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 7\textsuperscript{th}, 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

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%

**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

**Budget**

<table>
<thead>
<tr>
<th></th>
<th>FY15 Costs</th>
<th>FY16 Costs</th>
<th>Total Planned Funding (FY17-FY18)</th>
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<tr>
<td><strong>DOE Funded</strong></td>
<td>$0</td>
<td>$228</td>
<td>$250k*</td>
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*FY17 operating budget reduced to $125k

**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)
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.)
Project overview – Integrated approach

Establish an integrated and collaborative portfolio of catalytic and enabling technologies

CCB Catalysis Projects

- Catalytic Upgrading of Biochemical Intermediates
- Liquid Fuels via Upgrading of Indirect Liquefaction Intermediates
- Fast Pyrolysis and Upgrading
- Catalytic Fast Pyrolysis
- Recovering and Upgrading Biogenic Carbon in Biomass-Derived Aqueous Streams

Enabling Technologies

- Catalyst Development (ACSC)
- Computational Modeling (CCPC)
- Cost Guidance (CCM)

Collaborative outcomes

- Targeted Cost Reduction
- Improved Performance for Key Metrics
- Cost-guided Synthesis
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.

- **HGF, Capital Cost**
- **VPU C Efficiency**
- **Catalyst Cost**
- **Reactor Capital**
- **HT C Efficiency**
- **VPU Catalyst Replacement**

% Change to MFSP

Operating Costs ($/GGE product)

- 4% of MFSP: $12/GGE
- 11% of MFSP: $36/GGE
- 20% of MFSP: $72/GGE

Low Cost Catalyst
Base Case (ex-situ)
High Cost Catalyst
Management Approach

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

**Primary tool development, interface design, methodology testing**
- NREL
  - Frederick Baddour

**Decision making logic development, recycling incorporation**
- PNNL
  - Lesley Snowden-Swan

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**Assessment of SOT / Data Gathering**

**Implementation of Best Practices**

**Industrial Expert Review**

**Refinement**

**Industrial Expert Review**

**Finalized Module**

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**Data gaps**
- Immediate changes to design, assumptions, minor omissions

**ID of Critical Components**
- Incorporation into AOP, go/no-go, planned milestone efforts

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**Industrial Expert Review**

**Biannual methodology review**
- Annual user-interface review

**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)

**Industrial Expert and Independent Contractor Review**

- Industrial relevant cost databases
- **User-interface and module design**
- Recycling/Reclamation Cost Determination

**Catalyst Cost Estimation Tool Development**

- NREL

**Established cost estimation methods**

**Auxiliary Module Development**

- PNNL

**Determination of catalyst intrinsic value**

**TEA relevant materials and scales**
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

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

Materials Costs
- Operating Labor
  - Direct
  - Supervisory
  - Lab/QA
- Maintenance
  - Supplies
  - Labor
  - Site Services
- Equipment Capital
  - Installation
  - Piping
  - Instrumentation
- Production Site
  - Buildings
  - Land
  - Design & Constr.

Utility Flows
- Electricity
- Steam
- Cooling water
- Wastewater

Utility Costs

Factored Costs
- Contingencies
- Working Capital
- Administrative

Labor Costs
Maint. Costs
Equipment Costs
Site Costs
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

**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

**Manufacturing Scale**
Informed by FY15 *Ex situ* CFP Design report
**Challenge** – Many chemicals required for synthesis of pre-commercial catalyst require raw materials that lack industrial market data

\[
\text{Ni(acac)}_2 + 0.5 \text{ TOP} \rightarrow 10 \text{ OAm} \xrightarrow[\Delta]{\text{Supp.} \text{ Solv.}} \text{Ni Nanocatalyst}
\]

- **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

**Quote Information (Inputs)**

<table>
<thead>
<tr>
<th>Quantity, ( Q )</th>
<th>Units</th>
<th>Total Price, ( P ) ($)</th>
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<tbody>
<tr>
<td>100</td>
<td>g</td>
<td>25.72</td>
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<tr>
<td>500</td>
<td>g</td>
<td>60.20</td>
</tr>
<tr>
<td>2.5</td>
<td>kg</td>
<td>200.09</td>
</tr>
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</table>

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

<table>
<thead>
<tr>
<th>Quantity, ( Q )</th>
<th>Units</th>
<th>Total Price, ( P ) ($)</th>
<th>Quantity, ( Q ), in lb</th>
<th>Unit Price, ( p ), ($/lb)</th>
<th>Log(( Q ))</th>
<th>Log(( p ))</th>
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<tr>
<td>100</td>
<td>g</td>
<td>25.72</td>
<td>0.22</td>
<td>116.66</td>
<td>-0.66</td>
<td>2.07</td>
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<tr>
<td>500</td>
<td>g</td>
<td>60.20</td>
<td>1.10</td>
<td>54.61</td>
<td>0.04</td>
<td>1.74</td>
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<tr>
<td>2.5</td>
<td>kg</td>
<td>200.09</td>
<td>5.51</td>
<td>36.30</td>
<td>0.74</td>
<td>1.56</td>
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</table>

**Data Fit**

- Slope: -0.363
- Intercept: 1.803

**Calculated Bulk Pricing**

- Bulk Quantity = 2,000 lb
- Bulk Price = 4.04 $/lb
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
Research Progress: A Complete Scaffold

Ni(NO₃)₂ · 6 H₂O + (NH₄)₂HPO₄ → HNO₃/H₂O mix, support, dry → IW-Ni₂P/SiO₂ precursor → heat, cool passivate → IW-Ni₂P/SiO₂ catalyst

Processing Steps

<table>
<thead>
<tr>
<th>Cost ($/lb)</th>
<th>Step</th>
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<tr>
<td>0.05</td>
<td>mix</td>
</tr>
<tr>
<td>2</td>
<td>support</td>
</tr>
<tr>
<td>1</td>
<td>dry</td>
</tr>
<tr>
<td>3</td>
<td>heat</td>
</tr>
<tr>
<td>1</td>
<td>cool</td>
</tr>
<tr>
<td>1</td>
<td>passiv.</td>
</tr>
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</table>

Scaled by basis for purchase

<table>
<thead>
<tr>
<th>Catalyst</th>
<th>Material</th>
<th>Function</th>
<th>density</th>
<th>MW of precursor</th>
<th>amount unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>IW-Ni₂P/SiO₂</td>
<td>water</td>
<td>solvent</td>
<td>1</td>
<td>35 mL</td>
<td></td>
</tr>
<tr>
<td>ammonium phosphate dibasic</td>
<td></td>
<td>P-source</td>
<td></td>
<td>0.89 g</td>
<td></td>
</tr>
<tr>
<td>Conc. Nitric Acid</td>
<td></td>
<td>additive</td>
<td>1.51</td>
<td>1 mL</td>
<td></td>
</tr>
<tr>
<td>Ni(NO₃)₂ - 6 H₂O</td>
<td></td>
<td>metal source</td>
<td>290.79</td>
<td>1.96 g</td>
<td></td>
</tr>
<tr>
<td>Sipernat-22</td>
<td></td>
<td>support</td>
<td>9.50</td>
<td>10.00 g</td>
<td></td>
</tr>
</tbody>
</table>

Comprehensive approach to estimating novel catalyst costs

Σ costs

$10/lb IW-Ni₂P/SiO₂
Research Progress Roadmap

Method Development: Building the Catalyst Cost Estimation Tool

Implementation: Utilization of the Tool
The CCM tool successfully assessed the areas of greatest cost for CFP catalysts.

Materials Cost Allocation

- Ni(acac)$_2$ $\rightarrow$ Ni(OAc)$_2$ : 38% mat. cost red.
- TOP $\rightarrow$ PPh$_3$ : 18% mat. cost red.
Relevance: Cost-effective Synthesis with the ACSC

Utilizing the CCM to directing synthesis towards lower cost targets

**Base Case**

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

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

**19 nm**  
75% Yield  
$65/lb catalyst

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

**22 nm**  
50% Yield  
$64/lb catalyst

Ni(OAc)$_2$(OH)$_2$$_4$ + 1 PPh$_3$ $\xrightarrow{\Delta}$ 10 OAm

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

Ni(OAc)$_2$(OH)$_2$$_4$ + 4 PPh$_3$ $\xrightarrow{\Delta}$ 10 OAm
• 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
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.

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.

Established new collaboration with a small manufacturing business.
Future Work: Recycling and Decision Making

**Catalyst Material Balance**

- Sell to Smelter ($1-1.30/lb)
- Contains Precious Metals?
  - Yes
    - Metal Value Exceeds Recovery Cost?
      - Yes
        - Dissolve Support Separate and Dissolve Metals
      - No
        - Carbon Support?
          - Yes
            - Dissolve Metals
          - No
            - Clay, TiO₂, or ZrO₂ Support?
              - Yes
                - Leach Metals
              - No

- No
  - Metal Value Exceeds Recovery Cost?
    - Yes
      - Dissolve Support Separate and Dissolve Metals
    - No
      - Thermal Oxidation ($0.10-0.15/lb)

- Disposal ($3-7/lb) Seek user input

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

<table>
<thead>
<tr>
<th>Metal</th>
<th>Typical Recovery (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Iron</td>
<td>60</td>
</tr>
<tr>
<td>Cobalt</td>
<td>80</td>
</tr>
<tr>
<td>Nickel</td>
<td>80</td>
</tr>
<tr>
<td>Copper</td>
<td></td>
</tr>
<tr>
<td>Aluminum</td>
<td>30</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>70–80</td>
</tr>
<tr>
<td>Ruthenium</td>
<td>75–85</td>
</tr>
<tr>
<td>Rhodium</td>
<td>90–95</td>
</tr>
<tr>
<td>Palladium</td>
<td>95–98</td>
</tr>
<tr>
<td>Tungsten</td>
<td>50</td>
</tr>
<tr>
<td>Iridium</td>
<td>90</td>
</tr>
<tr>
<td>Platinum</td>
<td>96–98</td>
</tr>
<tr>
<td>Silver</td>
<td>97–98</td>
</tr>
<tr>
<td>Gold</td>
<td>97–99</td>
</tr>
</tbody>
</table>

**Support Material**

- Carbon: Typical Recovery Method
  - Combustion followed by acid extraction
- Silica: De-cooking and dissolution of silica
- Titania: De-cooking and extraction of metals
- Alumina: De-cooking and dissolution of alumina
- Clay: Dissolution of framework, extractions

Paraphrased comments from CCM reviewers:
- Copper is difficult to separate from precious metals during recovery. 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 decocking, to recover the metals.

**Metal Value Exceeds Recovery Cost?**

- Yes
  - Sell to Smelter ($1-1.30/lb)
- No
  - Disposal ($3-7/lb) Seek user input

**Recovered Metals as Soln. or Salt**
Future Work: A Tiered-complexity Approach to Operating Costs

- **Severity based operating costs**
- **μ-TEA plant template**

**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*

**Laboratory Procedure**
- Dissolution: 20-100°C
- Impregnation: 20-100°C
- Drying: 20-200°C
- Heat treatment: 200-700°C
- Pre-treatment: 200-400°C

**Parameterized scale-up templates**

**Rapid and accurate processing cost estimation**
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

**GREET Outputs**
- Cradle-to-gate impacts of catalyst production
- GHG emissions (kg CO$_2$e/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.
Acknowledgments

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Kenny Gruchalla

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John Frye
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Jennifer Dunn
Thathiana Pahola

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Questions
Additional Slides
Publications and Presentations

• Presentations

• Publications
<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>ACSC</td>
<td>Advanced Synthesis and Characterization project</td>
</tr>
<tr>
<td>ANL</td>
<td>Argonne National Laboratory</td>
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<tr>
<td>AOP</td>
<td>Annual operating plan</td>
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<tr>
<td>BETO</td>
<td>Bioenergy Technologies Office</td>
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<tr>
<td>CCB</td>
<td>Chemical Catalysis for Bioenergy Consortium; ChemCatBio consortium</td>
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<tr>
<td>CCM</td>
<td>Catalyst Cost Model Development project</td>
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<tr>
<td>CCPC</td>
<td>Consortium for Computational Physics and Chemistry</td>
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<td>CFP</td>
<td>Catalytic fast pyrolysis</td>
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<td>DOE</td>
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<td>EMN</td>
<td>Energy Materials Network</td>
</tr>
<tr>
<td>FY</td>
<td>Fiscal year</td>
</tr>
<tr>
<td>GGE</td>
<td>Gallon gasoline equivalent</td>
</tr>
<tr>
<td>HGF</td>
<td>Hot gas filter</td>
</tr>
<tr>
<td>HT</td>
<td>Hydrotreating</td>
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<tr>
<td>LANL</td>
<td>Los Alamos National Laboratory</td>
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<tr>
<td>LCA</td>
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<td>Description</td>
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<td>-----------</td>
<td>------------------------------------------</td>
</tr>
<tr>
<td>MFSP</td>
<td>Minimum fuel selling price</td>
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<td>Multi-Year Program Plan</td>
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<td>NETL</td>
<td>National Energy Technology Laboratory</td>
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<td>NREL</td>
<td>National Renewable Energy Laboratory</td>
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<tr>
<td>Ni(acac)$_2$</td>
<td>Nickel acetylacetonate</td>
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<td>Ni(OAc)$_2$</td>
<td>Nickel acetate hydrate</td>
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<td>PPh$_3$</td>
<td>Triphenylphosphine</td>
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<td>SOT</td>
<td>State of technology</td>
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<tr>
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<td>Techno-economic analysis</td>
</tr>
<tr>
<td>TOP</td>
<td>Trioctylphosphine</td>
</tr>
<tr>
<td>VPU</td>
<td>Vapor phase upgrading</td>
</tr>
<tr>
<td>wt%</td>
<td>Percentage by weight</td>
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