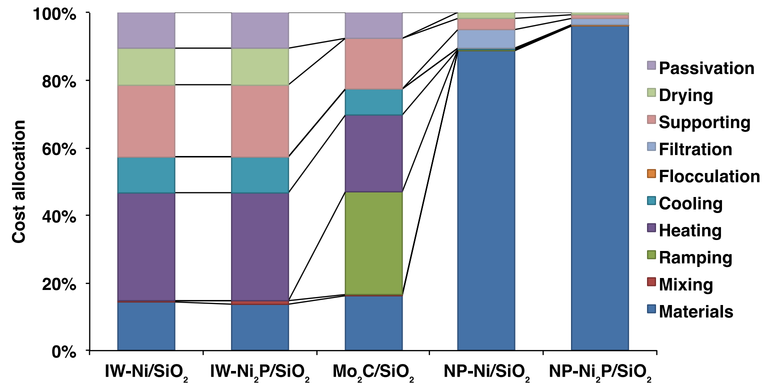
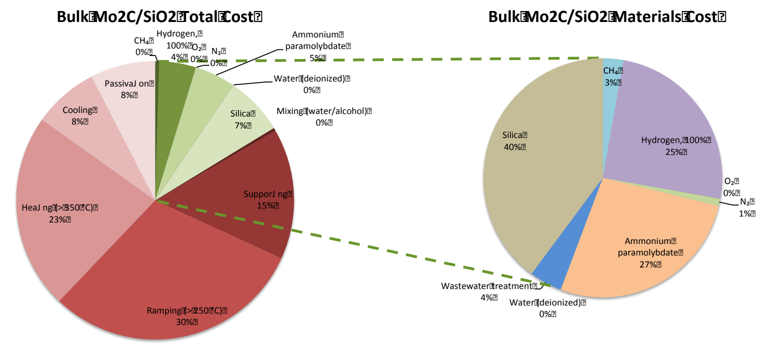
What information does *CatCost* provide to researchers?

- ***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)



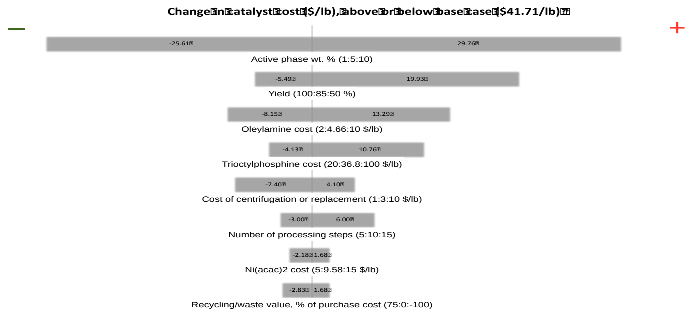
1 – Overview of CatCost

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 <u>pre-commercial catalysts</u>

Cost Sensitivity Analysis

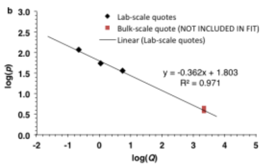
(assessing commercialization potential and risks)



Cost Analysis Framework

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

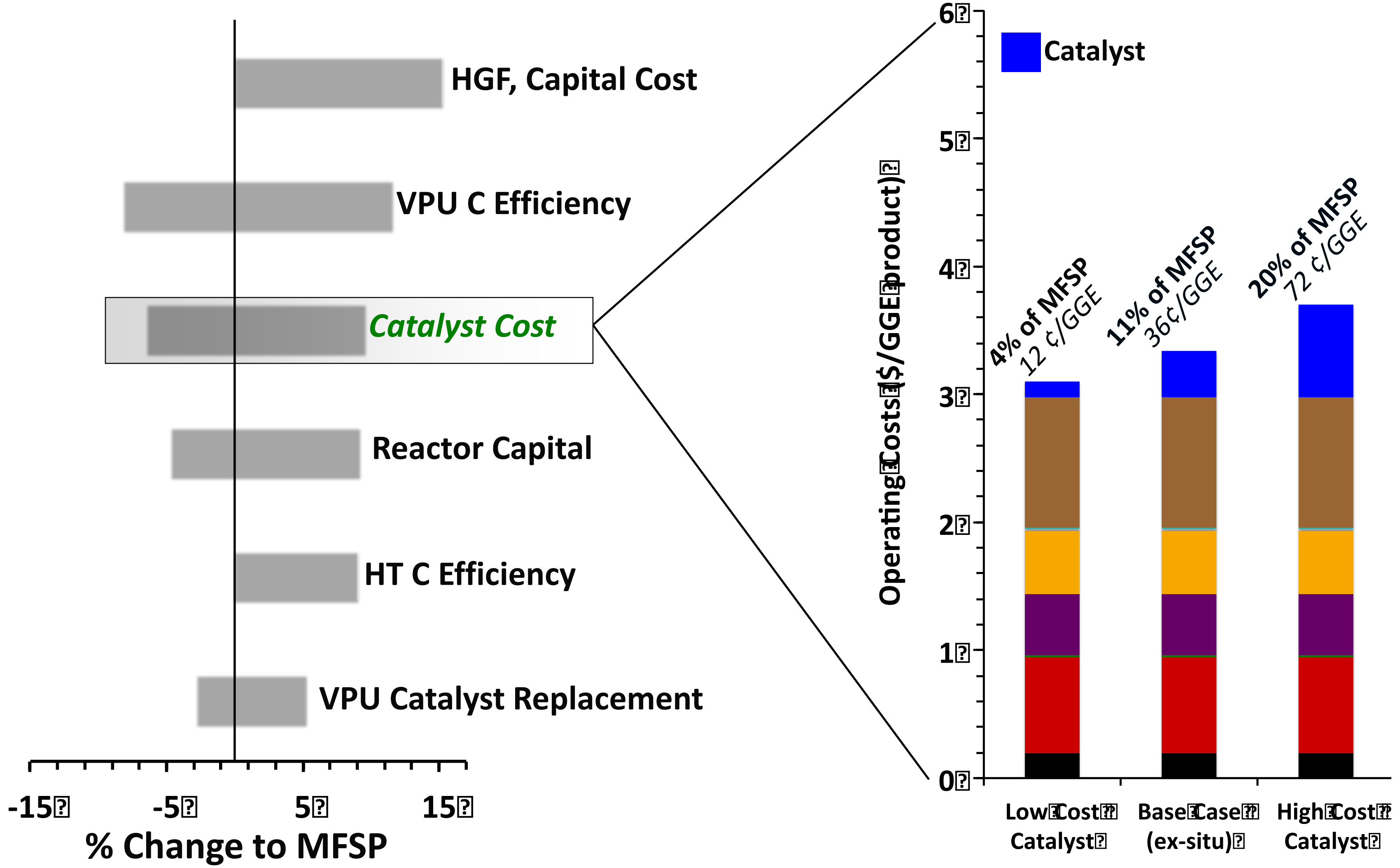
$$m_{AP} = {m_{LR}}/{MW_{LR}} \times \left(\frac{mol_{AP}}{mol_{LR}}\right) \times MW_{AP} \times yield$$



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

1 – The Uncertainty of Catalyst Cost

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



Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels Thermochemical Research Pathways with *In Situ* and *Ex Situ* Upgrading of Fast Pyrolysis Vapors
Abhijit Dutta, Asad Sahir, Eric Tan, David Humbird, Lesley J. Snowden-Swan, Pimphan Meyer, Jeff Ross, Danielle Sexton, Raymond Yap, and John Lukas

2 – 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

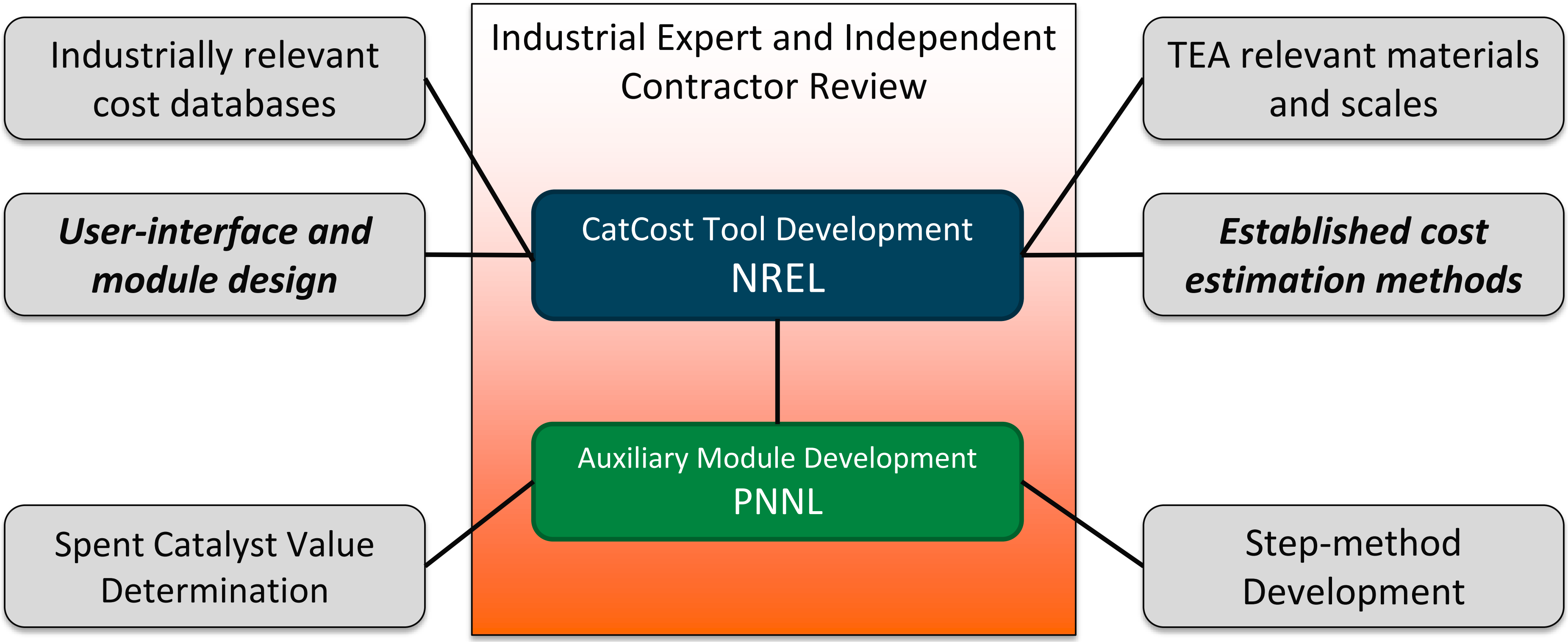
Data gaps
Immediate changes to design, assumptions, minor omissions

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

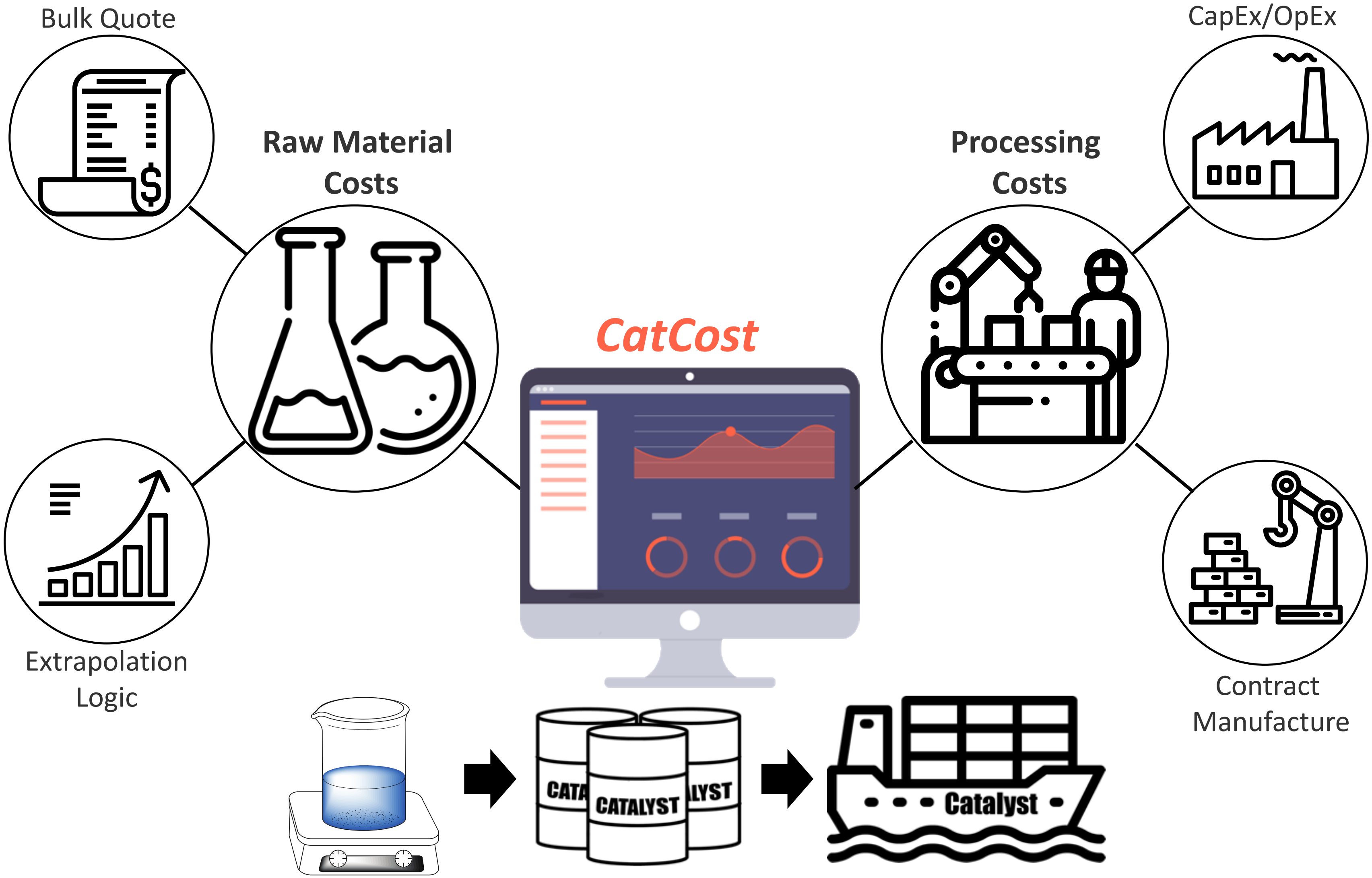
2 – Technical Approach



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 ✓

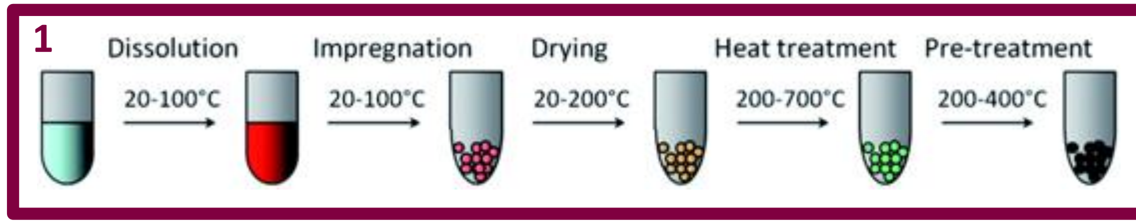
2 – Approach: The CatCost Framework



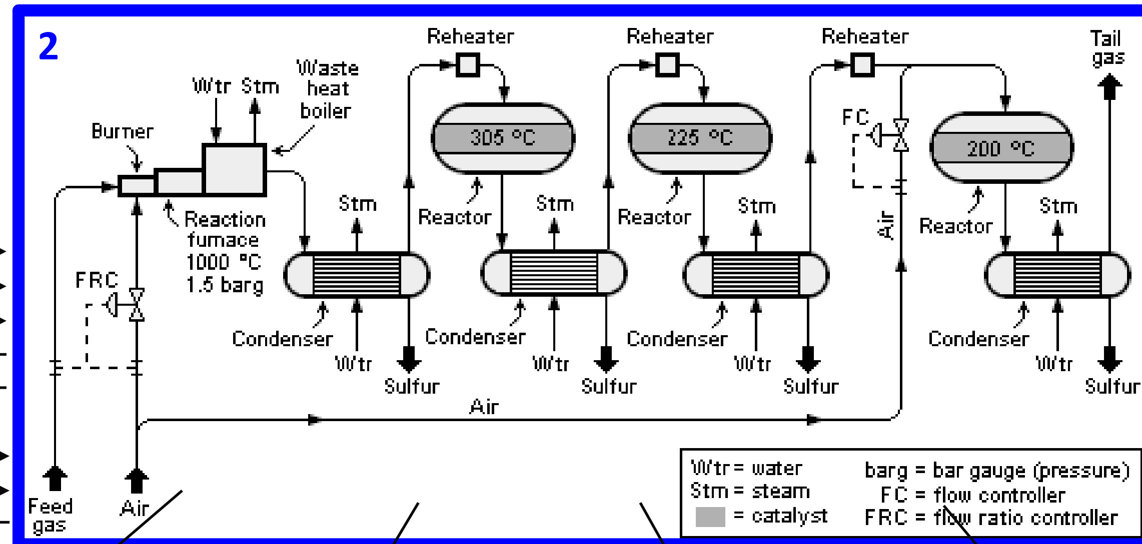
CatCost incorporates industry standard methods to accurately estimate manufacturing costs across scales

2 – 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

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

3 – Processing Costs *via* CapEx & OpEx Factors

Primary costs – estimate in detail:

- List of equipment, including purchase cost
- Direct labor (e.g. equipment operator) requirements and cost

Secondary costs – estimate using “factors”:

CapEx: installation, piping, buildings, etc.

OpEx: supervisory, administration, lab, insurance, etc.

These factors are widely available in process design textbooks

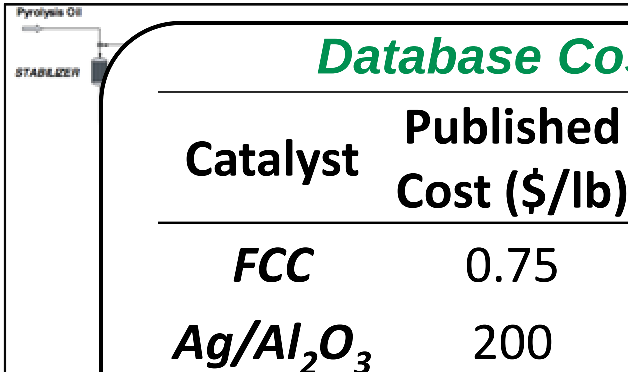
Factored approach enables a high level of customization but requires expertise in process design

3 – CapEx & OpEx Factors: Manufacturing Templates

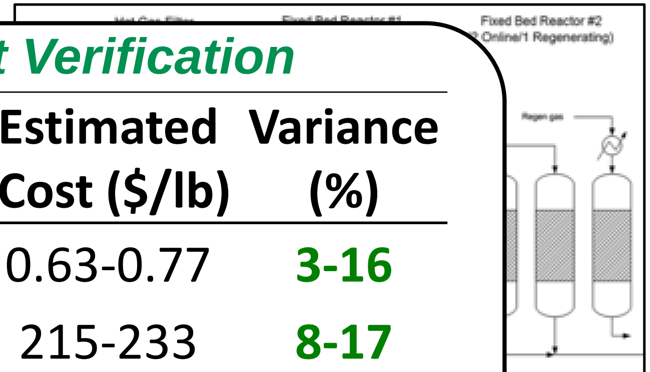
Equipment List | Factored Capital Costs | Factored Operating Costs (Annual)

I'm making a:

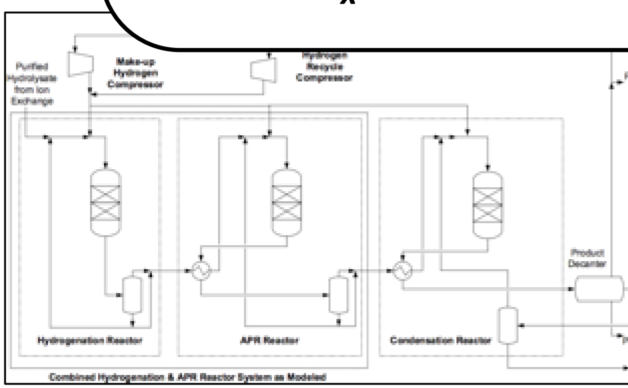
Zeolite

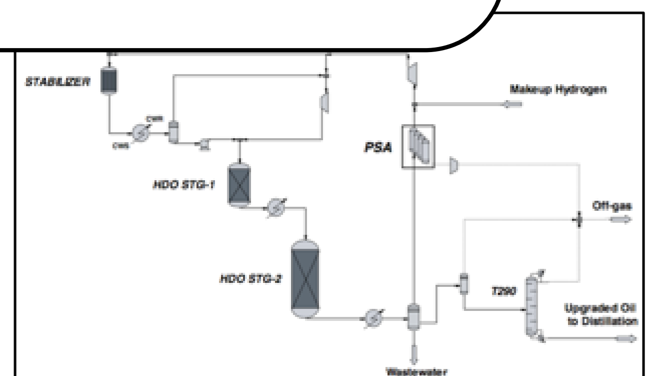


Nanoparticle Catalyst



Ox



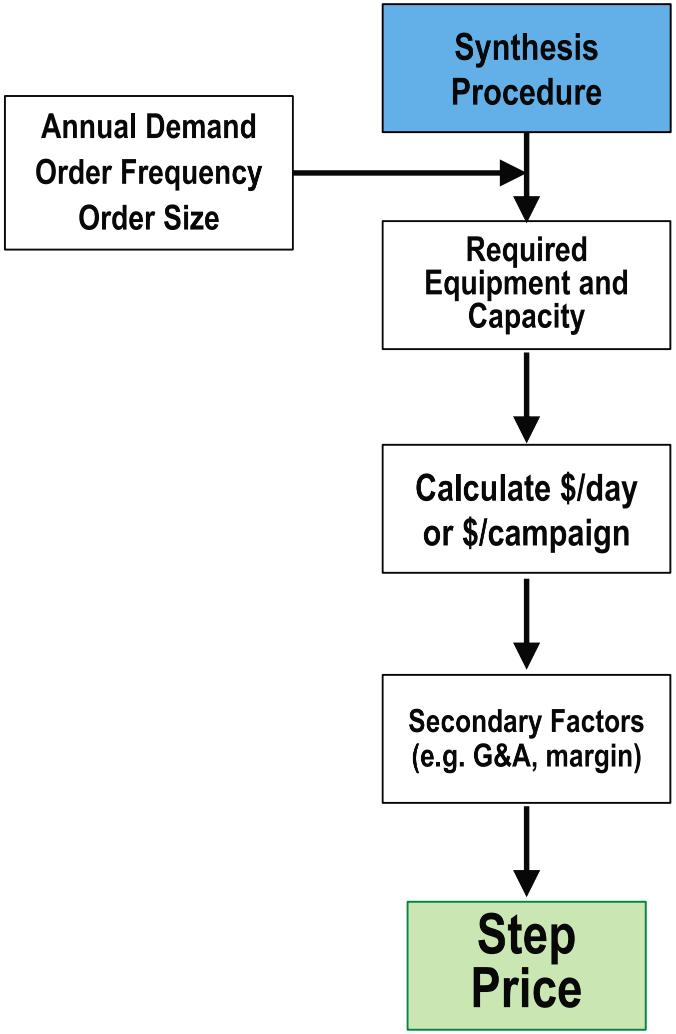


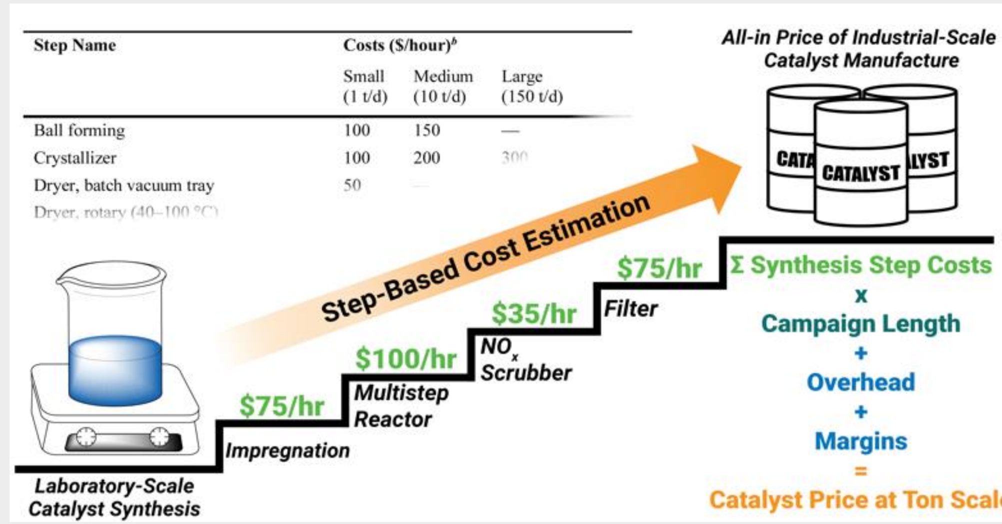
Database Cost Verification

Catalyst	Published Cost ($/lb)	Estimated Cost ($/lb)	Variance (%)
FCC	0.75	0.63-0.77	**3-16**
Ag/Al_2O_3	200	215-233	**8-17**
$BiMoO_x$	12.76	10.92	**16**

3 – CatCost Step Method (Toll Manufacturing)

Lab-scale step → ***Industrial Operation***



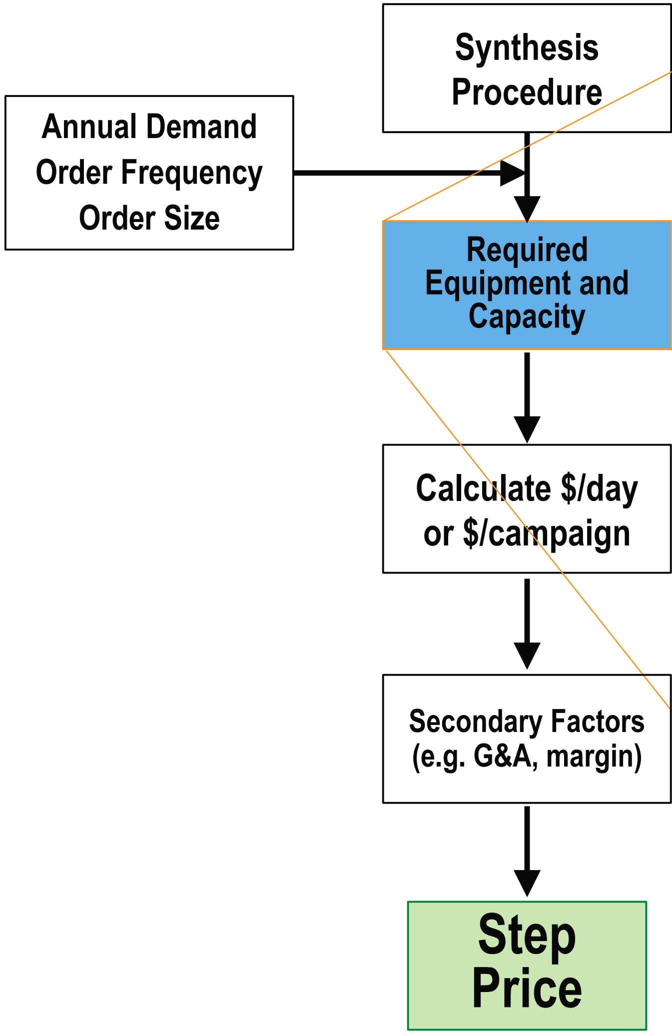


Baddour, F. G.; Snowden-Swan, L.; Super, J. D.; Van Allsburg, K. M. Estimating Pre-Commercial Heterogeneous Catalyst Price: A Simple Step-Based Method. *Org. Process Res. Dev.* **2018**, 22, 12, 1599-1605

Included databases of processing steps, estimated margins and hourly costs to simplify processing cost estimation

3 – CatCost Step Method (Toll Manufacturing)

Lab-scale step → Industrial Operation

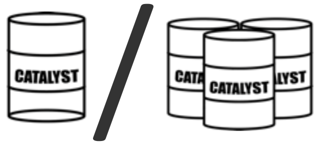


Step Costs ($/hr)			
Scale	*Small*	*Medium*	*Large*
Capacity, ton/day	*1*	*10*	*150*
Step Name			
Incipient wetness (impregnation)	75	100	200
NOx Scrubber	35	75	200
Mixing Reactor Simple	30	60	100
Reactor with steps	100	175	250
Crystallizer	100	200	300
Rotary Vac Filt	na	100	300
Belt Vac Filt	125	175	400
Plate and Frame Filt	75	na	na
Spray Dryer	na	300	550
Batch vac tray dry	50	na	na
Rotating dryer Low Temp (100-212 F)	75	100	200
Rotating Dryer Medium Temp 300 C	100	150	300
Hi Temp Kiln continuous indirect	na	na	325
Hi Temp Kiln continuous direct	na	na	400
High Temp Batch Kiln	75	na	na
Slurry mixer (Muller)	75	100	200
Extruder & Feeder	100	200	425
Ball Forming Unit	100	150	na
Milling	50	100	200
Dry Blending	50	100	200
Flare	50	75	150

Included databases of processing steps, estimated margins and hourly costs to simplify processing cost estimation

3 – CatCost In Practice

Select your scale



Processing Cost Estimation Inputs

Processing Cost Estimation Methods
CatCost includes two methods for estimation of processing costs:
> The **Step Method** *(3a only)*
Uses costs in $/hr for synthesis steps run at a contract manufacturer.
> The **CapEx & OpEx Factors** method *(3b-3e)*
Uses process design literature for a dedicated, new-build catalyst plant.

When compiling a catalyst estimate, **the user may choose either method, complete both to compare them, or combine the two** (e.g. if the user wants to estimate some steps of a synthesis using one method and some steps using the other). The 5a Outputs sheet displays both separate outputs from each method and a combined output summary.

Step Method Inputs

Synthesis Campaign Size	Base	
Order size (1-1000 tons)	100	ton
Equipment size	Large (150 ton/day)	
Synthesis time	0.7	days
Cleaning time	1.0	days
Total: Synthesis campaign length	1.7	days

Overhead and Selling Margin			
G&A Overhead	5	%	?
SARD Overhead	5	%	?
Selling Margin	16.3	%	?

CapEx & OpEx Factors Inputs

Production Capacity - Catalyst	Base		
Design Production, Annual	1.00E+03		?
Capacity Factor	1000	%	?
Actual Production, Annual	1.00E+03		?

Production Capacity - Operating Hours			
Operating Hours (Labor)	8760	hours	?
On-Stream Factor	90	%	?
Operating Hours (Production)	7884	hours	?
Design Production Rate	1.27E-01		?

Input your synthesis

2g K_2PtCl_4 + 8g TiO_2 in 20 mL H_2O

Metal Sources

User Input

Material Name	Quantity (Q)	Unit

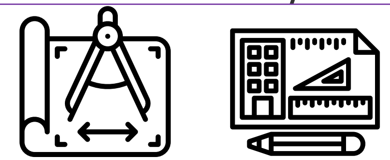
Supports

User Input

Material Name	Quantity (Q)	Unit

Tetraethylenepentamine, tanks, f.o.b.
Tetrahydrofuran, dms., c.l., t.l., f.o.b. works, list
Tetrahydrofuran, tanks, f.o.b. works, list
Titanium dioxide, anatase, bgs., 20-ton lots, frt. alld.
Titanium dioxide, rutile, reg. 20-ton lots, frt. alld.
Titanium dioxide, rutile, slurry shipments 50-ton lots, dr
Toluene di-isocyanate, (mixed isomers), 80%, 2,4- and 2
Toluene, C-grade, US Gulf, spot f.o.b. barges
Toluene, N-grade, US Gulf, spot f.o.b. barges
Trichloroethylene, US Gulf, spot ex-tank
Trichloroethylene, US Gulf, spot f.o.b. USG
Triethylene glycol, tanks, f.o.b. Gulf

Select a Template



Step Method: Inputs and Total Processing Costs

From CatCost "1 Inputs" Sheet

Order size in tons	100	ton
Order size in model units	-----	
Equipment size	Large (150 ton/day)	
Synthesis campaign length	1.666666667	days

Select a Process Template or Choose "Custom Step Process"

Custom Step Process
FCC Catalyst (USY w/ RE)
Magnesia/Alumina
Metal Carbide (Bulk)
Metal Carbide on Metal Oxide
Metal (Earth Abundant) on Metal Oxide
Metal (PGM) on Carbon
Metal (PGM) on Metal Oxide
Red Mud
Zeolite Beta (Bulk)
Zeolite Beta with Metal Active Site
Zeolite ZSM-5 (Bulk)

plate > /hr
plate > /campaign
plate > / catalyst
cess and Process Te
(Show all using "2" at top left, h
(USY w/ RE)
:-- show/hide Step Process Template: FCC Catalyst (USY w/ RE)

Generate Cost Insight

3 – Step Method Market Verification

Pt/C (2 wt. %)

Materials Costs[a]			
Material	***$/lb***	***lb/lb cat.***	***$/lb cat.***
H_2PtCl_6	10.00	0.053	0.53
Carbon support	9.09	1	9.09
N_2H_4	0.68	0.26	0.18
NaOH	0.18	0.025	0.00
NaCl disposal	0.09	10	0.90
Total			10.70
Step Costs			
Step	$/hr	$/day	
Incipient wetness	75	1800	
Reactor, multistep	100	2400	
Scrubber, NOx	35	840	
Filter, plate and frame	75	1800	
Reactor, simple	30	720	
Dryer, rotary (40–100 °C)	75	1800	
Total	390	9360	
Synthesis Campaign Costs			
Order size, tons	2		
Production scale	Small (1 ton/day)		
Step cost, $/day	9360		
Campaign length	2.5		
Campaign cost, $	23400		
Campaign cost, $/lb cat.	5.85		
Subtotal Before Overhead and Margin			
Materials cost, $/lb cat.	10.70		
Campaign cost, $/lb cat.	5.85		
Subtotal, $/lb cat.	16.55		
Overhead and Margin			
G&A, $/lb cat.[c]	0.83		
SARD, $/lb cat.[d]	0.87		
Margin, $/lb cat.[e]	9.12		
Total Estimated Price			
Est. price, $/lb cat.[h]	27.37		
Market Price			
Market price, $/lb cat.[a]	34.09		
Difference	20%		

Estimated Price: $27.37/lb*
Market Price: $34.09/lb*
Variance: 20%

*Excludes value of Pt metal

Ni/Al_2O_3 (21 wt. %)

Materials Costs			
Material	***$/lb***	***lb/lb cat.***	***$/lb cat.***
$Ni(NO_3)_2 \cdot 6H_2O$	2.50	1.04	2.59
Alumina (trilobes)	11.00	0.79	8.69
NaOH 50%	0.20	0.28	0.06
H_2O_2 50%	0.34	0.12	0.04
$NaNO_3$ landfill	0.50	0.02	0.01
H2 forming gas	1.10	0.45	0.50
Total			11.88
Step Costs			
Step	$/hr	$/day	
Incipient wetness	100	2400	
Dryer, rotary (40–100 °C)	100	2400	
Kiln, continuous indirect (300–1290 °C)	175	4200	
Scrubber, NOx	75	1800	
Crystallizer	200	4800	
Filter, rotary vacuum	100	2400	
Dryer, rotary (40–100 °C)	100	2400	
Kiln, continuous indirect (300–1290 °C) × 2	350	8400	
Total	1200	28800	
Synthesis Campaign Costs			
Order size, tons	20		
Production scale	Medium (10 ton/day)		
Step cost, $/day	28800		
Campaign length	3		
Campaign cost, $	86400		
Campaign cost, $/lb cat.	2.16		
Subtotal Before Overhead and Margin			
Materials cost, $/lb cat.	11.88		
Campaign cost, $/lb cat.	2.16		
Subtotal, $/lb cat.	14.04		
Overhead and Margin			
G&A, $/lb cat.	0.70		
SARD, $/lb cat.	0.74		
Margin, $/lb cat.[f]	5.11		
Total Estimated Price			
Est. price, $/lb cat.	20.59		
Market Price			
Market price, $/lb cat.	21.33		
Difference	3%		

Estimated Price: $20.59/lb
Market Price: $21.33/lb
Variance: 3%

USY-based FCC with rare earth

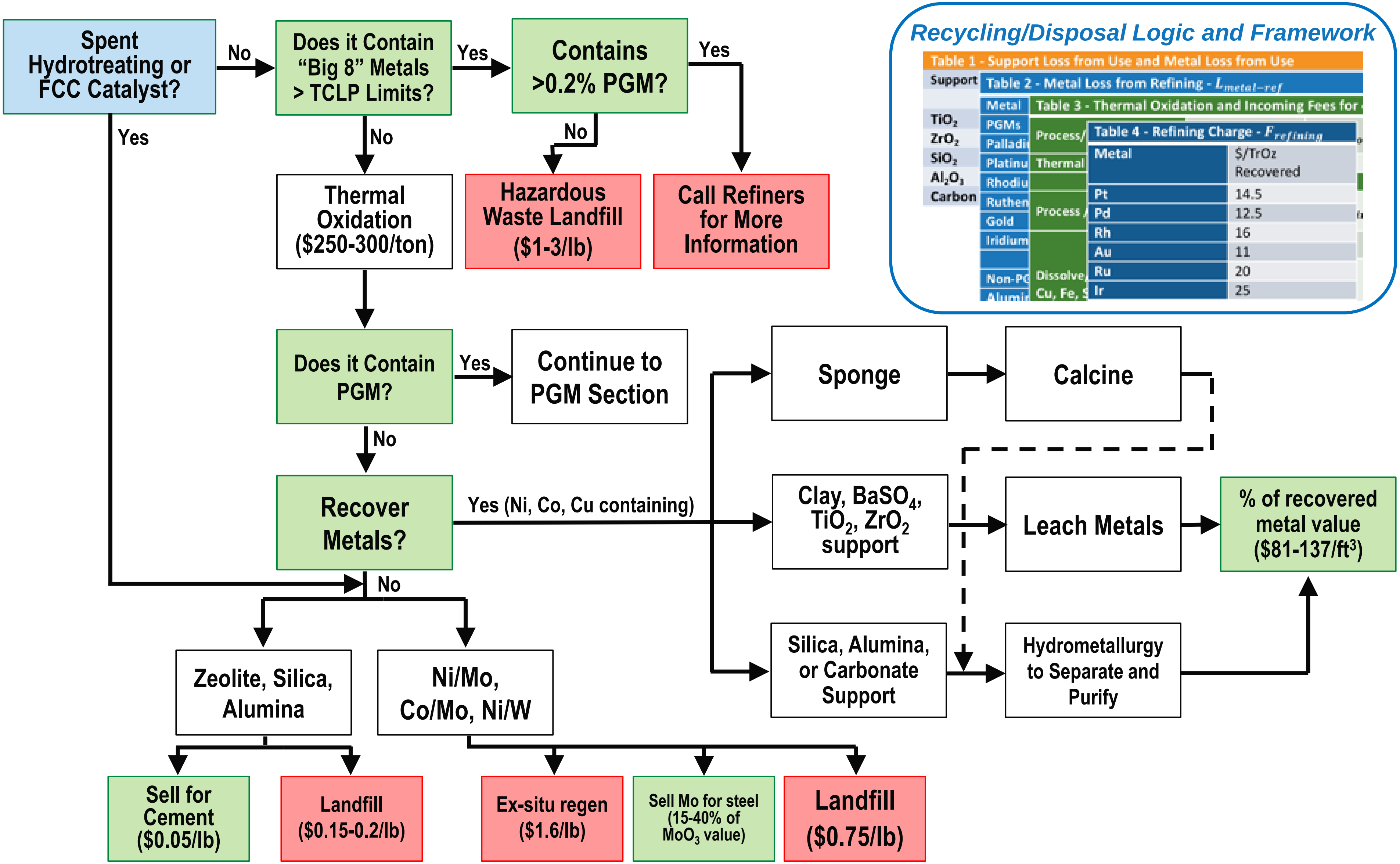
Materials Costs			
Material	***$/lb***	***lb/lb cat.***	***$/lb cat.***
Ludox sodium silicate	0.25	0.819	0.205
$Al(OH)_3$	0.3	0.14	0.042
NaOH 50%	0.2	0.074	0.015
H_2SO_4 98%	0.05	0.22	0.011
Clay	0.05	0.376	0.019
La_2O_3	1.5	0.035	0.053
HCl 31%	0.07	0.036	0.003
NH_4OH 28%	0.1	0.06	0.006
Total			0.352
Step Costs			
Step	$/hr	$/day	
Reactor, simple	200	4800	
Crystallizer	300	7200	
Filter, rotary vacuum × 2	600	14400	
Reactor, simple × 3	600	14400	
Kiln, continuous indirect (300–1290 °C)	325	7800	
Reactor, multistep	600	14400	
Filter, rotary vacuum	300	7200	
Reactor, multistep	600	14400	
Reactor, simple × 2	400	9600	
Dryer, spray × 2	1100	26400	
Reactor, simple × 4	800	19200	
Filter, rotary vacuum × 2	600	14400	
Dryer, rotary (100–300 °C)	300	7200	
Total	6725	161400	
Synthesis Campaign Costs			
Order size, tons	200		
Production scale	Large (150 ton/day)		
Step cost, $/day	161400		
Campaign length	4[b]		
Campaign cost, $	645600		
Campaign cost, $/lb cat.	1.61		
Subtotal Before Overhead and Margin			
Materials cost, $/lb cat.	0.35		
Campaign cost, $/lb cat.	1.61		
Subtotal, $/lb cat.	1.97		
Overhead and Margin			
G&A, $/lb cat.	0.10		
SARD, $/lb cat.	0.10		
Margin, $/lb cat.[g]	0.24		
Total Estimated Price			
Est. price, $/lb cat.	2.41		
Market Price			
Market price, $/lb cat.	2.73		
Difference	12%		

Estimated Price: $2.41/lb
Market Price: $2.73/lb
Variance: 12%

Step method in good agreement with market data

3 – Spent Catalyst Recycle vs. Disposal

Included decision-making logic and databases

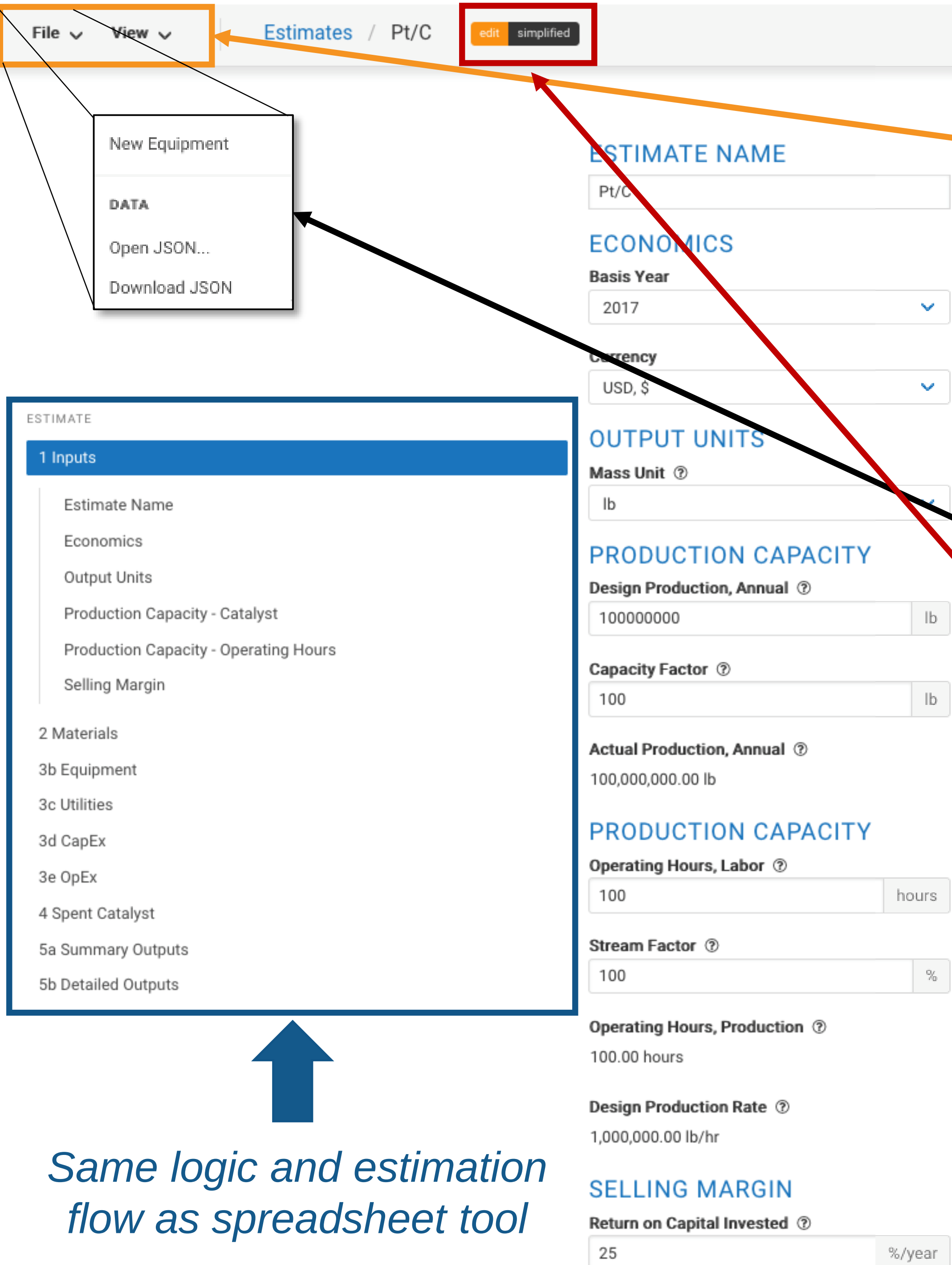


3 – Web UI Design

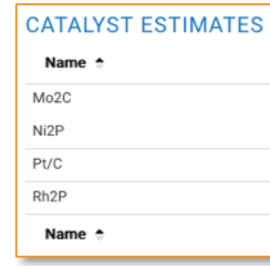
Our Web UI Offers:

- ***Seamless user experience*** with the same core functionality of the spreadsheet
- ***Powerful visualization*** tools for cost comparison of multiple catalysts
- ***Real-time*** variable adjustment
- ***Up-to-date*** pricing information from public databases though Datahub integration
- ***Exportable*** cost data

Advanced Webtool Features

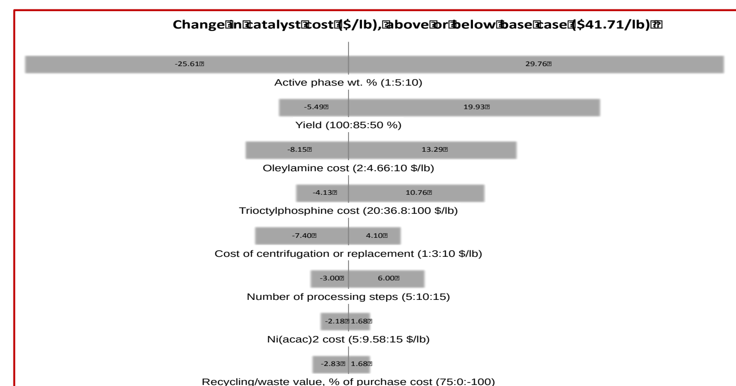


Create any number of locally saved, searchable estimates



Export/Import functions to share and view prepared estimates

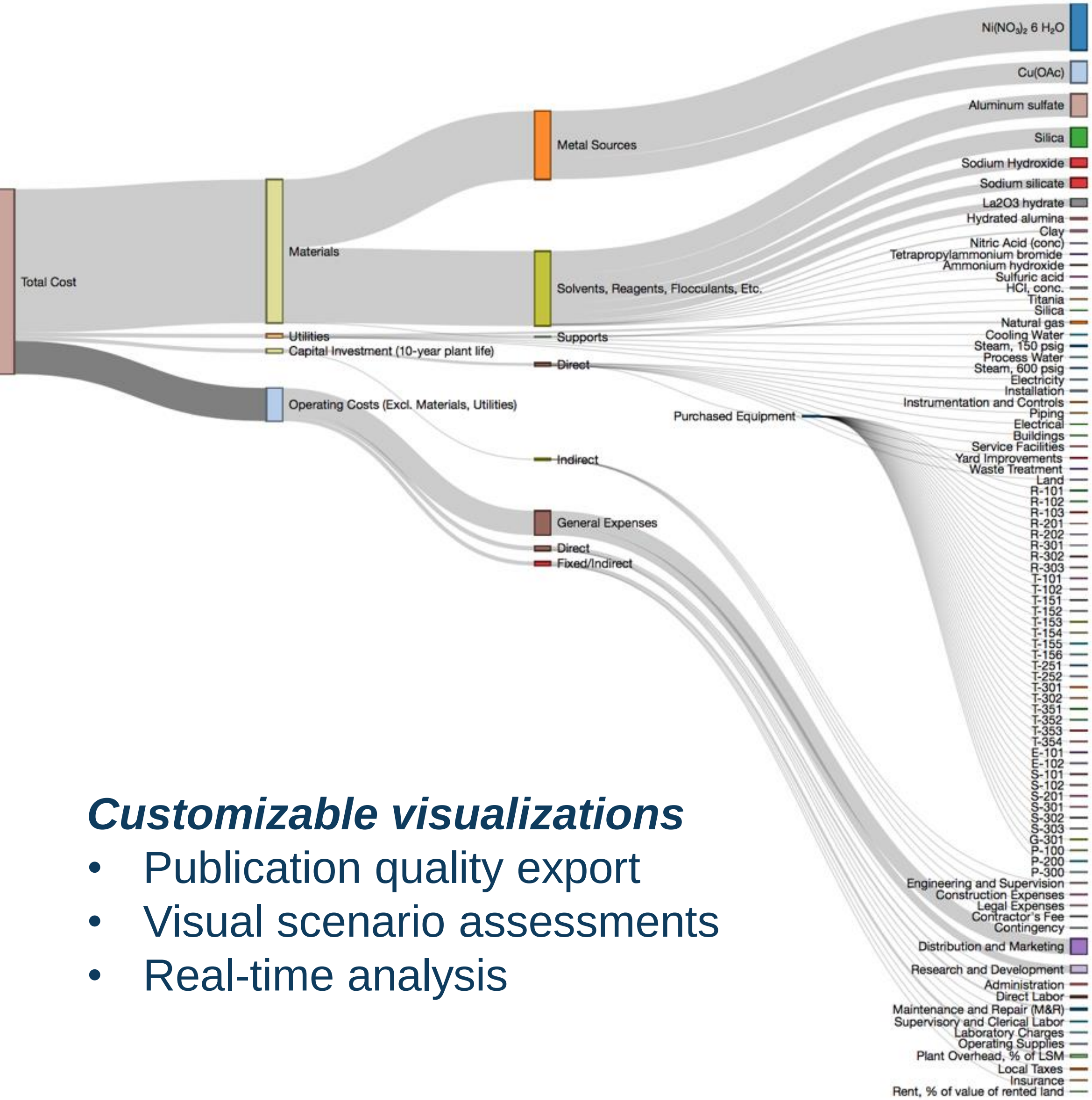
Enable simple or sensitivity mode



All estimates are securely saved on the user's computer

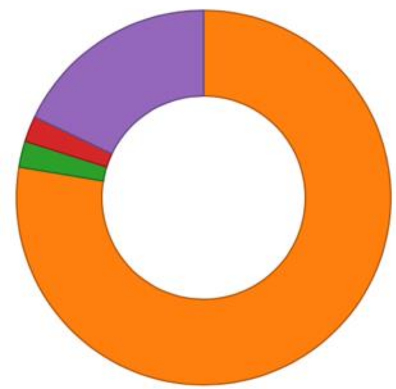
Same logic and estimation flow as spreadsheet tool

3 – Web UI: Interactive and Exportable Visualizations



Cost Estimate Breakdown

« ‹ Total Cost/

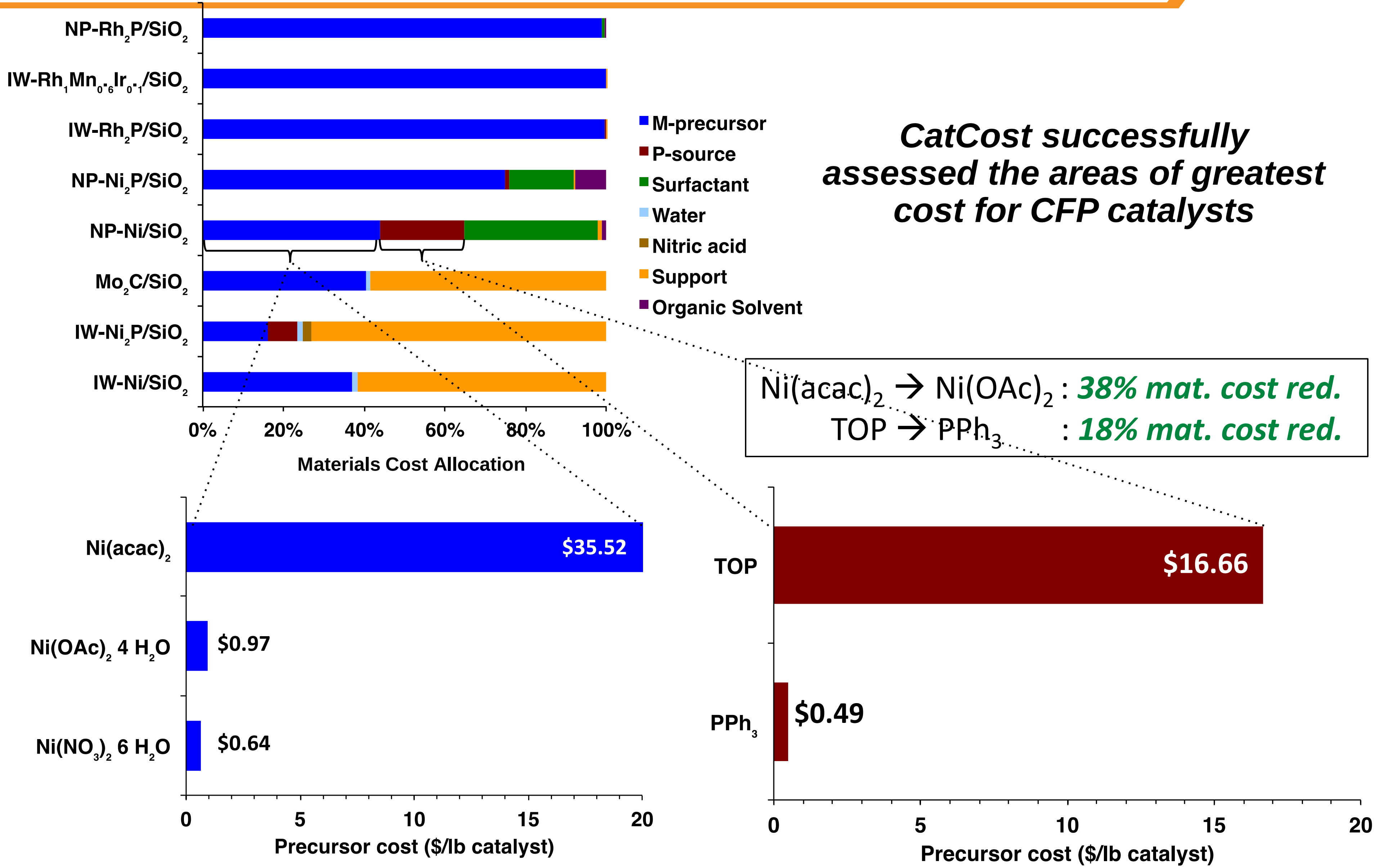


Category	Unit Cost	Annual Cost
Materials	$ 1.6103	$161,027,576
Utilities	$ 0.0468	$4,675,526
Capital Investment (10-year plant life)	$ 0.0459	$4,587,404
Operating Costs (Excl. Materials, Utilities)	$ 0.3716	$37,158,360

Customizable visualizations

- Publication quality export
- Visual scenario assessments
- Real-time analysis

4 – Ex-situ CFP as a Case Study



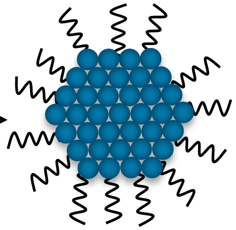
CatCost successfully assessed the areas of greatest cost for CFP catalysts

Ni(acac)$_2$ → Ni(OAc)$_2$: ***38% mat. cost red.***
TOP → PPh$_3$: ***18% mat. cost red.***

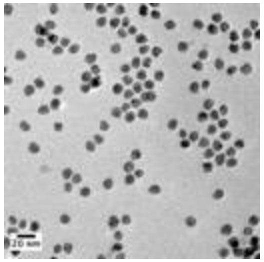
4 – Driving Towards Cost-effective Synthesis

Utilizing CatCost to direct synthesis toward lower cost targets

$Ni(acac)_2$ + 0.5 TOP —10 OAm, Δ→

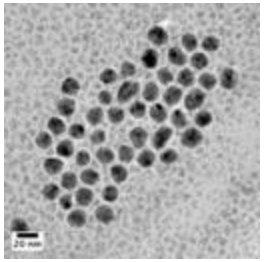


Ni nanoparticles



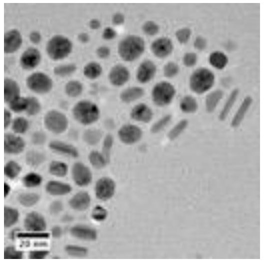
Base Case
11.1 ± 1.0 nm
85% Yield
$95/lb catalyst

$Ni(OAc)_2(OH_2)_4$ + 0.5 TOP —10 OAm, Δ→



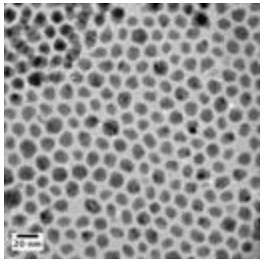
19 nm
75% Yield
$65/lb catalyst

$Ni(OAc)_2(OH_2)_4$ + 1 PPh_3 —10 OAm, Δ→



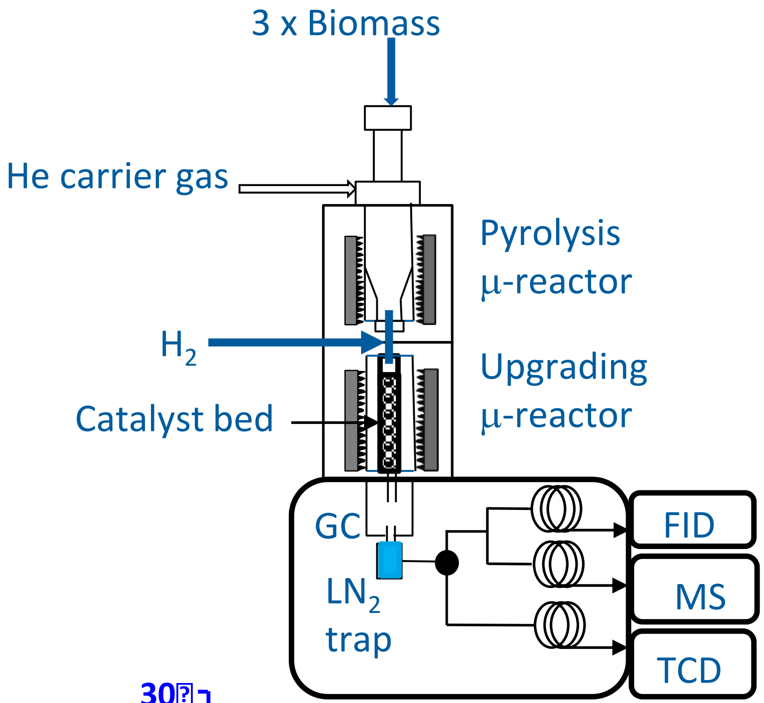
22 nm
50% Yield
$64/lb catalyst

$Ni(OAc)_2(OH_2)_4$ + 4 PPh_3 —10 OAm, Δ→

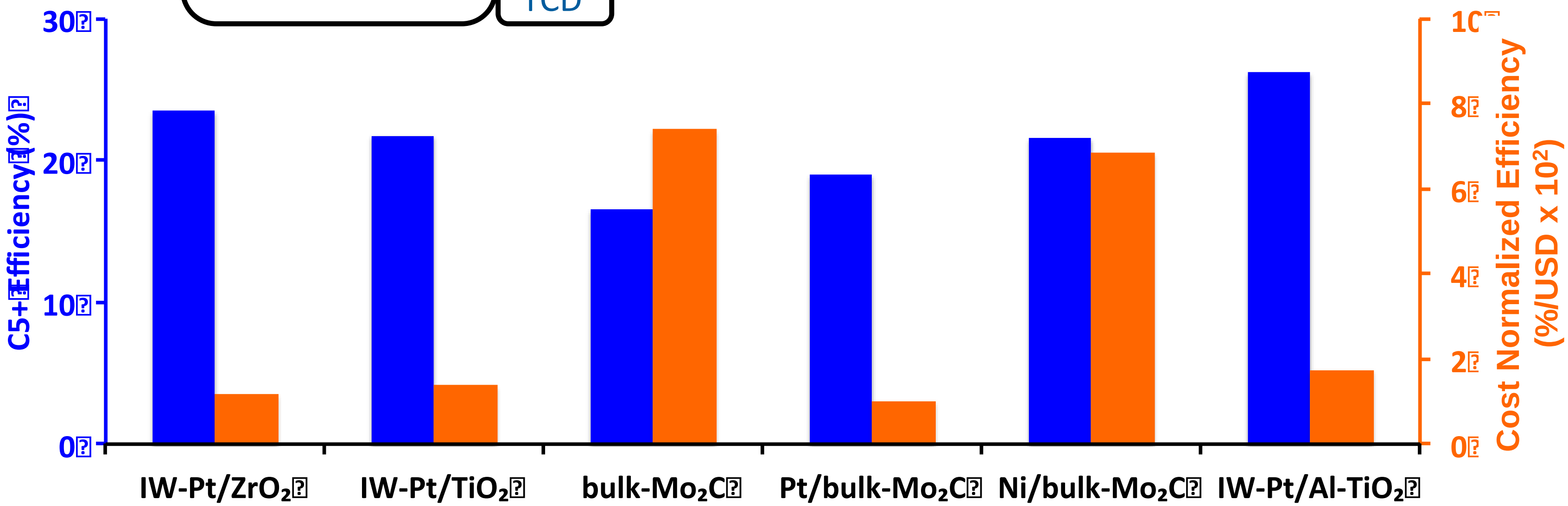


12.0 nm ± 1.8
85% Yield
$46/lb catalyst

4 – Assessing a Catalyst’s Value Proposition



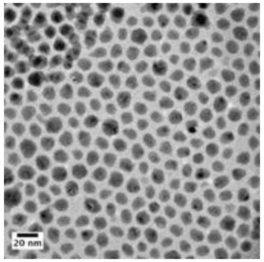
- Analysis with CatCost enables an early assessment of the ***value proposition of a catalyst***
- Catalyst performance metrics (e.g. lifetime, yields, regenerability) can be ***normalized by cost***



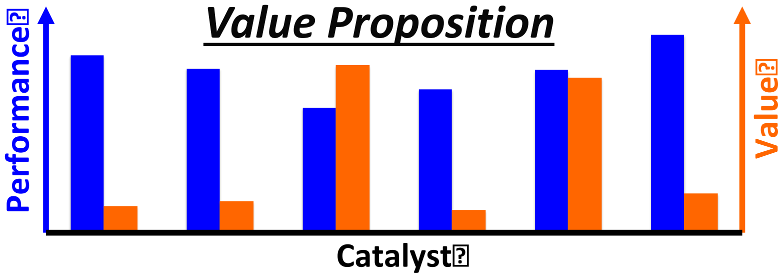
4 – Relevance

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



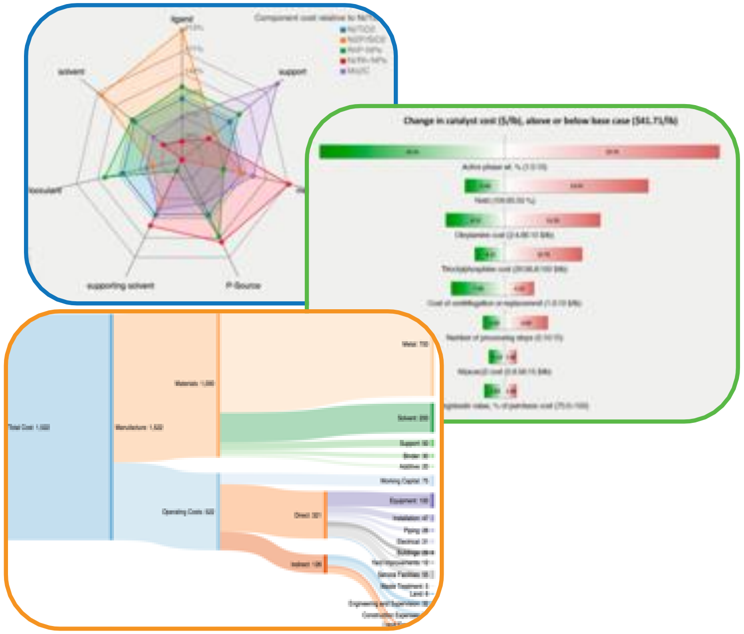
***CatCost*-generated cost metrics offer guidance for catalyst development**
CatCost can be used to ***guide materials development*** much like TEA guides research through performance targets

External R&D groups have demonstrated interest in *CatCost* and its capabilities University professors, national laboratory staff, and companies have reached out with positive feedback and it has been incorporated in 2 university curricula

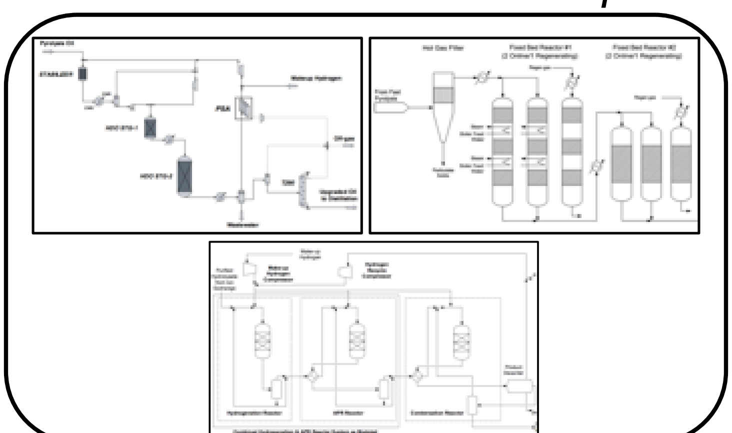
Average of 100 estimates performed monthly since October 1st launch on webtool

Summary

Interactive and Powerful Visualizations



Parameterized Process Templates



- A catalyst cost estimation tool has been developed with ***versatile materials pricing***, multiple ***processing cost estimation*** methods, and ***salvage value*** of catalysts.
- CatCost enables an ***assessment the value proposition*** of <u>pre-commercial</u> catalysts
- ***Rigorous industrial expert review*** of the CatCost tool has been conducted throughout development to ensure the relevance and veracity of the tool
- Future efforts will focus on increasing UI functionality and ***incorporation of additional templates***

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ChemCatBio
Chemical Catalysis for Bioenergy

Energy Materials Network
U.S. Department of Energy

Additional Slides

Peer Review FY17 Responses: Project Approach

Comment: It is ***difficult to predict the effects of economy of scale*** on catalyst. Finding companies interested in ***producing small commercial batches of catalyst may be difficult and cost*** far more than expected.

Address:

Implemented logic to differentiate calculated ***cost*** to produce and ***price*** to buy alleviates some economic ecosystem issues

Determined manufacturing margins for a number of classes of materials as a function of scale through contractor research

Comment: ***Web based system design*** will be powerful for both external relations and teams inside BETO

Address:

Increased funding allocation towards web development and visualization for deep integration with DataHub

Comment: Not obvious from the presentation but I ***encourage close collaboration with the TEA and Sustainability teams*** as well (suggested in future work)

Address:

- Comment likely because presentation did not emphasize existing relationship with TEA efforts
- Active collaboration with ANL established to enable CCM users to output valuable LCA relevant parameters to GREET for more detailed sustainability assessment

Peer Review FY17 Responses: Accomplishments and Progress

Comment: The accuracy of the tools could be checked by applying it to estimate the overall costs of an existing product.

Address: Accuracy of tool outputs verified to be within 20% for a number of large scale catalysts ZSM-5, Ag/Al_2O_3, $BiMoO_x$. Verification of Pt/C, Ni/Al_2O_3, and USY underway.

Comment: The source of the raw material cost estimates is unclear, catalog prices for KG quantities are not appropriate.

Address:

- Commercial open-source pricing data is now being built into a database within DataHub.
- Users are now able to input their own obtained quotes for commercial quantities.
- Catalog price scaling equations will always be least accurate method, but the logic will be included to allow users to build estimates and continue to refine as the obtain better prices
- Included documentation will alert users to accuracy limitations of scaling catalog data

Comment: Particularly important is to include the effects of preparing large quantities of new catalyst on the global supply of metal.

Address: Visualization and total raw material consumption values (including metals) will enable to users to perform this analysis

Peer Review FY17 Responses: Relevance

Comment: It should be kept in mind that the cost of actual catalyst in commercial plants (like the nth plant) most likely will be substantially lower than the estimated cost of pre-commercial catalyst. The relative cost of catalyst in the nth plant should therefore be expected to be a smaller percentage than currently used in several of the TEA analysis.

Address: Currently working to implement additional estimation modes that handle (1) grass-roots production and (2) production campaigns with no capital expenditure as determined by margins of operating contract manufacturers

Comment: The validity of the model has not been proven.

Address: Accuracy of tool outputs has since been verified to be within 20% for a number of large scale catalysts ZSM-5, Ag/Al_2O_3, $BiMoO_x$. Verification of Pt/C, Ni/Al_2O_3, and USY underway.

Other General Comments: Development of catalyst cost model tools and making them available cross teams and externally are highly valued not only for the BETO program but across academics and industry worldwide and already showing in short time value for teams assessments.

Hugely valuable not only to CCB consortium projects, but also to public bioenergy/biofuels community.

The catalyst cost model will be a great tool for determining pre-commercial catalyst cost to be used in the early techno-economic analysis on a consistent basis.

Presentations

1. CatCost Symposium: Tutorial on the Catalyst Cost Estimation Tool: Economic Insight for Catalyst Synthesis and Scale-up Research I & II, *AIChE Annual Meeting*, **October 2018**, Pittsburgh, PA.
    2. K. Van Allsburg; J. Super; L. Snowden-Swan; J. Schaidle; F. Baddour; "Introduction to Catalyst Cost Estimation" *AIChE Annual Meeting*, 369b
    3. K. Van Allsburg; "Tutorial on the CatCost Tool: FCC Catalyst Example" *AIChE Annual Meeting*, 369c
    4. K. Van Allsburg; J. Super; J. White; L. Snowden-Swan; J. Schaidle; F. Baddour; "Capability Highlight: A Simple Step Method for Estimating Processing Costs" *AIChE Annual Meeting*, 369d
    5. K. Van Allsburg; J. Super; J. White; L. Snowden-Swan; J. Schaidle; F. Baddour; "Capability Highlight: Estimation of Spent Catalyst Value" *AIChE Annual Meeting*, 369f
    6. K. Van Allsburg; "Tutorial on the CatCost Tool: Microfluidic Nanoparticle Synthesis Example" *AIChE Annual Meeting*, 431a
    7. J. Schaidle; "Commercialization Example: Catalytic Indirect Liquefaction of Biomass" *AIChE Annual Meeting*, 431b
8. K. Van Allsburg; L. Snowden-Swan; F. Baddour, "CatCost: An Estimation Tool To Aid Commercialization of Catalytic Materials," *Frontiers in Biorefining*, **November 2018**, St. Simons Island, GA.
9. K. Van Allsburg; F. Baddour; CatCost: An Estimation Tool to Aid Commercialization and R&D Decisions for Catalytic Materials" *ChemCatBio Webinar,* **September 2018**, Golden, CO.
10. F. Baddour; L. Snowden-Swan "Catalyst Cost Model Development: Introducing the CatCost Tool" *ChemCatBio/BETO Annual Face-to-Face Meeting*, **August 2018**, Golden, CO.
11. K. Van Allsburg; F. Baddour; "Introducing the CatCost Tool" ExxonMobil CRADA Annual Face-to-Face Meeting, **August 2018**, Golden, CO.
12. K. Van Allsburg; J. Super; J. White; J. Frye; L. Snowden-Swan; J. Schaidle; F. Baddour, "Cost insight for catalyst R&D and commercialization decisions with the catalyst cost estimation tool" 256th *ACS National Meeting & Exposition*, **August 2018**, CATL-170, Boston, MA
13. K. Van Allsburg; J. Super; J. White; J. Schaidle; L. Snowden-Swan; F. Baddour, "Catalyst cost estimation tool development: Reducing information barriers to commercialization" 255th *ACS National Meeting & Exposition*, **March 2018**, CATL-396, New Orleans, LA
14. Hensley J.; S. Habas; F. Baddour; C. Farberow; D. Ruddy; J. Schaidle; R. Brutchey; N. Malmstadt; H. Robota "Transitioning rationally designed catalytic materials to real "working" catalysts produced at commercial scale: Nanoparticle materials" 255th *ACS National Meeting & Exposition*, **March 2018**, CATL-384, New Orleans, LA.
15. Frederick Baddour, 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.
16. Kurt Van Allsburg, 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

1. F. G. Baddour; L. Snowden-Swan; J. D. Super; K. M. Van Allsburg, “Estimating Pre-Commercial Heterogeneous Catalyst Price: A Simple Step-Based Method” Org. *Process Res. Dev.* **2018**, 22, 12, 1599-1605.

2. M. B. Griffin; K. Iisa; H. Wang; A. Dutta; K. A. Orton; R. J. French; D. M. Santosa; N. Wilson; E. Christensen; C. Nash; K. M Van Allsburg; F. G. Baddour; D. A. Ruddy; E. C. D. Tan; H. Cai; C. Mukarakate; J. A. Schaidle “Driving towards cost-competitive biofuels through catalytic fast pyrolysis by rethinking catalyst selection and reactor configuration” *Energy Environ. Sci.* **2018**, 11, 2904-2918

3. J. A. Schaidle*, S. E. Habas, F. G. Baddour, C. A. Farberow, D. A. Ruddy, J. E. Hensley*, R. L. Brutchey, N. Malmstadt, H. Robota; “Transitioning Rationally Designed Catalytic Materials to Real “Working” Catalysts Produced at Commercial Scale: Nanoparticle Materials” *Catalysis, RSC Publishing*, **2017**, 29, 213, DOI: 10.1039/9781788010634-00213.

4. 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.

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

1 – Overview of CatCost

CatCost: A spreadsheet- and web-based **catalyst cost estimation tool** to enable rapid and informed cost-based decisions in the research and commercialization of catalysts

- ***An industrially reviewed*** and ***publicly-available*** catalyst cost estimation tool
- A ***first-of-its-kind*** tool for considering costs of ***novel and pre-commercial catalysts***

Available free-of-charge at catcost.chemcatbio.org