CatCost

An Estimation Tool to Aid Commercialization and R&D Decisions for Catalytic Materials

Documentation and User Guide

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CatCost is available at **catcost.chemcatbio.org**

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1 CatCost Overview and Version History

1.1 Purpose

Basic catalyst research can benefit from insight on catalyst cost trends and relationships. Early development of pre-commercial catalysts is generally guided by rigorous testing of catalytic performance and durability. However, information about catalyst manufacturing costs may be much more speculative, especially when advanced synthetic techniques not yet used in industry are required. Considering the significance of uncertainty in the cost of manufacture, better cost estimation methods for pre-commercial materials may allow better allocation of R&D resources, throughout the development process, by optimizing materials to meet cost targets in addition to performance and durability targets.

Resources for pre-commercial catalyst cost estimation have been limited prior to the release of CatCost. Evonik Industries provides a simple web-based calculator that estimates certain costs of a catalytic process based on catalyst purchase price, recovery costs, etc. However, it does not support estimation of the catalyst purchase price itself, making it suitable only for established materials. Aspen Technology, Inc. offers a capital cost estimation tool that would support some elements of cost estimation, but it is not catalyst-specific and requires a subscription. Catalyst manufacturers use sophisticated cost models, but their methods are often considered trade secrets. Therefore, the methods described herein represent the state of technology (SOT) for publicly available cost estimators.

The objective of CatCost is to support the catalysis community by integrating essential cost estimation methods into a user-friendly tool. It therefore allows users the opportunity to study a wide range of contributors to uncertainty in catalyst cost while doing little or no tool development of their own.

1.2 Estimation Modules in CatCost

The cost to synthesize a catalyst at industrial scale may be broken down into cost components that are well established in the process design literature.[1-4] These components have been implemented into CatCost by a combination of new and literature methods and organized by modules (Table 1.1). A module corresponds to a numbered worksheet in the Excel version of CatCost and to a page in the left-side navigation pane of a catalyst estimate in the web version.

CatCost has been developed with several core tenets to properly model the cost of catalyst manufacture, including: (i) solicitation of industrial review to maximize relevance of the tool to real industry design decisions, (ii) benchmarking and validation of the tool using a range of catalytic materials, and (iii) use of a tiered structure where users can select the level of complexity of the calculation and customize the tool to suit their needs for accuracy and sensitivity analysis (e.g. using CatCost-provided assumptions about capital and operating costs for greater speed or customizing with proprietary data from the user's company records for greater accuracy).

Table 1.1. Components of a catalyst cost estimate included in CatCost.	
Module Name	**Components of Catalyst Cost Analysis**
1 Inputs	Global Inputs (Estimate Name, Basis Year, Output Mass Unit) Processing Cost Estimation Inputs (synthesis scale, margins, etc.)
2 Materials	Yield and Stoichiometry Raw Material Selection and Pricing Material Losses During Handling
3a Step Method *(Excel-only in v1.0.0)*	Selection of Synthesis Steps with Costs in $/hr Calculation of Overall Synthesis Campaign Cost Process Templates for Common Catalyst Types
3b Equipment (CapEx & OpEx Factors Method)	Equipment List Including Sizes and Materials of Construction Scaling of Equipment from Reference Scale to Estimate Scale Purchased Cost, Installed Cost, and Labor Factor for Equipment Process Templates for Common Catalyst Types
3c Utilities (CapEx & OpEx Factors Method)	Process Utilities Consumption and Unit Costs Process Templates for Common Catalyst Types
3d CapEx (CapEx & OpEx Factors Method)	Factored Costs for Capital Expenditures: • Direct Costs (piping, buildings, land, etc.) • Indirect Costs (engineering, construction, contingency) • Working Capital
3e OpEx (CapEx & OpEx Factors Method)	Factored Costs for Operating Expenditures: • Direct Costs (labor, supervision, maintenance, supplies) • Indirect Costs (taxes, insurance, rent, overhead) • General Expenses (R&D, distribution, administration)
4 Spent Catalyst	Complete Treatment of the Value/Cost of Metals Recovery, Sale, or Disposal for Spent Catalysts: • Metal and Support Attrition During Catalyst Use (using data on specific metals, supports, and reactor configurations) • Value of Metals Content Including Spot Price Library • Metals Recovery and Refining Fees • Sale Values, where applicable • Landfill Costs for Different Hazard Classes
5 Outputs	Complete Catalyst Cost via Step Method Complete Catalyst Cost via CapEx & OpEx Factors Combined Catalyst Cost Using Both Methods in a Mix and Match Approach
Libraries *(bundled information to facilitate estimates; user-expandable)*	Materials Library, Step Library, Equipment Library, Spent Catalyst Library, Automated Unit Conversions (UnitConv), US Bureau of Labor Statistics Chemical Producer Price Index (ChemPPI), *Chemical Engineering* Plant Cost Index (CEPCI)

1.3 Industrial Review

The development of CatCost has been informed by thorough review with a team of industrial catalysis experts having extensive knowledge of catalyst synthesis and process economics. All members of the review team had experience in catalyst synthesis and many were selected for their knowledge in catalyst scale-up and industrial process design. Notably, the assembled members included senior members from the global petrochemical refining sector, the global catalyst manufacturing sector, and academic and industrial catalyst design and development, as well as consultants from these industries. This diversity of expertise generated feedback both on the validity of the underlying logic for catalyst estimation and the usability and implementation of these methods. The team provided guidance on the state-of-technology for publicly available cost estimators, the methods employed by CatCost, and the usability of the spreadsheet-based CatCost tool.

1.4 Overview of Web and Excel Versions

Two versions of CatCost are available, both of which use the same estimation logic and overall organization into modules and libraries. These versions include one based on Microsoft Excel (Office 365 version / Excel v16 recommended; tested on Excel 2011 and 2013) and a version that uses a web browser and does not require any software installation. The focus of the Excel version is customization and editable estimation logic, while the focus of the web version is ease of use and powerful visualizations. The web tool is written in JavaScript ES6 (ECMAScript 2015) and built with modern web technologies (e.g. Node JS, Node Package Manager (NPM), JavaScript Package Manager (JSPM), Aurelia, and Babel). Interactivity is added through the combination of modern data binding, an event-driven user interface, and charts designed with D3 and the Plotly API.

Note: the web version stores all user-entered content (estimates and libraries) locally in the browser used to access the tool. While the browser will check the CatCost website for an updated version of the tool each time it is run, no user-entered information is transmitted to or stored on CatCost/ChemCatBio web servers. No data entered, proprietary or otherwise, is transmitted to to CatCost, ChemCatBio, or the Data Hub. It is important to note that this means that in order to retrieve previously entered estimates or library entries, the same browser used to build them must be used, or the information must be downloaded as a JSON file. The user is therefore advised to back up their estimates and libraries using CatCost's import and export features as described in Chapter 10.

1.5 Version History

This is the first public version (1.0.0) of CatCost. As improvements and additions are made in future versions, a version history including a concise description of changes will be provided in this section of the documentation.

2 Accuracy, Sensitivity, and Scenario Analysis

The accuracy of estimates made using CatCost is highly dependent on the quality of the input information provided by users and on the relevance of its methods to the real industrial manufacturing procedures for a given material. The latter consideration of relevance means that CatCost estimates on established catalyst types such as zeolites will have a known and higher level of cost accuracy than estimates on pre-commercial materials for which the industrial synthesis procedures may not yet exist. For relatively established catalyst types using the CapEx & OpEx Factors method described in Chapter 7, CatCost estimates can be considered to fall into the "preliminary" or "study-grade" level of estimates as described in cost estimating literature.[5,6] This level is associated with an accuracy on the order of ± 15 % up to ± 40 %. However, *no warranty is made* as to the accuracy of CatCost estimates. The user is advised to focus on insights, such as identification of "problem" steps or materials for targeted R&D, the effect of process improvements, or comparisons between materials, rather than obtaining a single number. Overall, the philosophy of CatCost is to quickly provide estimates that are accurate for R&D decisions, while including flexible estimating techniques that power users can apply to customize and improve estimates.

Power users interested in obtaining greater accuracy are encouraged to customize CatCost estimates, for example replacing capital and operating factors from textbook sources with their own proprietary data. The Excel version is specifically designed for customization; while some sections of the workbook have been protected to reduce mishaps, there is no password and users should feel free to adjust the formulas and methods to adapt CatCost to their needs.

Sensitivity or scenario analysis, in which the effect of various input uncertainties (e.g. a range of possible prices for a raw material) on the uncertainty in overall outcomes (catalyst price), is a key tool in developing quantitative cost insight. In version 1.0.0, sensitivity analysis has been partially implemented in CatCost by inclusion of sensitivity input fields – for many inputs in CatCost, the user may enter not just a Base scenario value but also a Low and High scenario. In Excel, these inputs may be shown by use of +/− icons at the top of the screen along with dark red text indicating the presence of sensitivity inputs that can be expanded. In the web version, the sensitivity inputs may be shown or hidden using the "Edit" mode selector at the top right of the browser window, from which either "Simplified" or "Sensitivity Analysis" mode can be selected. The "Edit" mode selector also shows which mode is currently selected. The macros and tools that allow the effect of each sensitivity input on the bottom line catalyst cost to be evaluated will be added in a later version of CatCost. For now, only the Base scenario is used.

3 Global Inputs and Price Scaling: The *"1 Inputs"* Module and the *ChemPPI, CEPCI,* and *UnitConv* Libraries

The "1 Inputs" module contains basic parameters that are used throughout CatCost to perform an estimate. These parameters include an estimate name, basis year, and output mass unit in "Global Inputs," as well as some processing cost inputs. The Basis Year instructs CatCost to determine the cost to produce catalyst in that year, using cost indices to escalate the various cost components in CatCost's libraries to match costs in that year. Some users may simply want to choose the current year for their estimate (years 1984–2018 are selectable in v1.0.0), while others may want to choose a specific year to match other technoeconomic analyses or a government analysis standard, and still others may want to compare to historical price data. See below for more details on the cost escalation methods. The Output Mass Unit determines what unit to use for unit prices (e.g. $0.70/kg catalyst) and also sets the units of other input fields throughout CatCost. Processing Cost Estimation Inputs on "1 Inputs" are described in Chapter 5.

Note: Using the other modules without first completing "1 Inputs" will give unexpected results. Furthermore, the interpretation of information entered later on in a catalyst estimate depends on entries in "1 Inputs"; therefore, if settings on "1 Inputs" are made after entering information in later modules, the user is advised to check over the estimate carefully. For example, if the user selects an Output Mass Unit of "kg," the Catalyst Mass field on "2 Materials" will have units of kg as well. If the user then enters 1.5 kg for Catalyst Mass on "2 Materials" but then changes the Output Mass Unit to "ton," CatCost will interpret the Catalyst Mass as 1.5 ton instead of the 1.5 kg the user intended.

Cost escalation in CatCost is accomplished using two cost indices: the U.S. Bureau of Labor Statistics Chemical Producer Price Index,[7] incorporated in CatCost as the "ChemPPI" library, and the *Chemical Engineering* Plant Cost Index, available from *Chemical Engineering* magazine and other sources[8] and incorporated in CatCost as the "CEPCI" library.

Automated unit conversions are also incorporated into CatCost using the "UnitConv" library, which allows quantities like raw materials consumption in the synthesis to be entered naturally and automatically converted by the tool.

As time passes from the date a CatCost version has been released, some information must be updated for the tool to remain functional. We will attempt to update each of these items in future maintenance releases but the user is encouraged to check them when performing an estimate:

- ChemPPI and CEPCI must be updated in order to accommodate price entries and selection of a basis year (for v1.0.0, the years 1984–2018 are included)
- The direct labor rate on "3e OpEx" must match current conditions
- The factors on "3d CapEx" & "3e OpEx" should be relevant for many years, but may be updated as industry conditions change
- Libraries like the Step Library, Equipment Library, and Spent Catalyst Library should be robust on the order of 10 years (and are scaled via the appropriate price index to whatever basis year is selected) but should be checked by the user and/or updated with new information from textbooks, publications, etc.

4 Materials Costs: The *"2 Materials"* Module and *Materials Library*

4.1 The "2 Materials" Module and "Materials Library"

The "2 Materials" module of CatCost, coupled with the Materials Library, allows the convenient addition of raw materials to an estimate. This module allows the selection of a material from the library, conversion of units, and automatic stoichiometric and cost calculations. The first step to entering a synthesis into the "2 Materials" module is to define the scale by completing the fields in the "Materials Calculation Inputs" section of the module that include the stoichiometric parameters of a synthesis (Figure 4.1). The first input, "Yield Type," has three possible values: "% Yield," "Catalyst Mass," or "AP [Active Phase] Mass." Depending on this selection, the user enters either a % yield or a mass yield of catalyst or active phase in the next input cell. For the "% Yield" option, a molecular weight for the active phase and a stoichiometric ratio of the mols of active phase per mol of metal precursor must also be entered. The "% Yield" option assumes that the combined molar quantity of metal precursors entered into the synthesis comprise the limiting reagent. Next, the user enters the "Active Phase Weight Percent." The last input on the Materials Calculation Inputs is "Losses Due to Waste/Spoilage," which accounts for inevitable losses during storage and handling.

Figure 4.1. The "2 Materials" module in the Excel version of CatCost, showing the entry of stoichiometric parameters and individual raw materials with automated unit conversions and lookups from the Materials Library.

The user may then proceed to add materials to the estimate by selecting an empty cell in the "Material Name" column of "Metal Sources," "Supports," or "Other Materials" and using the dropdown button to select a material from the Materials Library. The user then enters a consumption for that material by typing both a quantity and a unit, which will automatically be converted to the estimate mass units. If a volume unit is entered but the Materials Library does not contain a density for that material, the calculation will fail with a "No Density" message.

The Materials Library of CatCost includes a large library of high-volume chemicals obtained from the ICIS Indicative Price Library. The Materials Library is designed to allow users to easily add new materials by adding a row to the table. Input fields in the Materials Library include the following (see notes in *italic text*):

- Material Name
- Material Type – *used for record-keeping only in v1.0.0*
- Molecular Weight (MW), g/mol – *used in stoichiometry calculations on "2 Materials"*
- Density (g/mL) – *used for unit conversions on "2 Materials"*
- Concentration (%) – *for record-keeping only in v1.0.0*
- Lab-Scale Log Fit? – *if "Lab" is selected, a lab-scale log fit is performed*
- Lab-Scale Columns – *show/hide using +/– at top*
  - Lab Quantity 1–4 – *must use same units, entered in "Lab Units"*
  - Lab Units
  - Lab Price 1–4 – *this is a <u>total</u> price, i.e. the price for the quantity of the material specified in the corresponding Lab Quantity column, <u>not</u> a unit price*
- Bulk Quote Price
- Bulk Quote Quantity
- Bulk Quote Units
- Quote Year – *used for price escalation to the estimate basis year*
- Quote Source
- Quote Access Date – *used for record-keeping only*
- Notes

Making selections and entries in these fields allows the Materials Library to automatically perform unit and price calculations. Users are encouraged to add their own materials to the library and to consider keeping their own "master copy" of CatCost with a library of materials appropriate to their estimates. For more details on the calculations performed by CatCost in "2 Materials" and the Materials Library, see the following sections.

4.2 Materials Consumption

Materials consumption calculations in CatCost rely on information from the pre-commercial or lab-scale synthesis of the catalyst of interest. The user supplies the lab-scale quantity of each reagent.

This laboratory-scale reaction stoichiometry serves as the basis of a materials balance and is scaled by CatCost to user-specified quantities. CatCost employs information about the yield and stoichiometry of the synthesis of interest to determine the scaling factor required to convert the user-input lab-scale quantities to the targeted plant design scale in mass units (M_{cat}; capital letters indicate plant design scale). The required information includes the reaction yield (*yield*), the stoichiometric ratio of the active phase to limiting reagent (mol_{AP}/mol_{LR}) in the balanced reaction formula (e.g. synthesis of Mo_2C from a reaction-limiting monometallic Mo precursor would have $mol_{AP}/mol_{LR} = 0.5$), and the molecular weights of both the limiting reagent (MW_{LR}) and the catalyst active phase as formulated in the balanced reaction formula (MW_{AP}). These inputs allow determination of the active-phase mass at lab scale (m_{AP}) (eq 4.1).

$$m_{AP} = \frac{m_{LR}}{MW_{LR}} \times \left(\frac{mol_{AP}}{mol_{LR}}\right) \times MW_{AP} \times yield \tag{4.1}$$

The total catalyst mass at lab scale (m_{cat}) can then be defined as the sum of the contributions of the active phase (m_{AP}) and the support material (m_{sup}) (eq 4.2).

$$m_{cat} = m_{AP} + m_{sup} \tag{4.2}$$

While the user may supply the mass of support material, if the supporting operation that generates the finished catalyst is assumed to be efficient (100% yield with no discarded support material or active phase), the m_{sup} can be restrained using the user-input weight percent loading ($wt\%$) of active phase in the catalyst (eq 4.3).

$$m_{sup} = \left(\frac{m_{AP}}{wt\%/100}\right) - m_{AP} \tag{4.3}$$

The scaling factor (k_{SF}) is then defined using the lab-scale (m_{cat}) and plant design scale (M_{cat}) catalyst mass quantities (eq 4.4).

$$k_{SF} = \frac{M_{cat}}{m_{cat}} \tag{4.4}$$

Each material's consumption (in any unit) at lab scale can then be scaled to the plant design scale in the same unit by multiplication with the (unitless or year^{-1}) scaling factor.

4.3 Materials Pricing

When planning catalyst manufacture, the best source for a raw material price is a quote from a credible supplier matching the characteristics of the actual purchase arrangement (e.g. quantity, purity, order frequency, delivery method, and location) most probable for the proposed plant. However, because many of these factors will be uncertain at the time of inquiry and suppliers may be reluctant to undertake the cost of a detailed estimate for a hypothetical purchasing plant that is very early in the design process, such price quotes may be difficult to obtain. Many CatCost users also lack access to in-house price databases used at catalyst companies for cost estimation.

Accordingly, freely available bulk pricing, industry catalog data, and, where necessary, extrapolation from lab-scale supplier pricing, are important for simple and rapid catalyst cost estimates. Among these methods, bulk prices ("bulk" scale is considered to be ≥ one ton) available on marketplace websites such as Alibaba may be useful because they already incorporate the best current market information. However, they may be systematically higher than the final settlement price of a transaction after negotiation.[9] When available, proprietary databases like the Process Economics Program (PEP) provided via subscription by IHS Markit Ltd are often useful. CatCost contains freely available prices from the ICIS Chemical Business catalog provided by the RELX Group.[10] In general, these databases do not include a comprehensive list of specialty chemicals and are especially lacking in the areas of inorganic and organometallic chemicals. In cases where none of the aforementioned databases provides a credible price, the final two raw materials cost estimation methods, extrapolation from lab scale and in-house synthesis, can be used.
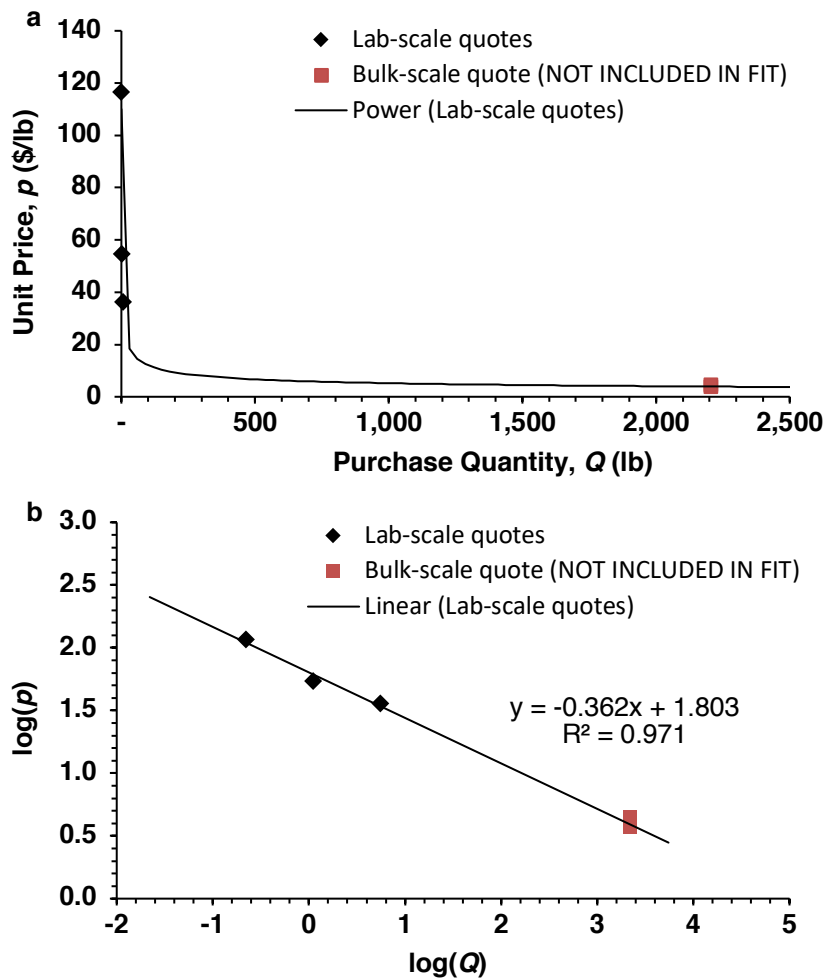
The first method employed for estimation of the cost of raw materials without bulk pricing information is extrapolation from lab-scale pricing. While lab-scale chemical supplier pricing reflects specific investment in that supply scale and order quantity[1] and is therefore not ideal for bulk price prediction, it has the advantage of ready availability on supplier websites. Furthermore, previous work by researchers at LBNL[9] has established suitable parameters and conditions under which this method provides acceptable accuracy in predicting bulk unit prices.

In the extrapolation method for bulk cost estimation, multiple lab-scale prices are fit to a power function (eq 5) relating the unit price p (obtained by dividing the quote price P by quote quantity Q) to quantity Q with two parameters. Using the terminology proposed by the authors of the LBNL report,[9] these parameters are the quantity discount factor (γ) and scaling parameter (b). In practice, fitting is done by log-log linear regression to p and Q data points, which yields γ as the fit slope and b as the fit intercept.

$$p(Q) = b \times Q^{\gamma} \tag{4.5}$$

An example of log-log regression fitting for a common metal precursor is shown in Figure 4.2. A series of price quotes from Acros Organics (through Fisher Scientific)[11] for nickel(II) acetate tetrahydrate in quantities ranging from 100 g to 2.5 kg was used to extrapolate the price of bulk $Ni(OAc)_2 \cdot 4H_2O$. The linear regression was performed on $\log_{10}(p)$ ($p = P/Q$) vs. $\log_{10}(Q)$ and produced $\gamma = -0.363$, $b = 1.803$, and $p(2{,}000 \text{ lb}) = 4.04$ \$/lb. This calculated bulk price compares favorably to an independently obtained bulk price quote from Alibaba,[12] which was not included in the linear regression. The bulk price quote lists \$8,250–10,000/tonne for $Ni(OAc)_2 \cdot 4H_2O$, which is equivalent to $p = 3.74$–4.54 \$/lb. A plot of p vs. Q for the lab- and bulk-scale price quotes, including the calculated $p(Q)$ trendline, is shown in Figure 4.2a. The same information is shown in Figure 4.2b with logarithmic axes, and the details of the calculation are tabulated in Figure 4.2c.

The second method for estimation of raw material costs in the absence of bulk pricing data is an in-house synthesis approach. Without assuming that the raw material would actually be produced in the catalyst synthesis plant through a sub-process, the method of breaking down a raw material into its own synthetic feedstocks and processing steps (using the methods described throughout this section) provides an alternative method of estimation when no other information is available. This approach requires knowledge of likely synthetic routes to the raw material of interest, as well as pricing information for the sub-process inputs.

Figure 4.2. Log-log linear regression fit to lab-scale price quote data (2016) for Ni(OAc)$_2$•4H$_2$O: a) plot of p vs. Q including indicative power fit, b) log-log plot of p vs. Q including linear regression fit showing agreement with bulk price quote (red), and c) details of price data and linear fit.

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

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

5 Processing Costs: General Comments and Estimation Parameters on *"1 Inputs"*

5.1 Two Methods for Processing Cost Estimation

CatCost contains two distinct methods for estimating "processing" costs in a catalyst synthesis. Processing costs can be understood to include all non-materials costs of an industrial synthesis, including capital equipment purchase and ongoing maintenance, plant design and construction, land purchase and upkeep, labor, process utilities, and other components of capital and operating costs. Estimating processing costs is the most complex and difficult part of assembling a catalyst cost estimate. In order to provide flexibility to users, CatCost includes two distinct approaches to estimating processing costs. These two approaches, the Step Method and the CapEx & OpEx Factors Method, are summarized below. All estimation methods assume production in the United States with respect to environmental regulations, default entries for regionally varying costs such as operating labor, and other aspects of production.

Step Method *(note: Excel version only in CatCost v1.0.0)*
- Assumes production at a contract catalyst manufacturer ("toller")
- Uses all-in hourly costs of operation in $/hour
- Requires a list of process steps and an order size in tons
- Based on methods used by tollers to provide price quotes
- Provides rapid estimates
- Modules: "3a Step Method"

CapEx & OpEx Factors Method
- Assumes construction of a new, dedicated catalyst plant for catalyst synthesis
- Uses detailed estimation of "primary" costs and fixed percentages for "secondary" costs
- Requires a list of process equipment including sizes, quantities, materials of construction, and auxiliary equipment such as pumps and motors, as well as process utilities consumption, and a production scale (e.g. kg/year)
- Based on estimating methods from the chemical engineering process design literature
- Provides detailed estimates that require more time and specialized knowledge to prepare
- Modules: "3b Equipment," "3c Utilities," "3d CapEx," and "3e OpEx"

Within CatCost, these two distinct methods are implemented separately as noted in the "Modules" bullets in the list above. When choosing a processing cost estimation method, the user should then complete only those modules listed for that method above. CatCost also allows the user to use both methods in a single estimate, for example using the convenience of the Step Method to evaluate the addition of a single process step to an existing process design assembled in CapEx & OpEx Factors. This is accomplished by the inclusion of a "combined outputs" section in the main CatCost outputs, described below. The two methods could also be completed using similar process steps to allow a comparison between them and thus between the scenarios of toller manufacturing and new-build synthesis plant. ***If combining the two methods (rather than comparing them), it is critical that no process step be entered in both methods, or this will overestimate the cost of producing***

catalyst (i.e. if a synthesis has 5 steps and steps #4 and #5 are entered in the Step Method, those steps should NOT be entered in CapEx & OpEx Factors).

Finally, process templates containing all of the necessary inputs for common catalyst types in each method are included in CatCost and described here in Chapter 8. These templates greatly reduce the time required to prepare an estimate for common catalyst types.

5.2   Processing Cost Estimation Inputs on "1 Inputs"

Processing Cost Estimation Inputs on "1 Inputs" set overall parameters that are used throughout CatCost. The inputs primarily concern the scale of catalyst synthesis in CatCost (Figure 5.1). The Step Method Inputs in this module include an order size in tons (values in the range of 1–1000 tons are accepted), which generates outputs including equipment size, synthesis campaign length, and selling margin as described in Chapter 6, as well as the values for several overhead items. The inputs for the CapEx & OpEx Factors method in this module include "Design Production, Annual" and a "Capacity Factor" in % which increases or reduces this value to obtain the "Actual Production, Annual." Both of these production items have units of catalyst mass per year (e.g. 1 million lb catalyst per year). The difference is that the "Design Production" is what is used to size the catalyst plant for construction, while the "Actual Production" refers to the actual amount of catalyst obtained once the plant begins operation and is used to determine operating costs and the allocation of capital costs. "Operating Hours (Labor)" should generally be set to 8760 hours (24/7 operation) as this sets the operating labor requirements. This indicates that the plant is staffed constantly. However, it is not producing catalyst at all times due to both planned and unplanned downtime, and this is accounted for by the "On-Stream Factor," which reduces the "Operating Hours (Labor)" to obtain the "Operating Hours, Production," the number of hours in which catalyst is actually produced. CatCost automatically computes a "Design Production Rate" that is used to scale equipment from a user-entered design or process template to the user's selection for the estimate's "Design Production, Annual." Finally, the user enters a "Plant Life" to allocate capital costs over the entire output of the plant (note: hard-coded as 10 years in web tool v1.0.0), as well as selecting either a pre-tax return on capital investment, flat margin (% of costs; not included in web tool v1.0.0), or both to determine a selling margin for the catalyst. For details on the implications of these inputs, please see the following chapters on processing cost in CatCost.

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)	200	ton	
Equipment size	Large (150 ton/day)		
Synthesis time	1.3	days	
Cleaning time	1.0	days	
Total: Synthesis campaign length	2.3	days	

Overhead and Selling Margin			
G&A Overhead	5	%	?
SARD Overhead	5	%	?
Selling Margin	13.4	%	?

CapEx & OpEx Factors Inputs

Production Capacity - Catalyst	Base		
Design Production, Annual	1.00E+07		?
Capacity Factor	100	%	?
Actual Production, Annual	1.00E+07		?

Production Capacity - Operating Hours			
Operating Hours (Labor)	8760	hours	?
On-Stream Factor	90	%	?
Operating Hours (Production)	7884	hours	?
Design Production Rate	1.27E+03		?

Plant Life			
Plant Life (for depreciation)	10	years	?

Selling Margin		
Calculate using (select):	ROI	
Return on capital invested (pre-tax)	25	%/yr
Flat margin (% of costs)		%

Figure 5.1. Processing Cost Estimation Inputs on "1 Inputs" within CatCost. These inputs primarily concern scale of catalyst synthesis.

6 Processing Costs via a Simplified Step Method: The *"3a Step Method"* Module

6.1 Overview and "3a Step Method"

NOTE: In CatCost v1.0.0, the Step Method is included in the Excel version only. It will be added to the web version in a future release.

The step method included in CatCost uses a simplified approach to processing cost estimation, in which all capital and operating costs associated with a particular process step (e.g. spray dryer, rotary vacuum filter, extruder) are captured in a single hourly cost at a specified production scale. This includes ancillary equipment for a process unit, such as pumps and motors. This approach is both attractive in its simplicity and highly relevant to real industrial conditions, as it is based on the procedures used by contract manufacturers of catalysts to provide price quotes for their services. The step method assumes that existing process equipment at a contract manufacturer (toller) is used to produce the catalyst, in contrast to the CapEx & OpEx Factors Method described later. The step method can be used on its own to assemble a complete synthesis process in CatCost, or as a way to rapidly add a step to an existing process design in the CapEx and OpEx Factors Method.

The "3a Step Method" module is quite simple. The user can choose a process template from a list of over 10 (described in Chapter 8) or enter a custom process. If entering a custom process or editing a process template, the user simply selects process steps from the available list. Some process steps will not be available at the synthesis scale (Small, Medium, or Large) that has automatically been chosen for the user-entered order size on "1 Inputs"; CatCost will suggest an alternate step in those cases. For each step, the tool will then automatically look up the correct hourly cost for each step and compute the campaign cost and cost per unit of catalyst. For more details on the basis for the Step Method, see the following sections or read the full publication.[13]

6.2 Background

The production costs for a novel catalyst may be estimated rapidly using a step-based method in which individual processing steps, corresponding to specific process equipment used by a contract manufacturer of catalysts, are selected from an established list. This estimation method and the names and costs of individual steps are based upon those used by contract catalyst manufacturers to provide price quotes for their paid manufacturing services. Each step corresponds to a process equipment unit at a particular scale and includes all capital and operating costs, such as equipment purchase, maintenance, operating labor, and utilities. A step-based approach to estimating the cost of catalyst manufacture enables researchers with minimal process design experience to successfully execute an estimate using an appropriate list of process equipment units that approximate a laboratory-scale synthesis.

For example, consider a synthetic chemist who has developed an improved catalyst synthesis that is based on an existing process, but requires an additional reaction step that has been successfully executed at the laboratory scale in a small autoclave. Determining the cost of the new process at industrial scale including this additional step would previously have required working with an

engineer who can properly size the reactor for large-scale production and price any new materials needed. The engineer would determine the cost to operate this reactor in an existing plant of appropriate size and provide the chemist the cost of new materials and the new production step (e.g. \$0.10/kg product). The researchers then determine whether the improved quality/performance or yield of catalyst achieved by adding this step is justified and, if so, proceed with developing a proposal for management approval. The step method detailed herein simplifies this process by providing a pre-determined list of common process steps for catalyst order quantities in the range of 1–1000 tons. This method can then be used by a researcher or team that does not have access to process design expertise, or with greater speed and accuracy by a team that does.

6.3 Preparing a Step Method Estimate

6.3.1 Inputs

A price estimate using the step method requires information on both the catalyst synthesis (Synthesis Inputs) and the market or application it will be used in (Business Inputs), as shown in Figure 6.1. This discussion will begin with Synthesis Inputs, which are based on a lab-scale synthetic procedure developed by the researcher or obtained from the literature.[14]

The step method presented herein relies on the assumption that the synthetic procedure translates readily into steps that are well known by the catalyst manufacturing industry.

6.3.2 Synthesis Inputs

The Synthesis Inputs include catalyst composition and preparation stoichiometry, raw materials consumption and pricing, and synthetic steps. Composition, preparation stoichiometry, and materials pricing are obtained as described above. Finally, the selection of industrially relevant process steps using the step method is conducted to complete the cost estimation.
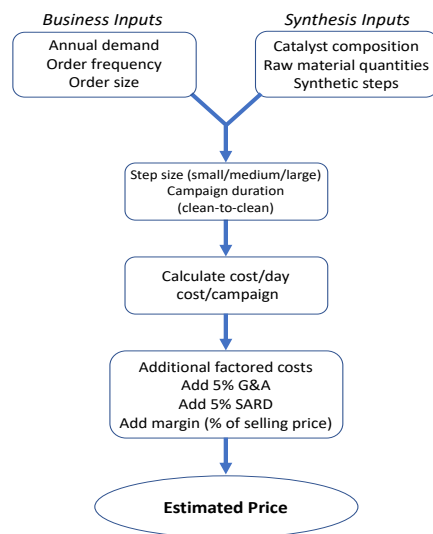
Figure 6.1. Flow of information in the step method from inputs to an estimated price.

The laboratory-scale synthetic procedure to prepare the catalyst serves as the basis for translation into industrially relevant process steps. A list of process steps and associated hourly costs for process equipment units commonly used in commercial catalyst synthesis is provided in Table 6.1. A user of the step method begins by selecting steps from this list that correspond to the synthesis steps used for their material at lab scale. Price estimates for three catalysts including Pt/C, Ni/Al$_2$O$_3$, and a modern fluid catalytic cracking (FCC) catalyst based on ultrastable zeolite Y (USY) were assembled using steps from Table 6.1 and are discussed below as part of the validation of the step method.

Table 6.1. Synthesis steps and hourly costs available in the step method.[a]

Step Name	Costs ($/hour)[b]			Substitute Step[c]
	Small (1 t/d)	Medium (10 t/d)	Large (150 t/d)	
Ball forming	100	150	—	
Crystallizer	100	200	300	
Dryer, batch vacuum tray	50	—	—	Rotary dryer
Dryer, rotary (40–100 °C)	75	100	200	
Dryer, rotary (100–300 °C)	100	150	300	
Dryer, spray	—	300	550	Rotary dryer
Extruder, with feeder	100	200	425	
Filter, belt vacuum	125	175	400	
Filter, plate and frame	75	—	—	Belt/rotary vacuum filter
Filter, rotary vacuum	—	100	300	Plate and frame filter
Flare	50	75	150	
Incipient wetness (impregnation)	75	100	200	
Kiln, batch (300–1290 °C)	75	—	—	Continuous kiln
Kiln, continuous direct (300–1290 °C)	—	225	400	Batch kiln
Kiln, continuous indirect (300–1290 °C)	—	175	325	Batch kiln
Mill	50	100	200	
Mixer, dry blender	50	100	200	
Mixer, slurry	75	100	200	
Reactor, simple (mixing)	30	60	200	
Reactor, multistep	100	175	600	
Scrubber, NO$_x$	35	75	200	

[a]Costs use a mid-2017 basis in the United States. [b]Hourly costs of operation ($/hour) for process equipment at small, medium, and large scale. Cleaning costs have the same hourly rate as operation. Dashes indicate that that step / process equipment unit is not commonly used at the specified scale; see substitute column for suggested alternative. These costs assume a 24-hour day. [c]For synthesis scale(s) at which that step is unavailable, indicated by a dash.

6.3.3 Business Inputs

For an accurate estimate, the Synthesis Inputs must be coupled with Business Inputs that consider the effect on price of intended catalyst use. The key business input to the step method is order size, which depends on knowledge of the catalytic application including catalyst charge, lifetime, order frequency, and any other factor affecting catalyst demand. In this way, the accuracy of the step method depends on testing[15] and technoeconomic analysis information on the catalyst and its application. In general, an economically viable catalyst will have a lifetime of at least 6–12 months, but because it is common practice to run multiple reactors in parallel and stagger catalyst replacement, the catalyst order frequency may not be equivalent to catalyst lifetime. A typical non-precious metal containing catalyst would be ordered twice per year. Catalysts containing gold, silver, or a platinum group metal (PGM) are typically ordered four times per year to minimize the cost of on-site and in-the-loop catalyst inventory.[16] From all this information the order size and frequency can be determined for the catalyst of interest. If ordering the catalyst from a contract manufacturer, the customer would provide this order size and frequency to the contract manufacturer or toller, who would then develop a price quote for a synthesis "campaign" to produce each order. In the step method described here, only the order size, in the range of 1–1000 tons, is needed to determine a price.

A step size (in tons/day) and campaign length can then be determined based on the desired order size. Determining the campaign length starts with selecting a synthesis scale, because a contract manufacturer has existing equipment at specific scales to choose from. These scales are defined here as Small (1 ton/day), Medium (10 tons/day), and Large (150 tons/day). The Small scale is used for 1–5 ton orders, the Medium scale for 5–70 ton orders, and the Large scale for 70–1000 ton orders. Determining the campaign length is then as simple as dividing the order size (tons) by the appropriate production scale (tons/day) and adding time for cleaning (0.5 days for Small; 1 day for Medium/Large). Standard protocol in the industry dictates that equipment is clean at the start and end of each campaign. Cleaning time is charged at the same rate as operating time because the requirements (operators, utilities, etc.) are similar. This entire process is depicted graphically in Figure 6.2.
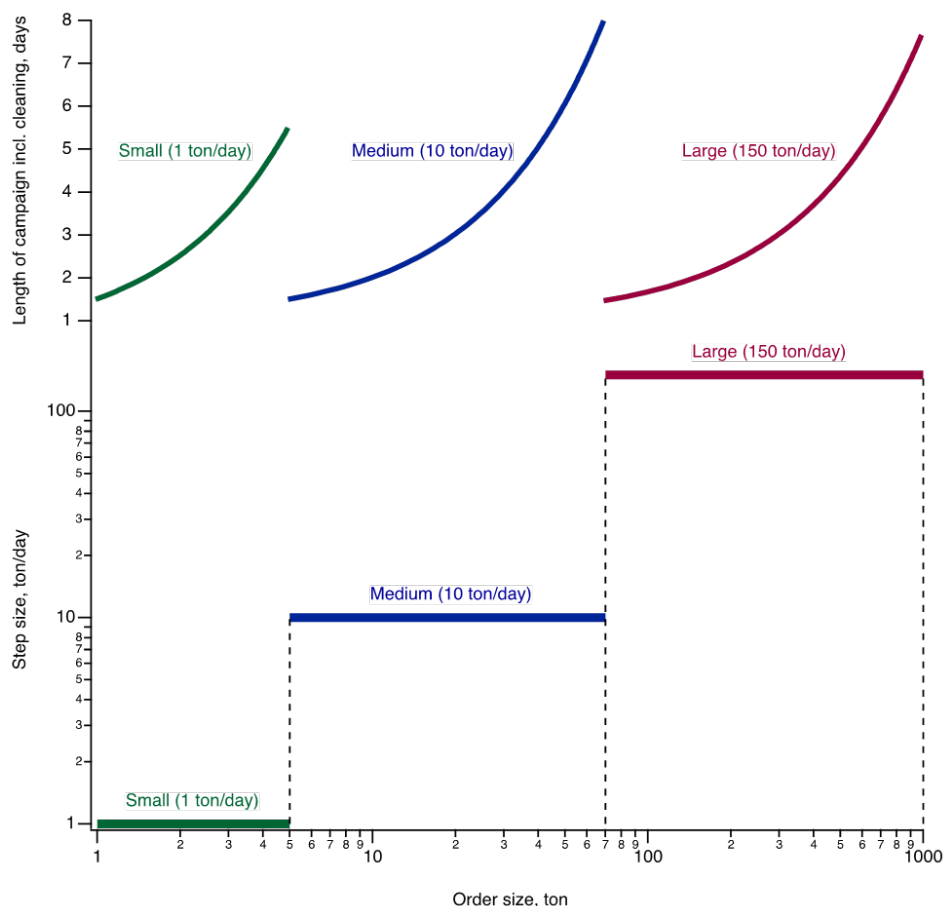
Figure 6.2. Step size (bottom, ton/day) and campaign length including cleaning (top, days) as a function of order size (tons), assuming 24-hour operation. Cleaning time is 0.5 days for Small and 1 day for Medium/Large.

6.3.4 Total Campaign Cost, Overhead, and Selling Margin

Having determined the production scale and campaign length, the hourly production cost is then calculated. Using the list of steps selected from Table 6.1 at the appropriate production scale (Small, Medium, or Large), the corresponding hourly costs are then added to determine a total hourly operating cost for the entire process. The costs in Table 6.1 are inclusive of all operating and capital costs including operating labor, maintenance, utilities, etc., and were determined through discussions with industry experts as well as literature review.[17] The costs have a mid-2017 basis assuming production in the United States. For escalation of these costs to other estimate basis years, the "ChemPPI" library is used. Note that because all the process equipment used in a synthesis is devoted to that customer's order throughout the campaign including cleaning, the hourly cost is constant for each unit/step. For steps in Table 6.1 that are not available at a particular production scale (e.g. a spray dryer at small scale), the alternative step suggested in the Substitute column may be selected instead. Using a 24-hour day, the daily production cost can then be calculated and multiplied by the campaign length in days to determine a total production cost for the next step in the catalyst price estimation process.

The final step of developing a catalyst price estimate using the step method is to add overhead costs and a selling margin. The raw materials and synthesis step costs are first added together as a subtotal. Then General and Administrative (G&A) costs are calculated as 5% of this subtotal, and Sales, Administrative, Research and Distribution (SARD) of 5% of both the subtotal and G&A.[4,8] Note that distribution entails loading the product on a dock at the catalyst production site; the customer pays the freight. For the purposes of a step method estimate, the selling margin can be considered solely as a function of the order size. In the corresponding author's experience with commercial catalyst manufacture, a single relationship between the selling margin and order size applies to a large majority of catalyst types, including but not limited to supported PGM, supported base metals, and metal oxides. As the order size increases, the margin decreases from ca. 33% of the selling price (50% of pre-margin costs) at the 2-ton scale to ca. 8% of the selling price at the 1000-ton scale, following a linear relationship between the logarithms of order size and margin (Figure 6.3). Note that the raw materials costs are generally included in the overhead and selling margin calculations because the contract manufacturer assumes the expense and risk of procuring the raw materials to meet the specifications and timeline of the catalyst purchaser. However, the costs of any noble metals would be excluded from the overhead and margin because they are provided by the catalyst user's pool account or offset by recoverable metals content.[16]

Margin (% of selling price) ≈ 39.192*(Order size, ton)^-0.23360

Margin (% of pre-margin costs) ≈ 60.976*(Order size, ton)^-0.28632
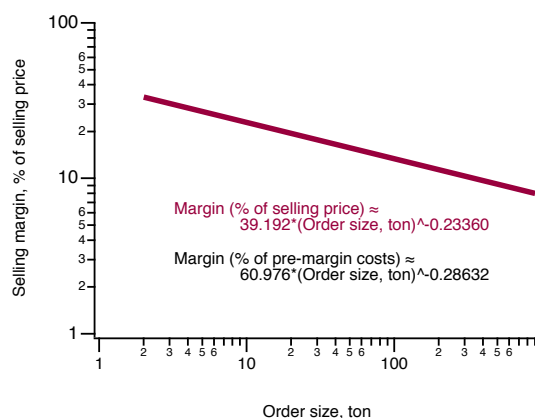
Figure 6.3. Selling margin (% of selling price) as a function of order size (ton).

6.4 Step Method Demonstration and Verification with Market Price Data

6.4.1 Catalyst Price Assessment: Pt/C

Using the procedures described in the previous section, the following example demonstrates the execution of the step method to estimate the price of a 2 wt. % Pt/C catalyst. This estimate uses the assumption of a precious metals pool account that is managed separately,[16] so the value of platinum content is excluded.

As described in the Synthesis Inputs section, the first step to estimating the price of the Pt/C catalyst is to determine the raw material requirements, catalyst composition, and synthesis method from the laboratory-scale procedure. In this example case, a researcher seeks to estimate the price of a 2 wt. % Pt/C catalyst that is prepared by wet impregnation of an activated carbon support with chloroplatinic acid (H_2PtCl_6). The price for the chloroplatinic acid does not include the value of Pt; it includes only the price of converting Pt metal to H_2PtCl_6 via oxidation in *aqua regia* because

of the pool account assumption mentioned above. In this procedure, a slurry of the Pt precursor and carbon is chemically reduced by the addition of hydrazine (N_2H_4) at 50 °C. Because the reaction liberates HCl upon reduction, the reaction vessel is fitted with a sodium hydroxide scrubber. The Pt/C material is then filtered and dried at 90–95 °C to remove 50% of the moisture and yield the final catalyst. This procedure was used to populate the raw materials requirements (lb/lb catalyst) shown in Table 6.2. Based on the lab-scale procedure, the industrial-scale process equipment units selected from Table 6.1 include incipient wetness, multistep reactor, scrubber, plate and frame filter, simple reactor, and rotary dryer (40–100 °C).

Proceeding to Business Inputs, the envisioned application of the Pt/C catalyst is a large-scale slurry hydrogenation plant with a hypothetical 8 ton/year catalyst demand. In order to minimize the value of Pt in the precious metals loop (i.e. to reduce inventory),[1616] an order frequency of 4 orders per year was assumed, giving an order size of 2 tons. Using this order size and the relationships illustrated in Figure 6.2, the Small (1 ton/day) scale was selected and the campaign length was determined as 2.5 days, including cleaning. A total campaign cost ($23,400/campaign), not including materials, overhead, or margin, was then calculated by multiplying the step cost total ($390/hr, $9360/day) from Table 6.1 by the campaign length (2.5 days).

Adding the raw materials and synthesis campaign costs gives a subtotal of $16.55/lb catalyst, as shown in Table 6.2. The final step of developing a catalyst price estimate using the step method is to add overhead costs and a selling margin. As described above, G&A (5% of subtotal), SARD (5% of [subtotal + G&A]), and selling margin (50% of [subtotal + G&A + SARD] at the 2 ton scale) are added to yield an estimated selling price of $27.37/lb for this Pt/C catalyst.

6.4.2 Comparison of Three Step Method Catalyst Estimates to Market Prices

Following the procedures outlined in the previous section for 2 wt. % Pt/C, price estimates were developed for 21 wt. % Ni/Al_2O_3 (at 20-ton scale) and a USY-based FCC catalyst with rare earth content (at 200-ton scale). The Ni/Al_2O_3 order size was based on a fixed bed reactor (catalyst charge of 10 tons) with an expected catalyst life of 6–12 months; this first order is intended to fill the reactor and have a spare charge. The FCC catalyst order size was based on 5 ton/day catalyst feed rate at a typical refinery, with 100 days of inventory. The components of these estimates are shown in Table 6.2 along with the Pt/C estimate. The step method-based estimates using the mid-2017 step costs for the three materials compare favorably with market price data,[18] also from mid-2017 in the US, within ± 20% relative to the market prices.

Table 6.2. Step method examples using a mid-2017 cost basis: Pt/C, Ni/Al₂O₃, and USY-based FCC catalysts.

Pt/C (2 wt. %)				Ni/Al$_2$O$_3$ (21 wt. %)				USY-based FCC with rare earth			
Materials Costs[a]				**Materials Costs**				**Materials Costs**			
Material	$/lb	lb/lb cat.	$/lb cat.	Material	$/lb	lb/lb cat.	$/lb cat.	Material	$/lb	lb/lb cat.	$/lb cat.
H$_2$PtCl$_6$	10.00	0.053	0.53	Ni(NO$_3$)$_2$·6H$_2$O	2.50	1.04	2.59	Ludox sodium silicate	0.25	0.819	0.205
Carbon support	9.09	1	9.09	Alumina (trilobes)	11.00	0.79	8.69	Al(OH)$_3$	0.3	0.14	0.042
N$_2$H$_4$	0.68	0.26	0.18	NaOH 50%	0.20	0.28	0.06	NaOH 50%	0.2	0.074	0.015
NaOH	0.18	0.025	0.00	H$_2$O$_2$ 50%	0.34	0.12	0.04	H$_2$SO$_4$ 98%	0.05	0.22	0.011
NaCl disposal	0.09	10	0.90	NaNO$_3$ landfill	0.50	0.02	0.01	Clay	0.05	0.376	0.019
Total			**10.70**	H2 forming gas	1.10	0.45	0.50	La$_2$O$_3$	1.5	0.035	0.053
				Total			**11.88**	HCl 31%	0.07	0.036	0.003
								NH$_4$OH 28%	0.1	0.06	0.006
								Total			**0.352**

Step Costs			**Step Costs**			**Step Costs**		
Step	$/hr	$/day	Step	$/hr	$/day	Step	$/hr	$/day
Incipient wetness	75	1800	Incipient wetness	100	2400	Reactor, simple	200	4800
Reactor, multistep	100	2400	Dryer, rotary (40–100 ℃)	100	2400	Crystallizer	300	7200
Scrubber, NOx	35	840	Kiln, continuous indirect (300–1290 ℃)	175	4200	Filter, rotary vacuum × 2	600	14400
Filter, plate and frame	75	1800	Scrubber, NOx	75	1800	Reactor, simple × 3	600	14400
Reactor, simple	30	720	Crystallizer	200	4800	Kiln, continuous indirect (300–1290 ℃)	325	7800
Dryer, rotary (40–100 ℃)	75	1800	Filter, rotary vacuum	100	2400	Reactor, multistep	600	14400
Total	**390**	**9360**	Dryer, rotary (40–100 ℃)	100	2400	Filter, rotary vacuum	300	7200
			Kiln, continuous indirect (300–1290 ℃) × 2	350	8400	Reactor, multistep	600	14400
			Total	**1200**	**28800**	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 ℃)	300	7200
						Total	**6725**	**161400**

Synthesis Campaign Costs		**Synthesis Campaign Costs**		**Synthesis Campaign Costs**	
Order size, tons	2	Order size, tons	20	Order size, tons	200
Production scale	Small (1 ton/day)	Production scale	Medium (10 ton/day)	Production scale	Large (150 ton/day)
Step cost, $/day	9360	Step cost, $/day	28800	Step cost, $/day	161400
Campaign length	2.5	Campaign length	3	Campaign length	4[b]
Campaign cost, $	23400	Campaign cost, $	86400	Campaign cost, $	645600
Campaign cost, $/lb cat.	**5.85**	**Campaign cost, $/lb cat.**	**2.16**	**Campaign cost, $/lb cat.**	**1.61**

Subtotal Before Overhead and Margin		**Subtotal Before Overhead and Margin**		**Subtotal Before Overhead and Margin**	
Materials cost, $/lb cat.	10.70	Materials cost, $/lb cat.	11.88	Materials cost, $/lb cat.	0.35
Campaign cost, $/lb cat.	5.85	Campaign cost, $/lb cat.	2.16	Campaign cost, $/lb cat.	1.61
Subtotal, $/lb cat.	**16.55**	**Subtotal, $/lb cat.**	**14.04**	**Subtotal, $/lb cat.**	**1.97**

Overhead and Margin		**Overhead and Margin**		**Overhead and Margin**	
G&A, $/lb cat.[c]	0.83	G&A, $/lb cat.	0.70	G&A, $/lb cat.	0.10
SARD, $/lb cat.[d]	0.87	SARD, $/lb cat.	0.74	SARD, $/lb cat.	0.10
Margin, $/lb cat[e]	9.12	Margin, $/lb cat[f]	5.11	Margin, $/lb cat[g]	0.24

Total Estimated Price		**Total Estimated Price**		**Total Estimated Price**	
Est. price, $/lb cat.[h]	27.37	Est. price, $/lb cat.	20.59	Est. price, $/lb cat.	2.41

Market Price		**Market Price**		**Market Price**	
Market price, $/lb cat.[a]	34.09	Market price, $/lb cat.	21.33	Market price, $/lb cat.	2.73
Difference	20%	Difference	3%	Difference	12%

[a]Excluding the value of platinum metal content. [b]Because of the complexity of zeolite synthesis, this campaign requires extra ramp-up and ramp-down time leading to an actual production rate of 67 ton/day. [c]General & Administrative costs (5% of subtotal). [d]Sales, Administrative, Research, and Distribution (5% of [subtotal + G&A]). [e]Estimated as 50% of [subtotal + G&A + SARD]. [f]Estimated as 33% of [subtotal + G&A + SARD]. [g]Estimated as 11% of [subtotal + G&A + SARD]. [h]Obtained by adding subtotal + G&A + SARD + Margin.

7 Processing Costs via a Detailed CapEx & OpEx Factors Method: The *"3b Equipment," "3c Utilities," "3d CapEx,"* and *"3e OpEx"* Modules and *Equipment Library*

7.1 Overview

The second approach to processing cost in CatCost is a detailed, factored processing cost estimation method, entitled CapEx & OpEx Factors. This approach, in contrast to the step method, assumes the construction of a dedicated process plant to synthesize the catalyst in question. The CapEx & OpEx Factors method allows significantly more detail and potentially more targeted insight than the step method, but requires more time and specialized knowledge/tools (e.g. AspenPlus) to generate. However, we have reduced these demands dramatically for common catalyst types by inclusion of process templates (Chapter 8).

The potential accuracy and flexibility benefits of a factored processing cost estimate result from the explicit consideration of a wide range of capital and operating components of processing cost. The methods for inclusion in CatCost were identified primarily through review of the process design literature used by chemical engineers for cost estimation. The methods selected for inclusion have been extensively used and validated, which means detailed information is available on the accuracy of each method and the associated error of each component for sensitivity analysis.

In this chapter, the methods are presented first and the implementation of these methods in CatCost is found in the last section.

7.2 Simplifying Estimates with Primary and Secondary Categories

In the process design literature, preliminary cost estimates for a new-build chemical synthesis plant are commonly made using a factored approach. This involves estimating a few components, which we will call "primary" costs, in detail and using factors (i.e. percentages) of the primary components to determine the other, "secondary" components.[4,6,19-23] The primary components commonly include raw materials purchase cost, direct operating labor cost, and equipment purchase cost. The secondary components comprise a wide variety of costs, such as ongoing supervisory labor or capital cost for piping, that tend to vary linearly with a particular primary component, within a known range. The accuracy afforded by this approach is on the order of ± 15 % up to ± 40 % (commonly called "preliminary" or "study-grade" in design literature),[5,6] which is appropriate for inclusion in CatCost.

Following this literature precedent, the procedure for estimating a catalyst cost using CatCost can be defined by three steps: (1) From the lab-scale synthesis procedure, develop a list of unit operations (e.g. jacketed, agitated reactor, spray dryer, ball mill) needed to conduct the synthesis at industrial scale. (2) Using the list of operations and the synthesis information, price primary components such as raw materials purchase cost, delivered-equipment purchase cost, ongoing direct labor, etc. (3) For secondary costs that vary directly with one of the primary outputs, use a factor (i.e. a percentage) to determine those costs from the primary output. This concept is depicted

in Figure 7.1, which shows secondary components of capital cost being determined as factors of the primary component, purchased equipment cost.
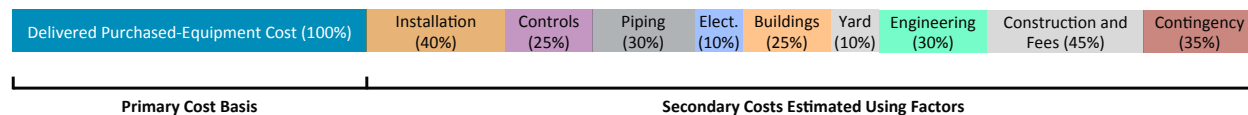
Delivered Purchased-Equipment Cost (100%)	Installation (40%)	Controls (25%)	Piping (30%)	Elect. (10%)	Buildings (25%)	Yard (10%)	Engineering (30%)	Construction and Fees (45%)	Contingency (35%)

Primary Cost Basis   **Secondary Costs Estimated Using Factors**

Figure 7.1. Illustration of the concept of primary cost components such as delivered purchased-equipment cost, calculated in detail for the process being studied, determining secondary cost components as factors (percentages) of the primary component.

7.3 Determining Primary Costs: Capital

Capital cost estimation for process plants begins with pricing each unit of process equipment. Equipment purchase cost is widely estimated by scaling a known price for a similar piece of equipment to the specific size needed in a process.[4,19-23] Rather than scaling linearly, these prices tend to follow power-law relationships (eq 7.1) with 0.6 being a common value for exponent *a*. The specific exponents to use for various pieces of equipment have been tabulated most extensively by Garrett and range from 0.38 to 0.90.[24] This method therefore requires only a valid price quote for each equipment type. For scaling purposes, the size of equipment is typically measured by a flowrate, heat-transfer area, volume, power rating, etc. Some authors have improved the accuracy of the scaling method by incorporating more than one parameter for a particular equipment type.[8,22,25] For example, Ulrich and Vasudevan scale process vessels not by volume alone, but as a function of both height and width to account for the relatively larger material requirements of extreme shapes.[22] It is also common to include factors for the cost of various materials of construction, e.g. carbon steel, stainless steel, aluminum. Importantly, some authors also include an exemplary price quote for each equipment type,[19,24] allowing complete algebraic determination of equipment cost at arbitrary size (within the extrapolation limits of these methods), which is what is needed for incorporation into CatCost.

$$\frac{price_2}{price_1} = \left(\frac{size_2}{size_1}\right)^a \tag{7.1}$$

A number of these equipment pricing methods have been compiled into web- or spreadsheet-based costing tools, most of which also facilitate the calculation of secondary costs (buildings, piping, installation, etc.) based on purchased-equipment cost. A useful review of these pricing tools has been published by Feng and Rangaiah.[25] Thus, there is precedent for the type of equipment costing used in CatCost.

CatCost includes a library of equipment cost correlations to allow the expert user to develop an equipment list and associated capital cost estimate from scratch. This library also forms the basis of the process templates (next chapter) so that users without design experience will be able to simply select a catalyst synthesis type, such as wet impregnation, zeolite, metal-organic framework, etc. and have the equipment list auto-populated.

7.4 Determining Primary Costs: Operating

Direct labor cost is the most common primary component of operating costs in published estimation methods.[4,22,23] Direct labor is defined here as the sum of labor requirements of each process unit. Items like supervisory labor and laboratory / quality assurance are figured as factors of direct labor. Direct labor can be readily calculated for a particular piece of process equipment *i* using the formula in eq 7.2. The (Operator Hours / Equipment Hours)$_i$ variable represents direct labor requirements for that piece of equipment; a value of 1.0 would indicate one full-time operator per process unit; a value of 0.5 would indicate an operator splitting his/her time between two units of this type. The local productivity adjusts the operator/equipment ratio to local labor productivity figures, which vary regionally. Both of these values are available in chemical engineering design texts.[4,22,23] The local hourly labor rate can be freely obtained from the U.S. Bureau of Labor Statistics or corresponding bodies abroad.

$$(Per\text{-}Unit\ Labor\ Cost)_i \ = \ \frac{\left(\frac{Operator\ Hours}{Equipment\ Hours}\right)_i}{(Local\ Productivity)} \ \times \ (Local\ Labor\ Rate) \qquad (7.2)$$

7.5 Determining Secondary Costs with Factors

The third and final step of processing cost estimation, determination of factored or secondary costs, is applied to capital costs using the equipment costs as primary components. There are three general approaches followed in the process design literature for this step. The first is the well-known Lang factor method.[26] In it, the sum of all individual purchased equipment costs is multiplied by a single factor, ranging from 4–5 for today's financial conditions,[4] which is designed to quickly estimate the cost of all other fixed capital components, including installation, piping, buildings, construction fees and labor, etc. (working capital is included separately). This method is not useful for CatCost because its errors are too large and it offers no insight on cost components or sensitivities in the final catalyst cost. The second and third methods add detail to the general approach taken by Lang, but along different dimensions. The second method, which has been described by both Hand[27] and Guthrie,[19] uses factors similar to the Lang factor, but includes one for each piece of equipment. This approach accounts for varying space requirements, installation complexity, etc. for various equipment types and is therefore much more process-specific than the Lang-factor method. However, it does not provide any breakdown of the individual components (e.g. piping) that comprise each process unit's factor. This shortcoming is addressed by the third method. The third method uses a sum of all equipment costs as in the Lang method, making it somewhat less process-specific than the second method. However, it uses separate factors for each component of capital cost, so that the user can see how much, for example, installation labor or insulation contributes to product cost.[4,22,23] This concept is depicted in Figure 7.1 and exemplary factors from two references are shown in Table 7.1. The table displays the slight variation in categories and factor values that is common in the literature. Furthermore, the user can customize the ranges used in the estimation to improve the usefulness of the sensitivity information this method provides. A blended approach combining the second and third methods described here has been incorporated into CatCost, in order to address their respective limitations and provide the best combination of detail and accuracy.

Table 7.1. Determination of secondary cost components from primary components in plant capital cost estimation: exemplary factors from literature.

Capital Cost Factors	Factor – ref. 4 (%)	Factor – ref. 23 (%)
Delivered Purchased-Equipment	100[a]	100[a]
Installation	39–47	30–60
Instrumentation and Controls	18–36	20–30
Piping (installed)	16–68[b]	20–80
Electrical (installed)	10–11	15–20
Buildings	18–25	15–30
Yard Improvements	10–15	20–30
Service Facilities	40–70	30–40
Engineering and Supervision	32–33	20–30
Construction Fees	34–41	not included[d]
Contingency	35–44	30
Total Fixed Capital	**397–504**	**455–605**
Working Capital	70–89	not included[d]
Total Capital Investment	**467–593[c]**	**455–605**

[a] By definition. [b] There are more detailed, but still deterministic, methods for accurately estimating components that tend to vary widely, like piping costs. [c] Since working capital is recovered at the end of the plant lifetime (though this inflow must be discounted), including it here gives the total upfront capital cost. [d] These categories in reference 4 are grouped into other categories in reference 23.

For estimation of secondary components in operating costs, direct labor is the most common basis (e.g. for items like laboratory costs and benefits) but other bases are also important. For example, total capital cost is among the best predictors for items like maintenance costs and certain utilities. Some items, such as energy costs, rely on equipment-specific requirements and modeling the local cost of energy commodities.

For each of the secondary cost categories, CatCost provides situation-dependent low, average, and high values for the determining factor. These values represent a synthesis and update of the various literature references to guide user input and form the basis of future sensitivity analyses. These values are intended to be a starting point for users to adjust and learn about the effect of these factors on their catalyst cost estimates.

7.6   Implementation in CatCost

The processing cost methods described above were incorporated into a functional, extensible, and user-friendly CapEx & OpEx Factors method within CatCost. This method allows detailed and accurate cost estimations while automating much of the process to reduce the time required to generate an estimate.

7.6.1 The "3b Equipment" Module and Equipment Library

The foundation of the CapEx & OpEx Factors method in CatCost is the equipment list for the industrial catalyst synthesis process, found in module "3b Equipment." This equipment list generates or influences the majority of capital and operating cost components in CatCost and

corresponds naturally to the process steps a catalyst engineer is accustomed to designing. In this module, users select process equipment (such as 'Reactor, jacketed, agitated') from the CatCost Equipment Library, which we believe to be the largest publicly available process unit library with over 200 pieces of equipment from highly respected sources.[4,8,19,22-24] CatCost prompts the user for a sizing parameter, such as tank size in m^3 or pump power in kW. It also allows the user to select the material of construction for each piece of equipment according to process requirements, such as corrosion resistance (Figure 7.2).

Equipment List: Zeolite for FCC

Inputs at Reference Design Production Rate

Equipment Type	User Label	Material of Construction	Quantity	Size	Size Unit	Within Size Limits?
Reactor, jacketed, agitated		Carbon steel	2	11.4	volume, m3	Yes
Reactor, jacketed, agitated		Carbon steel	2	75.7	volume, m3	Yes
Crystallizer, batch evaporative		Carbon steel	3	75.7	Volume, ft3	Yes
Filter, rotary-drum vacuum		Carbon steel and Polypropylene wet	2	100.0	Filtering area, ft2	Yes
Reactor, jacketed, agitated		Carbon steel	1	5.7	volume, m3	Yes
Reactor, jacketed, agitated		Carbon steel	1	0.8	volume, m3	Yes
Evaporator, forced circulation		Carbon steel	1	600.0	Heat transfer area, ft2	Yes
Reactor, jacketed, agitated		Carbon steel	1	11.4	volume, m3	Yes
Dryer, indirect-heat steam-tube rotary (Seider)		Stainless steel	1	738.3	Heat-transfer area, ft2	Yes
Reactor, jacketed, agitated		Carbon steel	1	24.0	volume, m3	Yes
Reactor, jacketed, agitated		Carbon steel	1	28.4	volume, m3	Yes
Filter, rotary-drum vacuum		Carbon steel and Polypropylene wet	1	100.0	Filtering area, ft2	Yes
Muller mixer		Carbon steel	3	100.0	Volume, ft3	Yes
Dryer, spray (Sinnott)		304 stainless steel	3	2881.8	evap rate kg/h	Yes
Reactor, jacketed, agitated		Carbon steel	1	1.1	volume, m3	Yes
Reactor, jacketed, agitated		Carbon steel	1	30.3	volume, m3	Yes
Filter, rotary-drum vacuum		Carbon steel	1	255.0	Filtering area, ft2	Yes
Reactor, jacketed, agitated		Rubber-lined	1	3.8	volume, m3	Yes
Reactor, jacketed, agitated		Rubber-lined	1	30.3	volume, m3	Yes
Filter, rotary-drum vacuum		Carbon steel and Polypropylene wet	1	255.0	Filtering area, ft2	Yes
Dryer, steam-tube 2.4 m diameter, 350-1200 m2 (Perry's)		Carbon steel	2	1161.7	Free tube surface area, m2	Yes
Cooling tower w/ pumps, field assembled		Carbon steel	2	1577.0	flow, L/s	Yes
Pump, single stage centrifugal	misc	Carbon steel	40	20.0	flow, L/s	Yes
Blower, centrifugal (turbo)	misc	Aluminum	20	400.0	Brake horsepower	Yes
Tank, cone roof (Seider)	misc	Carbon steel	10	3000.0	Volume, gal	Yes
Tank, cone roof (Seider)	misc	Carbon steel	15	150000.0	Volume, gal	Yes

Figure 7.2. The sizing inputs section of the equipment list for a Zeolite for FCC process design, showing Equipment Type selection from the Equipment Library by dropdown list, User Label, Material of Construction, and the scaling inputs Quantity and Size. Note that the Size Unit from the Equipment Library is provided and varies between equipment items. Finally, a "Within Size Limits?" check is included to help users identify when their process design might be better suited by an alternate equipment type.

Based on the user inputs to the equipment list, CatCost automatically looks up and calculates key outputs for each equipment item and for the process plant as a whole. These outputs include the equipment purchase price, using established cost correlations that incorporate factors for varying materials of construction and which automatically notify the user of equipment which is sized outside the pricing correlation's range of validity; factors that multiply with the equipment purchase price to produce an installed cost (which includes the equipment and associated fittings, support structures, installation labor, etc.); and direct labor requirements for each piece of equipment (Figure 7.3).

Equipment List: Zeolite for FCC							
Inputs at Reference Design Production Rate			Scaling to Current Design Production Rate		Outputs at Current Design Production Rate		
Equipment Type	Quantity	Size	CatCost Scaled Quantity	CatCost Scaled Size	Purchase Cost	Installed Cost	Labor Factor
Reactor, jacketed, agitated	2	11.4	2	34.1	951,934	1,618,289	0.6
Reactor, jacketed, agitated	2	75.7	5	90.9	4,927,969	8,377,547	1.5
Crystallizer, batch evaporative	3	75.7	3	227.1	615,051	1,107,091	0.5
Filter, rotary-drum vacuum	2	100.0	2	300.0	648,854	1,096,563	0.4
Reactor, jacketed, agitated	1	5.7	1	17.0	293,852	499,548	0.3
Reactor, jacketed, agitated	1	0.8	1	2.3	97,279	165,374	0.3
Evaporator, forced circulation	1	600.0	1	1800.0	557,904	1,166,018	0.3
Reactor, jacketed, agitated	1	11.4	1	34.1	475,967	809,144	0.3
Dryer, indirect-heat steam-tube rotary (Seider)	1	738.3	2	1107.4	792,022	1,298,915	1.0
Reactor, jacketed, agitated	1	24.0	1	72.1	827,476	1,406,709	0.3
Reactor, jacketed, agitated	1	28.4	1	85.2	938,388	1,595,259	0.3
Filter, rotary-drum vacuum	1	100.0	1	300.0	324,427	548,281	0.2
Muller mixer	3	100.0	3	300.0	1,110,297	1,554,416	0.6
Dryer, spray (Sinnott)	3	2881.8	7	3705.2	10,206,592	16,738,810	7.0
Reactor, jacketed, agitated	1	1.1	1	3.4	116,116	197,398	0.3
Reactor, jacketed, agitated	1	30.3	1	90.8	985,495	1,675,341	0.3
Filter, rotary-drum vacuum	1	255.0	1	765.0	411,878	696,074	0.2
Reactor, jacketed, agitated	1	3.8	1	11.4	293,674	499,246	0.3
Reactor, jacketed, agitated	1	30.3	1	90.8	1,281,143	2,177,943	0.3
Filter, rotary-drum vacuum	1	255.0	1	765.0	514,848	870,093	0.2
Dryer, steam-tube 2.4 m diameter, 350-1200 m2 (Perry's)	2	1161.7	6	1161.7	11,022,680	18,077,195	3.0
Cooling tower w/ pumps, field assembled	2	1577.0	2	4731.0	6,539,254	7,847,104	1.2
Pump, single stage centrifugal	40	20.0	40	60.0	714,475	928,817	0.0
Blower, centrifugal (turbo)	20	400.0	24	1000.0	3,605,466	5,372,144	2.4
Tank, cone roof (Seider)	10	3000.0	10	9000.0	270,513	508,565	0.0
Tank, cone roof (Seider)	15	150000.0	15	450000.0	3,018,918	5,675,567	0.0

Figure 7.3. Another screenshot of the Equipment List in "3b Equipment" on Excel, this time showing the automated scaling built into CatCost. The green vertical bar indicates cells that have been hidden for view in order to allow comparison from the reference design scale for this equipment list of 100 M lb/yr, which has been automatically scaled to this estimate's production scale of 300 M lb/yr. The outputs section contains purchase cost, installed cost, and a labor factor. Purchase cost is calculated using material of construction-specific pricing correlations and scaled from the correlation year to the estimate basis year. For each piece of equipment, factors for the number of labor operators and for installation cost as a multiple of purchase price are retrieved from the CatCost database.

Once the user has established a baseline process design scenario, evaluating the effect of changing production scale is easy and automated. CatCost automatically adjusts the size of equipment items entered in the base case (see Figure 7.3, showing scaling of a 100 M lb/yr base case to 300 M lb/yr). If this scaling sizes a piece of equipment below its pricing correlation's minimum size, the price of a minimum size unit is used; similarly, if the equipment called for is too large for a pricing correlation, CatCost automatically generates two or more of that piece of equipment to replace the oversized unit, while never using fewer than the number specified in the base case (if pumps are needed in two locations then at least two pumps are needed). The rest of the logic in the processing module carries these changes through, allowing a user to rapidly see how the fraction of catalyst cost contributed by, for example, capital investment changes with production scale. Figure 7.4 shows the results of scaling a 100 M lb/yr base case to two new production scales.

Model Summary	Test Case: 10 M lb/yr			Base Case: 100 M lb/yr			Test Case: 300 M lb/yr		
	Annual Basis	Product Basis	%	Annual Basis	Product Basis	%	Annual Basis	Product Basis	%
Capital Costs	$/year	$/lb		$/year	$/lb		$/year	$/lb	
Fixed Capital Investment (FCI)	749,742	0.07	2.6	2,564,410	0.03	2.5	6,412,481	0.02	2.4
Working Capital	124,775	0.012	0.4	421,943	0.004	0.4	1,053,965	0.004	0.4
Total Capital Investment (TCI)	**874,517**	**0.09**	**3.0**	**2,986,354**	**0.03**	**2.9**	**7,466,446**	**0.02**	**2.8**
Expected Return on Capital Investment									
Return on Investment, Annual	**2,186,292**	**0.22**	**7.6**	**7,465,884**	**0.07**	**7.2**	**18,666,115**	**0.06**	**6.9**
Operating Costs									
Variable									
Raw Materials	19,000,447	1.90	66.0	73,004,466	0.73	70.0	193,013,398	0.64	71.2
Process Utilities	1,311,012	0.13	4.6	4,110,122	0.04	3.9	10,330,366	0.03	3.8
Labor, Supplies, Maintenance, Lab	1,001,105	0.10	3.5	2,044,540	0.02	2.0	4,257,181	0.01	1.6
Fixed									
Taxes, Insurance, Rent, Overhead	881,834	0.09	3.1	2,106,735	0.02	2.0	4,704,183	0.02	1.7
General Expenses									
Admin, Dist., Mkting., R&D	3,529,381	0.35	12.3	12,598,787	0.13	12.1	32,697,205	0.11	12.1
Total Operating Cost	**25,723,779**	**2.57**	**89.4**	**93,864,650**	**0.94**	**90.0**	**245,002,332**	**0.82**	**90.4**
Total Cost	**28,784,588**	**2.88**	**100.0**	**104,316,888**	**1.04**	**100.0**	**271,134,894**	**0.90**	**100.0**
Recovery Value	(3,687,263)	(0.37)	(12.8)	(36,872,631)	(0.37)	(35.3)	(110,617,892)	(0.37)	(40.8)
Total Cost with Recovery	**25,097,325**	**2.51**	**87.2**	**67,444,257**	**0.67**	**64.7**	**160,517,002**	**0.54**	**59.2**

Figure 7.4. An example of the automated scaling incorporated into CatCost, which allows easy scenario analysis to observe the relative significance of, for example, capital investment to total product cost at various production scales.

7.6.2 The "3c Utilities" Module

The "3c Utilities" module is quite simple, containing only consumption inputs per unit catalyst and unit costs for six process utilities: cooling water, process water, low-pressure steam, high-pressure steam, electricity, and natural gas. The Excel version of the module is shown in Figure 7.5. Entries in this module should correspond to the process design entered on "3b Equipment."

Figure 7.5. The "3c Utilities" module in the Excel version of CatCost.

7.6.3 The "3d CapEx" and "3e OpEx" Modules

The outputs from the equipment list form the basis for estimation of the remainder of CatCost's processing cost components, as described in Section 7.5. In the factored capital costs module "3d CapEx," cost components like piping, installation, buildings, land, etc. are calculated from the total equipment purchase price using percentage factors. Default factors are provided from Peters & Timmerhaus,[4] one of process design's most respected resources, and the user can change any or all of the factors according to their own process design knowledge or to evaluate cost scenarios (Figure 7.6). The factored operating costs module on "3e OpEx" is similar (Figure 7.7), but with

32

most costs based on the sum of direct labor requirements rather than the purchased equipment cost. The cost bases vary in the operating factors. Notably, Distribution and Marketing and Research and Development costs exclude the value of any precious/noble metals content using the "4 Spent Catalyst" module, so for catalysts containing these metals the calculation will not be complete until "4 Spent Catalyst" has been completed.

CapEx & OpEx Factors: Factored Capital Expenditures

Cost Item	Base	Units	Total Cost ($)	
Direct Capital				
Purchased Equipment	100	% of purchased equipment cost	51,542,469	
Installation	60	% of purchased equipment cost	30,964,982	
Instrumentation and Controls	26	% of purchased equipment cost	13,401,042	
Piping	31	% of purchased equipment cost	15,978,165	
Electrical	10	% of purchased equipment cost	5,154,247	
Buildings	29	% of purchased equipment cost	14,947,316	
Yard Improvements	12	% of purchased equipment cost	6,185,096	
Service Facilities	55	% of purchased equipment cost	28,348,358	
Waste Treatment	5	% of purchased equipment cost	2,577,123	
Land	6	% of purchased equipment cost	3,092,548	
Total Direct	**334**	**% of purchased equipment cost**	**172,191,348**	
Indirect Capital				
Engineering and Supervision	32	% of purchased equipment cost	16,493,590	
Construction Expenses	34	% of purchased equipment cost	17,524,439	
Legal Expenses	4	% of purchased equipment cost	2,061,699	
Contractor's Fee	19	% of purchased equipment cost	9,793,069	
Contingency	37	% of purchased equipment cost	19,070,714	
Total Indirect	**126**	**% of purchased equipment cost**	**64,943,511**	
Total Fixed Capital Investment (FCI)	**460**	**% of purchased equipment cost**	**237,134,859**	
Working Capital	75	% of purchased equipment cost	38,656,852	?
Total Capital Investment (TCI)	**535**	**% of purchased equipment cost**	**275,791,710**	

Figure 7.6. Factored Capital Costs on "3d CapEx."

CapEx & OpEx Factors: Factored Operating Expenditures

Cost Item	Base	Units	Cost ($/year)	Cost ($/lb catalyst)	
Direct Labor					
Direct Labor Operators (rounded up)	22	operators			
Direct Labor Hours per Year	192,720	hr/yr			
Direct Labor Rate	43	$/hr			
Direct Labor Cost (DL)			**8,286,960**	**0.0276**	
Direct Operating Costs					
Supervisory and Clerical Labor	18	% of DL	1,491,653	0.0050	
Laboratory Charges	15	% of DL	1,243,044	0.0041	
Maintenance and Repair (M&R)	5	% of FCI	11,856,743	0.0395	
Operating Supplies	15	% of M&R	1,778,511	0.0059	
Total: Labor, Supplies, Maintenance, Lab (LSM)			**24,656,911**	**0.0822**	
Fixed/Indirect Operating Costs					
Local Taxes	2.5	% of FCI	5,928,371	0.0198	
Insurance	0.8	% of FCI	1,897,079	0.0063	
Rent, % of value of rented land	10	% of land	309,255	0.0010	
Plant Overhead, % of LSM	60	% of LSM	14,794,147	0.0493	
Total: Taxes, Insurance, Rent, Overhead			**22,928,852**	**0.0764**	
General Expenses					
Administration	20	% of LSM	4,931,382	0.0164	
Distribution and Marketing	10	% of op. costs excluding PGM/noble metals content	6,294,919	0.0210	?
Research and Development	5	% of op. costs excluding PGM/noble metals content	3,147,459	0.0105	?
Total: Admin, Dist., Mkting., R&D			**14,373,760**	**0.0479**	

Figure 7.7. Factored Operating Costs on "3e OpEx."

8 Process Templates for the Step Method and CapEx & OpEx Factors Method

8.1 Making estimates faster and more accessible

Many users of CatCost are not expected to have the experience in industrial chemistry or the access to process simulation tools, such as AspenPlus, needed to generate a detailed synthesis process design at industrial scale. Furthermore, even for experienced users, developing such a design may involve sizing 10–30 pieces of equipment with materials of construction, performing materials and energy balances, and undergoing optimization and revision to obtain a credible process design, a significant effort that may require days or weeks to complete. For this reason, a key feature of CatCost in both the Step Method and the CapEx & OpEx Factors method for processing cost estimation is the inclusion of process templates, in which complete process models have already been developed and entered in CatCost for easy selection by the user. We expect that this will aid both casual users or non-engineers who may have difficulty developing such designs on their own, and power users for whom the process designs will be an excellent starting point that they can then customize for greater accuracy and specificity. The bundled process templates were chosen to encompass the largest potential user-base and minimize the required user input to generate accurate estimates for the largest number of potential catalysts.

8.2 Step Method templates

Templates in the step method consist of selected process steps (e.g. spray dryer) with alternates for different production scales in order to accommodate the entire 1–1000 ton range of step method order size (Figure 8.1). Twelve different step method templates are included in CatCost, and the user can easily select from among them or enter a custom process as shown in Figure 8.2.

54	**Step Process Template: FCC Catalyst (USY w/ RE)**					
55						

56	Step Method Template Name	Totals:	Cost ($/hr)	Cost ($/campaign)	Cost ($/kg catalyst)
57	FCC Catalyst (USY w/ RE)		1535	92083	50.75

Notes for Template

A modern FCC catalyst based on Ultrastable zeolite Y with rare earth at 200-ton scale.

Note that substitute steps are included to accommodate Small, Medium, and Large scales using formulae in the Quantity column.

	Step Name	Quantity	Cost ($/hr)	Cost ($/campaign)	Cost ($/kg catalyst)	Note
65	Reactor, simple (mixing)	1	29	1732	0.95	-
66	Crystallizer	2	192	11546	6.36	-
67	Filter, rotary vacuum	0	N/A at small scale	N/A at small scale	N/A at small scale	Substitute with plate and frame at small scale
68	Filter, plate and frame	4	289	17320	9.55	Substitute with belt or rotary vacuum at M/L scale
69	Reactor, simple (mixing)	4	115	6928	3.82	-
70	Kiln, continuous indirect (300–1290 °C)	0	N/A at small scale	N/A at small scale	N/A at small scale	A.k.a. calciner. Sub with batch kiln at small scale
71	Kiln, batch (300–1290 °C)	1	72	4330	2.39	A.k.a. calciner. Sub with continuous kiln at M/L scale
72	Reactor, multistep	1	96	5773	3.18	-
73	Filter, rotary vacuum	0	N/A at small scale	N/A at small scale	N/A at small scale	Substitute with plate and frame at small scale
74	Filter, plate and frame	1	72	4330	2.39	Substitute with belt or rotary vacuum at M/L scale
75	Reactor, multistep	1	96	5773	3.18	-
76	Mixer, slurry	2	144	8660	4.77	Muller
77	Dryer, spray	0	N/A at small scale	N/A at small scale	N/A at small scale	Substitute with rotary dryer at small scale
78	Dryer, rotary (40–100 °C)	1	72	4330	2.39	-
79	Reactor, simple (mixing)	4	115	6928	3.82	-
80	Filter, rotary vacuum	0	N/A at small scale	N/A at small scale	N/A at small scale	Substitute with plate and frame at small scale
81	Filter, plate and frame	2	144	8660	4.77	Substitute with belt or rotary vacuum at M/L scale
82	Dryer, rotary (100–300 °C)	1	96	5773	3.18	For higher temp use kiln

88 <– show/hide Step Process Template: FCC Catalyst (USY w/ RE)

Figure 8.1. Screenshot of CatCost showing an exemplary step method process template: Production of an FCC catalyst at "Small" (1 ton/day) scale. Steps in green are not available at all production scales, so formulae automatically select the correct unit for that production scale for inclusion.

Figure 8.2. Overview screenshot of the Step Method section of CatCost, showing the range of 12 process templates included, as well as the ability to enter a custom process, and to easily select from this list for inclusion in an estimate.

8.3 CapEx & OpEx Factors templates

Process templates in the CapEx & OpEx Factors method include a list of equipment items including size, quantity, and material of construction for a specified production scale of catalyst (see Figure 8.3 for an example of a process template equipment list and Figure 8.4 for the overall

selection of a process template from the list), as well as a list of utilities consumption per mass unit of catalyst (see Figure 8.5).

Equipment List: Metal Carbide on Metal Oxide					
Inputs at Reference Design Production Rate					
Equipment Type	User Label	Material of Construction	Quantity	Size	Size Unit
Bin	F-101	Carbon steel	1	120.8	Volume, ft3
Feeder, belt	F-102	Carbon steel	1	96.4	Volumetric flow rate, ft3/hr
Reactor, jacketed, agitated	R-101	Carbon steel	1	4.8	volume, m3
Heater, general purpose (box furnace)	H-101	Carbon steel tubes	1	7170000.0	Heat duty, Btu/hr
Reactor, jacketed, agitated	R-102	Carbon steel	1	5.5	volume, m3
Heat exchanger, U-tube shell and tube	H-102	Carbon steel	1	2.5	area, m2
Compressor, rotary twin-screw, electric motor (preferred)	C-101	Carbon steel	1	8.6	Consumed power, hp
Blower, centrifugal (turbo)	C-102	Carbon steel	1	0.5	Brake horsepower
Compressor, rotary twin-screw, electric motor (preferred)	C-103	Carbon steel	1	22.2	Consumed power, hp
Blower, centrifugal (turbo)	C-104	Carbon steel	1	48.2	Brake horsepower
Flare, elevated (40 ft)	U-102	Below 60 Btu/ft3	1	3053.6	Waste gas flow rate, lb/hr
Bag filter	U-103	Carbon steel	1	70.6	Gas flow rate, actual ft3/min
Tank, cone roof (Seider)	S-101	Carbon steel	1	500.0	Volume, gal
Tank, cone roof (Seider)	S-102	Carbon steel	1	2000.0	Volume, gal
Tank, cone roof (Seider)	S-103	Carbon steel	1	2000.0	Volume, gal

Figure 8.3. Screenshot from CatCost showing the equipment list from one of the CapEx & OpEx Factors Templates: Metal Carbide on Metal Oxide, including equipment items, sizes, quantities, and materials of construction.

2	
3	**CapEx & OpEx Factors: Equipment Costs**
4	
5	Select a Process Template or Choose "Custom Process"
6	Nanoparticles - Flow Synthesis
7	
8	Equipment Cost Totals for Selected Template
9	Purchase Cost $ 16,645,631
10	Installed Cost $ 16,645,631
11	Labor Factor (# of operators) 79.5
12	
13	
14	**CapEx & OpEx Factors Equipment Lists: Custom Process and Process Templates**
15	Show/Hide Individual Process Templates Using +/- at left (Show all using "2" at top left, hide all using "1" at top left)
16	
17	**User Entry: Custom Process**
83	<– show/hide User Entry: Custom Process
84	**Process Template: Metal Carbide on Metal Oxide**
130	<– show/hide Process Template: Metal Carbide on Metal Oxide
131	**Process Template: Nanoparticles - Flow Synthesis**
177	<– show/hide Process Template: Nanoparticles - Flow Synthesis
178	**Process Template: Wet Impregnation - Metal on Metal Oxide**
219	<– show/hide Process Template: Wet Impregnation - Metal on Metal Oxide
220	**Process Template: Zeolite for FCC**
286	<– show/hide Process Template: Zeolite for FCC

Figure 8.4. Overview screenshot from CatCost showing selection of a process template or custom process in the Equipment list section of the CapEx & OpEx Factors Method.

CapEx & OpEx Factors: Utilities Costs

Selected Process Template

Zeolite for FCC

Note: ordinarily this is set by the entry on 3b Equip but can be overridden

Process Utilities Consumption and Cost for Selected Template

Utility	Consumption per kg catalyst	Units	Unit Cost	Units	Cost ($/kg catalyst)	Cost ($/year)	
Cooling Water	0.116220472	kgal	0.14	$/kgal	0.0163	1,627,087	?
Process Water	0	kgal	1.3	$/kgal	-	-	
Steam, 150 psig	0.001574803	ton	5	$/ton	0.0079	787,402	
Steam, 600 psig	0	ton	5.7	$/ton	-	-	
Electricity	0.17	kWh	0.055	$/kWh	0.0094	935,000	
Natural gas	0.005905512	MMBtu	3	$/MMBtu	0.0177	1,771,654	

?

		Cost ($/kg catalyst)	Cost ($/year)
Totals		0.0512	5,121,142

Utilities Process Templates

Custom Process

Utility	Consumption per kg catalyst	Units
Cooling Water		kgal
Process Water		kgal
Steam, 150 psig		ton
Steam, 600 psig		ton
Electricity		kWh
Natural gas		MMBtu

Metal Carbide on Metal Oxide

Utility	Consumption per kg catalyst	Units
Cooling Water	0.000229775	kgal
Process Water	3.44662E-06	kgal
Steam, 150 psig	0.00014978	ton
Steam, 600 psig	0.000744137	ton
Electricity	0.47435654	kWh
Natural gas	0.00501571	MMBtu

Nanoparticles - Flow Synthesis

Utility	Consumption per kg catalyst	Units
Cooling Water	0	kgal
Process Water	0	kgal
Steam, 150 psig	0	ton
Steam, 600 psig	0	ton
Electricity	0.26	kWh
Natural gas	0	MMBtu

Wet Impregnation - Metal on Metal Oxide

Utility	Consumption per kg catalyst	Units
Cooling Water	0.001431831	kgal
Process Water	2.14775E-05	kgal
Steam, 150 psig	0.000782148	ton
Steam, 600 psig	0.003885863	ton
Electricity	7.296509343	kWh
Natural gas	0.0261919	MMBtu

Zeolite for FCC

Utility	Consumption per kg catalyst	Units
Cooling Water	0.116220472	kgal
Process Water	0	kgal
Steam, 150 psig	0.001574803	ton
Steam, 600 psig	0	ton
Electricity	0.17	kWh
Natural gas	0.005905512	MMBtu

Figure 8.5. Screenshot from CatCost showing the Utilities portion of the CapEx & OpEx Factors method, with the ability to select from process templates to match those in the Equipment list.

9 Spent Catalyst Value: The *"4 Spent Catalyst"* Module and *Spent Catalyst Library*

9.1 Overview and "4 Spent Catalyst" Module

While the procedures outlined so far for estimating materials and processing costs allow CatCost to provide a complete estimate of the initial purchase/synthesis cost of a catalyst at industrial scale, the initial cost of filling a catalytic reactor is only part of the story. Accurate comparisons of catalytic materials must consider the differing values of catalysts at the *end* of their useful life. CatCost provides a Spent Catalyst Value module for this purpose, enabling comparisons between, for example, a molybdenum carbide catalyst with a relatively low purchase cost and a platinum-based catalyst with a high purchase cost but with significant spent catalyst value.

Within CatCost, the "4 Spent Catalyst" module estimates the value of three distinct options for spent catalysts: metals recovery, sale, and landfill. CatCost presents the value of each of the options and automatically chooses the most favorable option (i.e. if the cost to recover metal from a catalyst exceeds the value of the metal content to be recovered, CatCost first looks for sale value, and then finally chooses to landfill the catalyst if neither metals recovery nor sale were more favorable). Notably, CatCost presents the spent catalyst value as an individual line item in the catalyst cost outputs (Figure 9.1) so that the user can choose whether to include it in catalyst cost comparisons. This approach also allows the technoeconomic analysis-oriented user to enter the reactor filling and catalyst disposal inflows/costs at the appropriate times in a discounted cash-flow analysis of a catalytic process plant.

Cost Item	Unit Cost $/kg catalyst	Campaign cost $ for 200 tons
Total Catalyst Cost	857.65	155,610,078
Spent Catalyst Value (SCV)	549.37	99,675,389
Total Catalyst Cost, Including SCV	308.29	55,934,690

Figure 9.1. Excerpt from CatCost outputs showing the separate line item for Spent Catalyst Value.

The inputs to CatCost for the "4 Spent Catalyst" module are shown in Figure 9.2 below. These inputs, shared by the Excel and web versions of CatCost, allow the tool to look up values from the Spent Catalyst Library (described below) and to perform calculations. Built-in logic allows CatCost to determine the best-value option for the spent catalyst based on these inputs. For details of the logic being used, see the following sections. The first two inputs to "4 Spent Catalyst," "Metal to recover" and "Support," allow CatCost to estimate the attrition losses during catalyst use and metals refining, as well as to look up the appropriate spot metal price from the Spent Catalyst Library. The third input, "Metal wt. % of AP" (the weight fraction of the recoverable metal in the active phase; for example, for a Rh_2P active phase this number is 86.92%), is used with the "Active Phase Weight Percent" field on "2 Materials" to determine the metal content in fresh catalyst. The fourth input, "Catalyst Bulk Density," may be entered in units of either lb/ft^3 or kg/m^3 and is used in calculation of refiner "incoming" and "metal contaminant" fees (described below), both of which have a volumetric basis (e.g. $105/ft^3$). CatCost automatically converts the

user-entered density according to the units chosen and conveniently provides a "Bulk Density Lookup Tool" with densities for common catalyst materials on the right side of the Excel spreadsheet and bottom of the web tool module. The fifth input, "Planned reactor configuration" accepts values of "Fixed Bed" and "Slurry/Fluidized Bed" and affects the calculation of attrition losses mentioned above, since fluidized beds cause greater catalyst attrition. The sixth input, "Has trace Sn, Cu, Fe > 2% of AP?" addresses the difficulty of recovering precious metals from catalysts contaminated with over 2% (by wt. % of the active phase) of any of the named metals, and triggers a "metal contaminant" fee in addition to fees charged to catalysts without these contaminants. The seventh and final input, in contrast to the forgoing inputs, determines to the sale value, if any, and landfill cost of the spent catalyst. It is entitled "Classification for Sale or Landfill" and accepts options such as "Zeolite, Silica, Alumina" and "Hazardous (e.g. RCRA metals)." For more information on the meaning of these options and selecting the appropriate classification for a catalyst, see the following sections.

Figure 9.2. Inputs section of "4 Spent Catalyst" module in Excel, showing an estimate completed for a Rh/C catalyst.
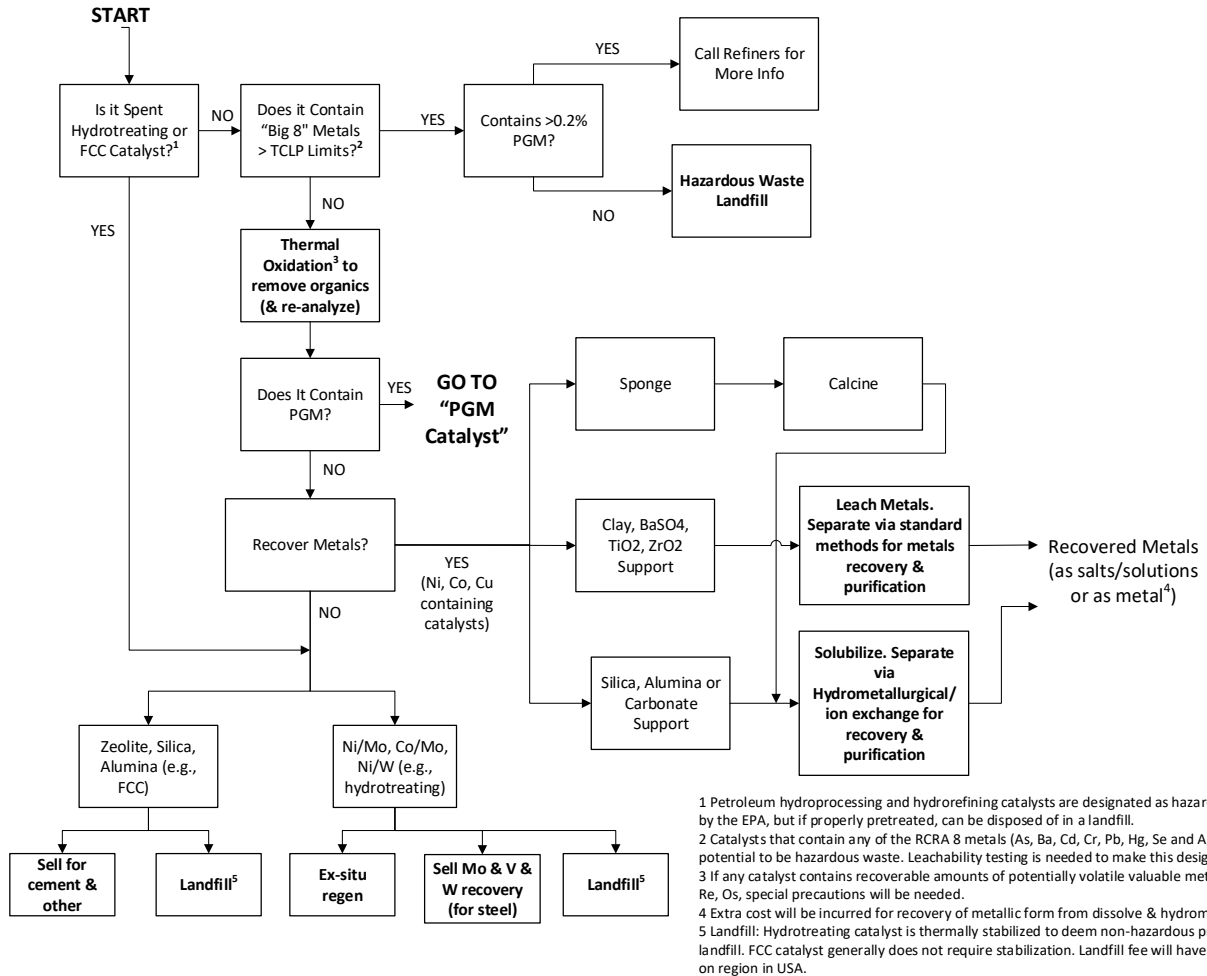
9.2   Spent Catalyst Recovery/Disposal Details and Calculation Logic

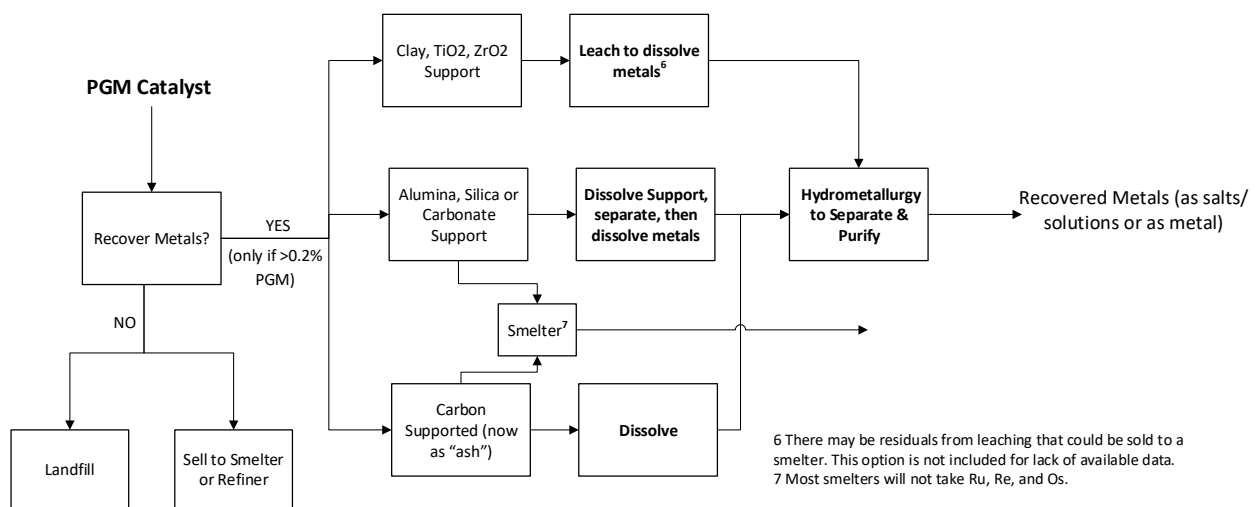### 9.2.1   Overview of options for managing spent catalyst

Figure 9.3 illustrates commonly available options for managing spent catalyst and key decision points for each. This decision logic has been incorporated in CatCost such that the "options" mentioned below are automatically selected to maximize spent catalyst value. In general, spent catalysts can be sent to a catalyst refiner and processed to reclaim metals, sold for other uses (e.g., steel, cement, or smelter), or disposed of in a landfill. Note that it is already assumed that plants employing catalytic materials will regenerate them as long and as often as it is economical to do so. Starting at the top of Figure 9.3 ("START"), spent hydrotreating and fluidized catalytic cracker (FCC) catalysts used in petroleum refineries are generally landfilled or sometimes sold to a cement or steel mill. Hydrotreating catalysts are designated as hazardous waste by the US Environmental Protection Agency (EPA) through the Resource Conservation and Recovery Act (RCRA),[28] but if properly stabilized, can be deemed safe to handle and transport. These materials, once properly pretreated, can be regenerated, sold for their Mo, V or W content to be used in steel, or landfilled. FCC catalysts are generally not considered hazardous and do not require stabilization due to the highly encapsulated nature of the catalyst structure. For non-hydroprocessing/hydrorefining catalysts, the first step is to determine whether or not the spent material is hazardous waste (per RCRA and/or state regulations). If it is, the material may either be sent to a hazardous landfill, or it is possible that it may be sold to a catalyst refiner if there is enough PGM and they are equipped to process the material. For non-hazardous material, it first goes through a thermal oxidation step

to remove residual volatiles, coke, and most of the sulfur resulting from catalytic processing. For non-PGM catalysts, it may or may not be economically justified to reclaim metals (e.g., Ni, Co, Cu) from the spent material. If the recovery option is chosen, the type of processing used will depend on the support. For Al_2O_3, SiO_2 or carbonate supports, the support is first solubilized with an appropriate solvent (e.g., NaOH or H_2SO_4). The metals are then recovered from the insoluble residue via filtration, and hydrometallurgical processing is used to further purify and recover the metals. For clay, $BaSO_4$, TiO_2, and ZrO_2 supports, the metals are leached (e.g., with a HCl / sodium chlorate mixture) from the support and then concentrated into a solution form for recovery and purification. For a metal "sponge" in which a high-surface-area metal is used as a catalyst with no supporting material, the sponge is first calcined and then solubilized and recovered similarly to silica- and alumina-supported catalysts.

For PGM catalysts, (see "PGM CATALYST" in Figure 9.3), it must first be decided whether or not to recover the metal, which depends on the identity of the PGM(s) and amount present in the spent material. Generally, if the material contains less than 0.2% PGM, the recovery option will be uneconomical and/or technically difficult. In this case, the material could either be landfilled or sold to a smelter or catalyst refiner (to add to their stockpile for later refining). If the recovery option is chosen, the processes described above for the oxide supported materials are applied. For carbon supported material, the initial thermal oxidation step destroys the support and the remaining metal is dissolved and recovered via hydrometallurgy.

START

Is it Spent Hydrotreating or FCC Catalyst?[1]

NO → Does it Contain "Big 8" Metals > TCLP Limits?[2]

YES → Contains >0.2% PGM?

YES → Call Refiners for More Info

NO → **Hazardous Waste Landfill**

NO → **Thermal Oxidation[3] to remove organics (& re-analyze)**

Does It Contain PGM?

YES → **GO TO "PGM Catalyst"**

NO → Recover Metals?

YES (Ni, Co, Cu containing catalysts) →

Sponge → Calcine

Clay, BaSO4, TiO2, ZrO2 Support → **Leach Metals. Separate via standard methods for metals recovery & purification** → Recovered Metals (as salts/solutions or as metal[4])

Silica, Alumina or Carbonate Support → **Solubilize. Separate via Hydrometallurgical/ion exchange for recovery & purification**

NO →

Zeolite, Silica, Alumina (e.g., FCC)
- **Sell for cement & other**
- **Landfill[5]**

Ni/Mo, Co/Mo, Ni/W (e.g., hydrotreating)
- **Ex-situ regen**
- **Sell Mo & V & W recovery (for steel)**
- **Landfill[5]**

YES (start) → Is it Spent Hydrotreating or FCC Catalyst?

1 Petroleum hydroprocessing and hydrorefining catalysts are designated as hazardous waste by the EPA, but if properly pretreated, can be disposed of in a landfill.
2 Catalysts that contain any of the RCRA 8 metals (As, Ba, Cd, Cr, Pb, Hg, Se and Ag) has the potential to be hazardous waste. Leachability testing is needed to make this designation.
3 If any catalyst contains recoverable amounts of potentially volatile valuable metals, e.g., Ru, Re, Os, special precautions will be needed.
4 Extra cost will be incurred for recovery of metallic form from dissolve & hydrometallurgy.
5 Landfill: Hydrotreating catalyst is thermally stabilized to deem non-hazardous prior to landfill. FCC catalyst generally does not require stabilization. Landfill fee will have dependency on region in USA.

PGM Catalyst

Recover Metals?

YES (only if >0.2% PGM) →

Clay, TiO2, ZrO2 Support → **Leach to dissolve metals[6]** → **Hydrometallurgy to Separate & Purify** → Recovered Metals (as salts/solutions or as metal)

Alumina, Silica or Carbonate Support → **Dissolve Support, separate, then dissolve metals**

Smelter[7]

Carbon Supported (now as "ash") → **Dissolve**

NO →
- Landfill
- Sell to Smelter or Refiner

6 There may be residuals from leaching that could be sold to a smelter. This option is not included for lack of available data.
7 Most smelters will not take Ru, Re, and Os.

Figure 9.3. Spent catalyst management options and associated costs.

The mathematical logic used for calculation of aggregated costs for each of the spent catalyst options is described in the following paragraphs. Default values for the key variables used in these calculations are given in the tables contained in the Spent Catalyst Library (described in Section 9.3).

9.2.2 Metals Recovery Option:

If the option to reclaim spent catalyst is chosen, the value associated with reclaiming metal from the spent catalyst is counted as a credit towards the manufacturing cost to calculate an overall adjusted catalyst cost:

$$C_{adjusted} = C_{manufacturing} - V_{reclaimed}$$

Where $C_{adjusted}$ is the overall adjusted cost of the catalyst in $/lb catalyst purchased with $C_{manufacturing}$ and $V_{reclaimed}$ defined below.

$C_{manufacturing}$ = manufacturing cost ($/lb catalyst purchased)

$V_{reclaimed}$ = reclaimed catalyst value ($/catalyst purchased)

$V_{reclaimed}$ is calculated as:

$$V_{reclaimed} = V_{metal} - C_{recovery}$$

V_{metal} is the salvage value of the metal ($/lb catalyst purchased) and is calculated as

$$V_{metal} = (1 - L_{metal-use}) \times (1 - L_{metal-ref}) \times M_{loading} \times P$$

Where

$L_{metal-use}$ = metal loss from use phase (lb metal lost/lb metal on fresh catalyst)

$L_{metal-ref}$ = metal loss from catalyst refining process (lb metal lost/lb metal on spent catalyst)

$M_{loading}$ = metal loading on catalyst (lb/lb fresh catalyst)

P = metal spot price ($/lb)

$C_{recovery}$ is the cost to recover the metal ($/lb catalyst purchased) and is calculated by summing the fees for each of the processing steps shown in the block diagrams (Figure 9.3) (thermal oxidation, dissolution/leaching and hydrometallurgy, and refining charge for Platinum Group Metal (PGM) catalysts):

$$C_{recovery} = (1 - L_{solids-use}) \times (F_{thermox} + F_{Incoming}/\rho) + (F_{refining} \times M_{loading}) \times (1 - L_{metal-use}) \times (1 - L_{metal-ref})$$

Where

$F_{thermox}$ = thermal oxidation fee ($/lb catalyst treated)

$F_{incoming}$ = incoming fee for metals recovery processing (typically dissolution/leaching + hydrometallurgy) (lb/ft³ catalyst treated)

ρ = catalyst bulk density (lb/ft³)

$F_{refining}$ = refining fee ($/lb PGM metal recovered)

$L_{solids-use}$ is the total catalyst solids lost during the use phase (resulting from loading, attrition, metal not staying attached, and unloading), (lb catalyst loss/lb fresh catalyst), and is calculated as:

$$L_{solids-use} = (L_{support-use}) \times (1 - M_{loading}) + (L_{metal-use}) \times M_{loading}$$

Where

$L_{support-use}$ = loss of support during use phase (lb support/lb fresh catalyst)

CatCost default values for the variables used in the above equations are given in Section 9.3.

9.2.3 Sale Option:

If the spent catalyst is sold for other purposes, the overall Adjusted Catalyst Cost is calculated as:

$$C_{adjusted} = C_{manufacturing} - (1 - L_{solids-use}) \times (V_{sale})$$

Where V_{sale} is the sale value available from various buyers. The applicable sale values are given in Section 9.3.

In the case of a molybdenum containing catalyst, V_{sale} is calculated as

$$V_{sale} = M_{moly} \times (1 - L_{metal-use}) \times 1.5 \ \times (P_{MoO3}) \times (X)$$

Where

M_{moly} = Loading of Mo on catalyst (lb Mo/lb catalyst purchased)

P_{MoO3} = Price of MoO₃ ($/lb)

$X = 0.15\text{-}0.40$ (adjustment factor, fraction of MoO₃ value)

(Factor of 1.5 is the molecular weight ratio of MoO₃ to Mo)

9.2.4 Landfill Option:

If neither metals recovery nor sale is a viable option for a spent catalyst, it must be landfilled at additional cost. This is particularly likely in the following scenarios:
1) Hydroprocessing and hydrorefining catalysts are deemed RCRA hazardous waste by the US EPA but can be treated/stabilized to render the waste non-hazardous and subsequently disposed of in a non-hazardous waste landfill.
2) If a spent catalyst contains any of the RCRA metals ("Big 8"), Toxicity Characteristic Leaching Procedure (TCLP) testing is needed to determine whether or not it is hazardous waste.   The TCLP limits are provided in the Spent Catalyst Library (next section) (hazardous determination is accomplished solely through testing and working with a company's regional regulatory authorities).
3) If a PGM catalyst contains less than 0.2% PGM, the PGM cannot be easily recovered so it would likely go to landfill.

The adjusted catalyst cost in the case of the landfill option is calculated as:

$$C_{adjusted} = C_{man} + C_{landfill}$$

Where $C_{landfill}$ is the overall cost to landfill ($/lb catalyst purchased) and is calculated as:

$$C_{landfill} = (1 - L_{solids-use}) \times (F_{thermox} + F_{landfill})$$

Where

$F_{landfill}$ is the landfill fee ($/lb catalyst landfilled)

Typical landfill fees included in CatCost are given in Section 9.3.

9.3 The Spent Catalyst Library

The Spent Catalyst Library included in CatCost provides default values for the variables used in calculations in "4 Spent Catalyst," as described in the previous section. The user may change or add to the entries in the Spent Catalyst Library to suit their estimation needs. The Spent Catalyst Library contains the same information described below, but implemented into five tables with slightly different grouping and different numbering than in this report.

Table 9.1 gives average losses of the support and active phase metal during catalyst use, which are used in the calculation of spent catalyst solids remaining after unloading of the reactor. Table 9.2 presents typical metal losses that occur during catalyst refining. Table 9.3 lists average thermal oxidation and incoming fees charged for the different support types. Table 9.4 lists typical fees charged by the catalyst refiner. Table 9.5 lists estimated catalyst bulk densities. The Toxicity Characteristic Leaching Procedure (TCLP) limits are listed in Table 9.6 and include a 20-fold dilution of waste (weight basis) in acetic acid, per EPA Test Method 1311.[29] Also listed are the corresponding minimum concentrations of metals that would need to be present in the spent catalyst material to possibly exceed the TCLP limits (assuming 100% of the metal leaches out of the spent catalyst). This table is provided here and in CatCost for informational purposes only and

hazardous determination is accomplished solely through testing and working with the proper regulatory authorities. The list of applicable landfill fees for calculation of spent catalyst disposal is listed in Table 9.7. Table 9.8 presents typical selling prices for spent catalyst sold for other uses, such as cement, a smelter, or metals refiner.

Table 9.1. Average values of support and metal losses from use phase.

Support	Fixed		Slurry/Fluidized	
	$L_{support-use}$	$L_{metal-use}$	$L_{support-use}$	$L_{metal-use}$
TiO_2	2%	10%	3%	13%
ZrO_2	2%	10%	3%	13%
SiO_2	2%	3%	2%	4%
Al_2O_3	2%	3%	2%	4%
Carbon	2%	2.5%	6%	5%
Carbonate	5%	5%	5%	5%
Sponge of metal	n/a	5%	n/a	5%
Clay	5%	5%	5%	5%

Table 9.2. Metal loss from refining.

Metal	High	Low	Average
PGMs			
Palladium	4%	1%	3.5%
Platinum	3%	1%	3.0%
Rhodium	10%	5%	7.5%
Ruthenium	25%	15%	20.0%
Gold			10.0%
Iridium			10.0%
Non-PGMs			
Aluminum (Claus, misc)			70%
Cobalt			20%
Copper CuZn	25%	15%	20%
Iron			40%
Molybdenum	30%	20%	25%
Nickel			20%
Silver	2%	3%	2.5%
Tungsten NiW	25%	15%	20%

Table 9.3. Thermal oxidation fees ($F_{thermox}$) and incoming fees ($F_{incoming}$) for metals recovery processing (typically dissolve/leach + hydrometallurgy).

Process/ Variable	Support	$F_{thermox}$ (low) $/lb	$F_{thermox}$ (high) $/lb
Thermal Oxidation	All	0.125	0.15

Process / Variable	Support	$F_{incoming}$ (low) $/ft^3$	$F_{incoming}$ (high) $/ft^3$
Incoming Fee for Processing – (<2% Cu, Fe, Sn of PGM)	Carbon	94	115
	Al_2O_3, SiO_2, TiO_2, ZrO_2, carbonate, clay	108	123
	Sponge[a]	81	92
Incoming Fee for Processing– (>2% Cu, Fe, Sn of PGM)[b]	Carbon	115	130
	Al_2O_3, SiO_2, TiO_2, ZrO_2, carbonate, clay	126	137
	Sponge[a]	95	103

[a] Estimated at 30% less costly than with hard supports.
[b] Applies to catalysts that contain Cu, Fe, or Sn at >2% of the main PGM or non-PGM metal.

Table 9.4. Refining Charge - $F_{refining}$.

Metal	$/TrOz Recovered
Pt	14.5
Pd	12.5
Rh	16
Au	11
Ru	20
Ir	25
Ag	11.5

Table 9.5. Catalyst bulk densities provided to users as a guide.

Catalyst	ρ (lb/ft^3)	Note
Activated C powder	42	Containing 50% moisture
Activated C granules	46	Containing 50% moisture
Metal on Al_2O_3	45	dry extrudate
Metal on TiO_2	65	dry extrudate
Metal on ZrO_2	66	dry extrudate
Al_2O_3/SiO_2, 44%/51%	50	dry extrudate
SiO_2, 3/16"	30	dry spheres
Sponge Ni, Co, or Cu	71.25	Dry basis; average of 67.5-75 lb/ft3

Table 9.6. RCRA metals and Toxicity Characteristic Leaching Procedure limits, along with *estimated* minimum concentrations in a catalyst that would be expected to cause a material to exceed the TCLP limit and be regulated under RCRA.

Metal	TCLP Limit, mg/L	Minimum Concentration in Catalyst, wt%
As	5	0.01%
Ba	100	0.20%
Cd	1	0.002%
Cr	5	0.01%
Pb	5	0.01%
Hg	0.2	0.0004%
Se	1	0.002%
Ag	5	0.01%

Table 9.7. Landfill Fees ($F_{landfill}$).

Catalyst Type	Fee (per pound catalyst)	Notes
Zeolite, Silica, Alumina	$0.15-0.20/lb	e.g. FCC
Ni/Mo, Co/Mo, Ni/W	$0.75/lb	Includes stabilization
PGM	$1-3/lb	May include stabilization
Hazardous Waste	$1-3/lb	E.g., contains Big 8>TCLP limits

Table 9.8. Sale Values (V_{sale})

Catalyst Type	Value	Notes
Zeolite, Silica, Alumina	$0.05/lb catalyst	e.g. for cement
PGM	$1-1.30/lb catalyst	e.g. to smelter or refiner, typically <0.2% PGM

10 Web Tool Data Import/Export and Visualizations

10.1 Importing/Exporting Data in the CatCost Web Tool

The CatCost webtool has been designed with data import and export functionalities to allow users to export any dataset they have in the CatCost tool to their local machine in the form of a .json file. CatCost can export any individual library (e.g. the *Materials Library*, the *Equipment Library*, or the *Spent Catalyst Library*), any individual estimate, or the complete portfolio of estimates from the *Catalyst Estimates* page. These .json files can then be imported into the webtool to resume work on an estimate and can be easily shared with colleagues. This section outlines the import and export features of the CatCost tool and how they can be used effectively to save and share estimates and cost libraries.

Exporting data from CatCost is easy, and this option is always located in the "File" dropdown menu (Figure 10.1). It is important to note that the "Download JSON file" option is contextual, meaning that it will download the information that is displayed on whatever page you are currently on. For example, notice in Figure 10.1 that when on the main "Estimates" page the file menu displays the option to "Download Estimate Set JSON file". This option downloads all estimates in the CatCost tool to a single .json file. On all other pages, the download JSON button in the file dropdown menu will only download the data from that page. For example, while browsing the "Materials Library" page the option to "Download Materials Library JSON file" is displayed (Figure 10.2).
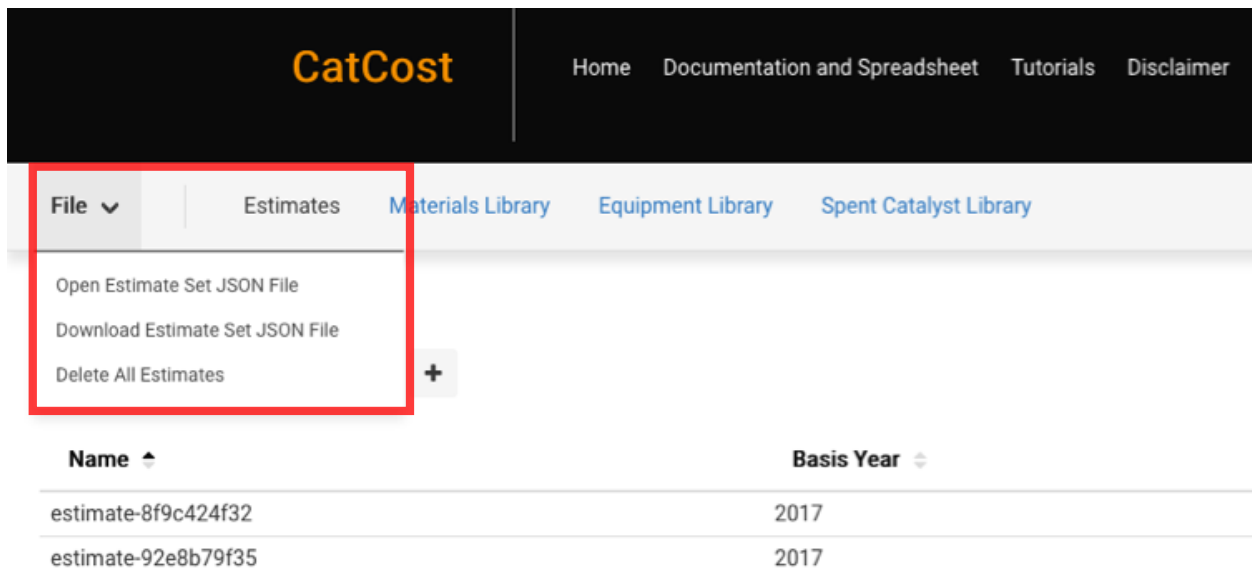

Figure 10.1. File menu import and export options available from the main "Estimates" page.
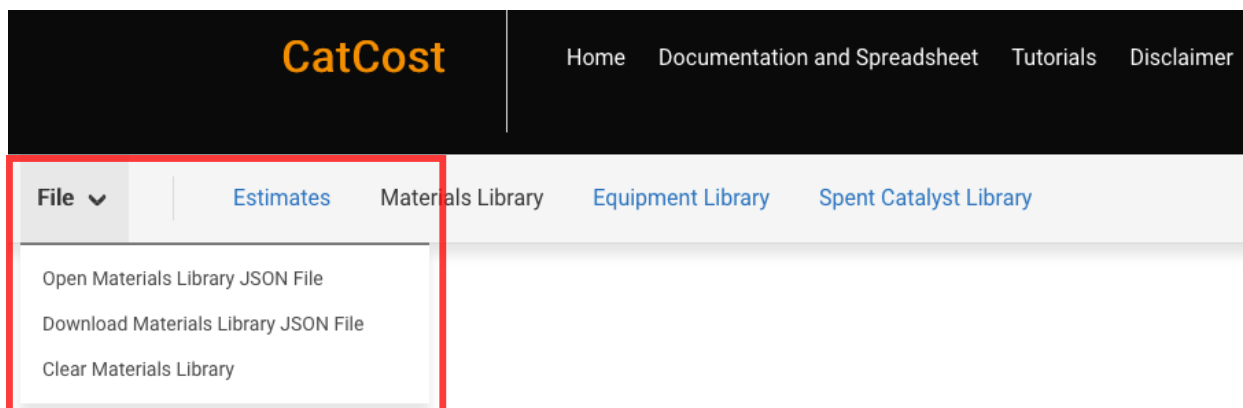
Figure 10.2. File menu import and export options available from the main "Materials Library" page.

Importing data is just as simple and uses the same contextual options as described above for exporting data. To import an estimate set simply visit the main "Estimates" page, hover the cursor over the file menu shown in Figure 10.1, and select the "Open Estimate Set JSON file" option and a dialog for importing estimates will appear. You may then choose from the following two options, to open a dataset from the ChemCatBio Data Hub or to upload your own estimate file. At the top of the dialog you can select to download a set of default catalyst estimates that the CatCost team has made available on the Data Hub (these may be limited at the initial release of the tool). To import an estimate that has previously been created in the CatCost tool, simple drag and drop the file from your local machine to box highlighted in the left pane of Figure 10.3. CatCost will then verify the contents of the file to ensure it is compatible with the current version of the tool, and if successful the filename will appear in green and the "Import from File" button will change from gray to green as shown in the right pane of Figure 10.3. The page will then be refreshed and populated with the estimate or library that was just imported.
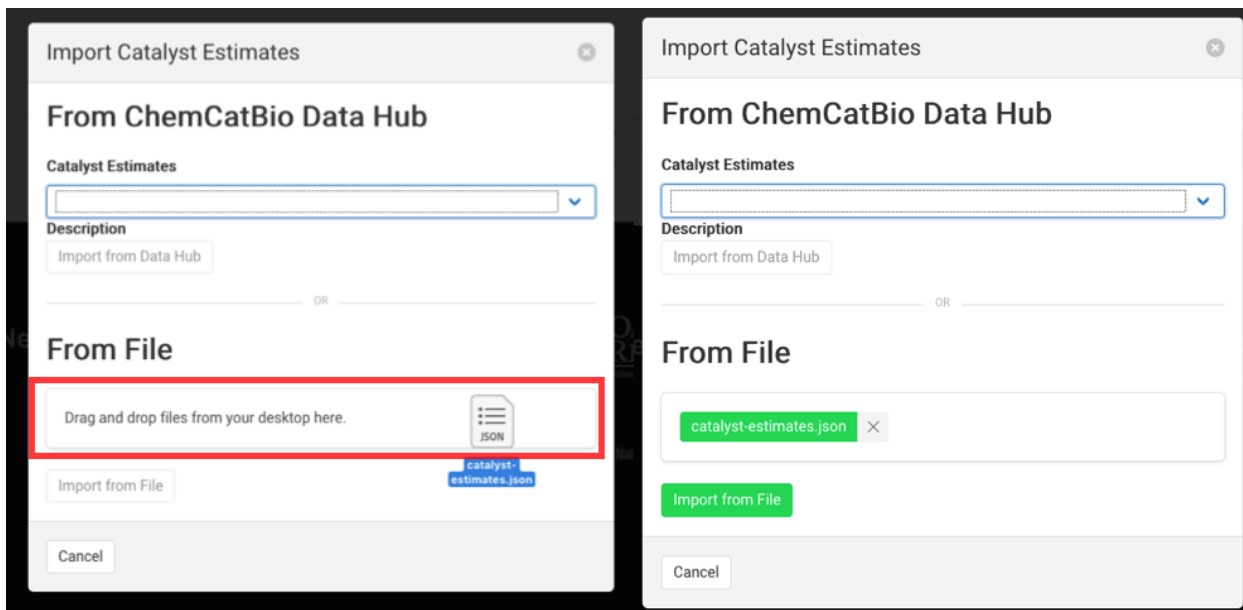

Figure 10.3. The import dialog for Catalyst Estimates (Left) and a successfully verified .json ready for import (right).

Important Note: This import operation is contextual and can be performed from any page of the CatCost tool. Be careful to only select .json files that correspond to the correct data type for the open page. For example, only select .json files that contain a "Materials Library" for import while on the "Materials Library" page; otherwise the file will fail to import. The data type is displayed at the top of each import dialog box.

Python scripts that are currently under development will be provided to aid users in transferring estimates and libraries between the Excel and web versions of CatCost. This will allow users to easily apply the benefits of each tool to a single estimate.

Note: the web version stores all user-entered content (estimates and libraries) locally in the browser used to access the tool. While the browser will check the CatCost website for an updated version of the tool each time it is run, no user-entered information is transmitted to or stored on CatCost/ChemCatBio web servers. No data entered, proprietary or otherwise, is transmitted to to CatCost, ChemCatBio, or the Data Hub. It is important to note that this means that in order to retrieve previously entered estimates or library entries, the same browser used to build them must be used, or the information must be downloaded as a JSON file. The user is therefore advised to back up their estimates and libraries as described above.

10.2 Visualizations in the CatCost Web Tool

The web version of CatCost has the added functionality of powerful visualizations that can be manipulated in real time. The initial release of the CatCost webtool (v1.0.0) includes three visualization options that enable users to interact with their cost estimate beyond the capabilities of Excel, including a Sankey Diagram, an interactive cost breakdown "donut chart," and a customizable pie chart as shown in Figure 10.4b-d. These visualizations can be accessed while editing an estimate by placing the cursor over the "Visualize" menu on the estimation navigation toolbar as shown in Figure 10.4a and selecting one of the visualization options.
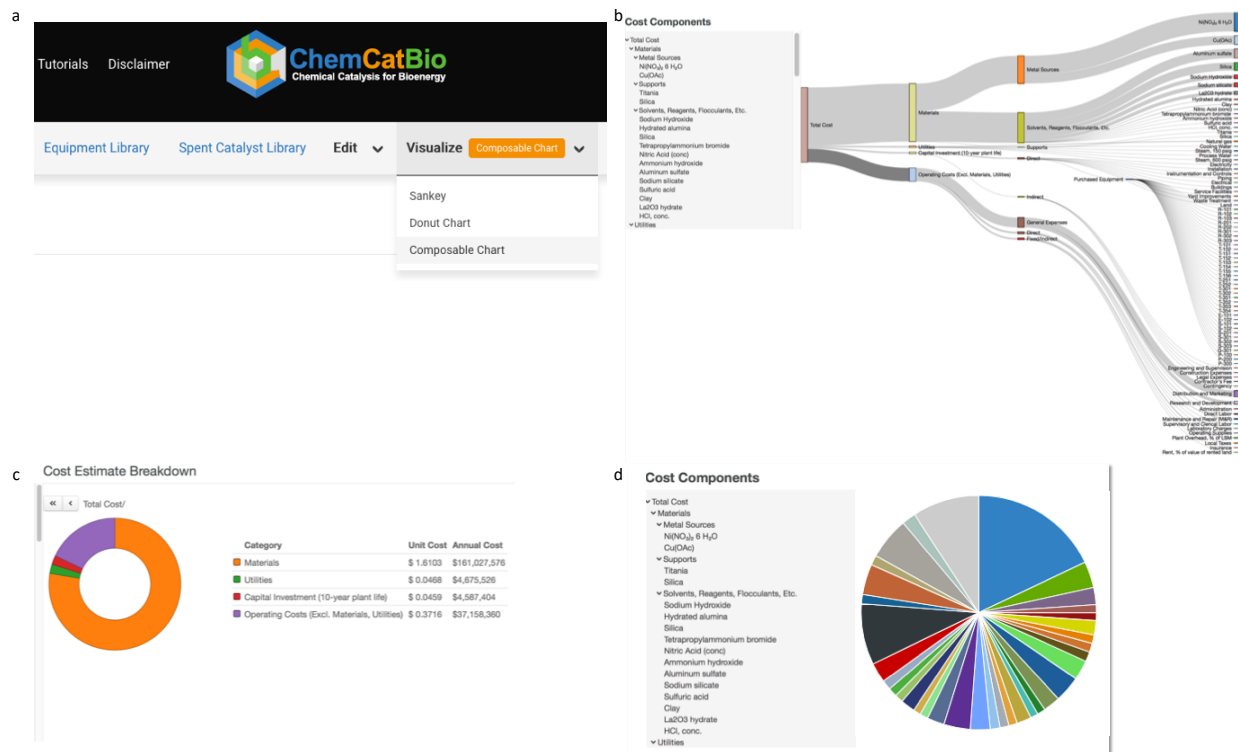
Figure 10.4. The drop-down menu to access the interactive visualizations of cost data (a) including the Sankey diagram (b) interactive donut chart (c) and composable pie chart and (d).

The Sankey diagram highlights the hierarchical relationships of all cost contributors and enables the visualization of the flow of cost through an estimate. The data shown can be adjusted by clicking on any of the cost contributors, which collapses all sub-cost contributors in that category and removes them from display. The "donut" chart has been designed to facilitate analysis by allowing users to "drill" into any section and view what cost components contribute to that section simply by clicking on any cost component of interest either on the chart itself or from the table. The pie chart allows users to build their own graphics directly from the interface, selecting only the categories they wish to be visualized with a simple check/uncheck option available for each category.

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