CatCost: Better Cost Information for Catalyst R&D





Problem: High commercialization risk

- Catalyst cost is a major contributor to commercialization risk for catalytic processes
- Up to 10% of capital cost and \pm 10% uncertainty in MFSP for biomass conversion
- No publicly available tools to evaluate cost

Solution: "CatCost" Catalyst Cost Estimation Tool

- Enables early-stage comprehensive cost analysis
- No process design / TEA experience needed
- Improves cost-responsiveness of catalyst R&D



Developed at NREL and PNNL with guidance of industry experts

<u>Free and public</u> release Fall 2018

catcost.chemcatbio.org

Excel- and web-based versions available

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1	Catalyst Cost Model: Pt/TiO	2 Show/Hic	le Sensitivity Inputs	Using +/- above	2	
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3	Materials Calculation In	nputs				
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5	Stoichiometric Calculations	Base Units				
6	Yield Type: % Yield or Mass?	Catalyst Mass	2			
7	Finished Catalyst Mass Yield	1 kg				
8	Stoichiometric Ratio AP/metal		7			
9	Active Phase Molecular Weight	g/mol	7			
10	Active Phase Weight Percent	2 %	7			
11	Active Phase Mass at Prep Scale	0.0200 kg				
12	Catalyst Mass at Prep Scale	1.0000 kg				
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14	Losses Due to Waste/Spoilage	3 %	?			
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16	· · · · · · · · · · · · · · · · · · ·					
17	Metal Source(s)					
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19	User Input		Pricing Calculations			
20	Material Name	Quantity (Q) Unit	Q in kg	Q in mol	Q (kg/kg catalyst) Uni	t Price (2016 \$/kg)
21	Pt(NH3)4(NO3)2	0.04 kg	0.0397	0.1025	0.0397	20,002.71
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4 1	0 Instructions 1 Inputs 2 Materials 3a	Step Method 3b Equip	3c Utilities 3d Cape	Ex 3e OpEx	4 Spent Catalyst 5a Su	immary Outputs +
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CatCost: Estimation Methods

1. Raw Materials Pricing

- Built-in library of common materials
- Guidance for obtaining quotes
- Extrapolation from lab-scale prices



3. A Simple "Step Method" to Supplement Process Templates

- All-in costs in \$/hr for typical unit ops. (e.g. Belt Filter, Reactor, Spray Dryer)
- Quick addition of new catalyst types or steps to existing process templates

2. Detailed Process Templates for Common Catalyst Types

- E.g. metal/metal oxide, zeolite, MOFs, flow/batch nano, metal carbides
- Including equipment, labor, utilities, CapEx, OpEx (industry-standard methods)



- 4. Complete Spent Catalyst Value
- Including precious metals recycling, catalyst attrition, landfill/disposal costs

Metals Reclamation Calculations
Catalyst solids after use
Metal content in fresh catalyst
Metal losses during use (typical)
Metal losses during refining (typical)
Recoverable metal
Recoverable metal, troy ounces
Spot price
Recoverable metal value

Unrs 0.98 kg/kg catalyst 0.0200 kg/kg catalyst 10 % 0.0175 kg/kg catalyst 0.5514 oz t/kg catalyst 31,873.61 \$/kg metal 556.51 \$/kg catalyst

Integrating the best methods in catalyst cost estimation into a powerful analysis tool

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CatCost: A Convenient and Powerful Tool for Researchers

Flexible for a Variety of Uses



Enabling better R&D decisions by providing catalyst researchers with actionable cost information

- Built-in, industry-vetted analysis features
- Extensively reviewed by industrial experts
- Powerful visualizations
- Verified (± 20%) with market cost data for high-volume commercial catalysts



<u>Free public</u> release in the fall of 2018 at catcost.chemcatbio.org

Contact the team at CatCost@nrel.gov





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Chemical Catalysis for Bioenergy

Energy Materials Network

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