

Technoeconomic Analysis Tool for Carbon Mineralization Processes

User Manual

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Disclaimer:

This is a beta version of the Carbon Mineralization TEA Tool. The results and analysis given by this tool are to be used as a relative estimation of economic performance by prospective carbon mineralization projects. Hence, results should not be taken as a definitive solution. Using this tool is done at your own risk. The author is not liable for damage resulting from the tool's use.

Introduction:

The purpose of this tool is to compare a wide array of prospective Carbon Mineralization (CM) projects. Using inputs of annual CO₂ sequestration, alkaline feed, and process steps, the tool will output the proposed project's net present value, material usage, capital and operating expenses, and net CO₂ sequestration. Essentially, the tool performs a large mass balance. That is, based on the desired annual CO₂ sequestration rate and the type of mineral product produced, the tool calculates the amount of alkalinity (magnesium and calcium) required for the entire process. This balances the amount of alkalinity required to enter the system (as alkaline feed) with the amount leaving the system (as a mineralized product containing CO₂). The general flow of the tool's mass balance is found in Section 1.5.

This tool contains a process model based on the six-step process shown in Figure 1. Each step is controlled separately and has the option to be skipped and removed from the calculations, presenting a versatile tool that can model processes of varying complexity. Within each step, you may view the mass balance, energy and material usage (operating expenses), and equipment selection (capital expenses).

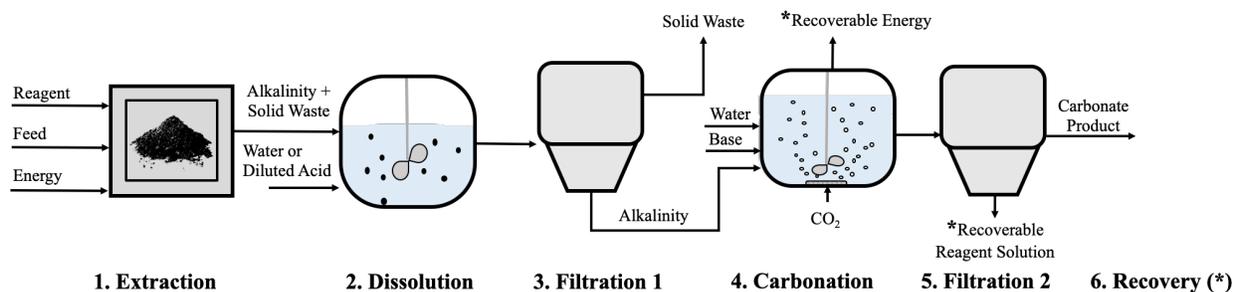


Figure 1: Process Flow Diagram

Within the tool, cells are organized by color, as shown in the color key in Figure 2. Generally, green cells require an input value, blue cells provide an output value, and red and gray cells can be ignored.

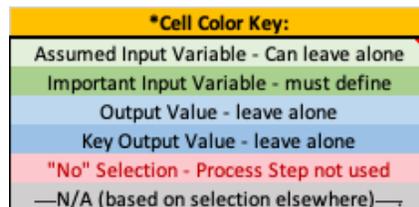


Figure 2: Cell Color Key within the Tool

Further, the tool consists of several tabs (located at the bottom of the spreadsheet) which have different purposes. Primary Tabs are colored green and contain the most important information for assessing CM projects. Data Input Tabs (yellow) are used for reference throughout the tool and are able to be edited by the user. Reference Tabs (red) contain back-end calculations of various parameters, and should not be altered. Finally, the orange dHrxn Calculator offers a more rigorous option for calculating energy requirements for chemical reactions. It may be edited, and its results may be manually input into the Process Tab, but it is not essential for the primary model calculations.

1.1 Navigating the Tool: A Quick Guide

Below is a generalized step-by-step guide to quickly navigate the tool. Explanation of different process steps is given in Section 2 of this manual, and detail about other model parameters and model outputs is given in Section 3. Additional instructive comments are included in the tool as comments, visible when hovering the cursor over a cell with a red marker in the top right corner, as shown below in Figure 3.

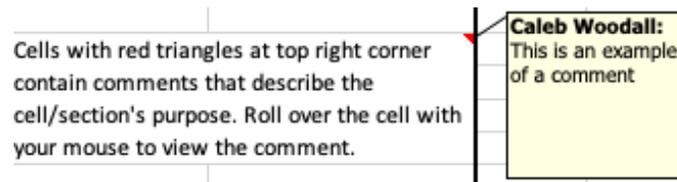


Figure 3: Example of a cell comment

1. Save the tool template for your new analysis: File → Save as → (name your file)
2. Open the tool to the Summary Tab. Find the title **Model Control Panel** (Cell E1).
3. In “Process Name”, enter a name for the process to be referred to throughout the tool, or leave as is.
4. Enter the desired annual CO₂ sequestration rate in “Target CO₂ Sequestered”
5. Select the alkaline feed to be used in the drop-down menu in “Alkaline Feed”
6. Select the alkaline cation to be targeted in “Selected Target Cation”
7. Enter the particle size of the alkaline feed in “Feed Particle Size”
8. Enter the “Cost of Alkaline Feed”
9. Enter the “Cost of CO₂ Supply”
10. Select the “Target Market Product”
 - a. If selected “Carbonate Product,” select the “Target Carbonate Product”
11. Enter the “Product Selling Price”
12. Enter operation times, “Project Life,” and “Project Starting Year”. “Project Life” impacts the project’s net present value calculation.
13. Look below at the figure which the tool’s model is based on.
 - a. Determine which steps apply to your process. As you navigate to the modules for each step below the figure, select Yes/No in “Use this step?”
14. Navigate to “0. Feed Preparation” (Cell E37)
15. Decide whether the feed preparation steps available are necessary, and select Yes/No accordingly.
 - a. If “Yes,” fill respective green input cells below.
16. Proceed to the modules for each process step (1. Extraction, 2. Dissolution, etc.)
 - a. Decide which steps are necessary, select Yes/No accordingly, then enter information in every available green cell.
17. Navigate to the next column of modules, **Other Model Parameters** (Cell I2).
18. In the Efficiency Assumptions module, enter values in all green cells.
 - a. Based on selections in previous process steps, some cells in Efficiency Assumptions are not applicable and are gray.
19. In Economics module:
 - a. Enter a “Discount Rate” (for net present value calculations)
 - b. Enter any applicable “Tax Credit”
 - c. Enter the “Current CEPCI Value” (for equipment costing), or leave as is

- d. Select an “Equipment Costing Model”
20. In Transport module:
 - a. Select Yes/No for whether the feed is transported to the project site.
 - i. If Yes, enter the distance and transport method accordingly.
 - b. Select Yes/No for whether the product is transported from the project site to the consumer.
 - i. If Yes, enter the distance and transport method accordingly.
21. At this point, all essential parameters have been set, and results are shown in the next column of modules, **MODEL OUTPUTS** (Cell M1).
22. In the **Process Summary** module, view the **CO2 Sequestration** results. This includes:
 - a. The CO2 “Sequestered as Carbonate”
 - b. The CO2 “Emitted from Process”
 - c. The CO2 “Emitted from Transport”
 - d. The CO2 “**Net Sequestered**” – the difference of the CO₂ sequestered as carbonate and the CO₂ emitted from the process and transportation.
23. Next, view the **Process Economics** results. This includes:
 - a. The “Total Transport Expense”
 - b. The “Total Capital Expense”
 - c. The “Total Operating Expense.” Here, a negative value means the product revenue is greater than the cost of materials and energy.
 - d. The “**Project Net Present Value**” (i.e., NPV). Here, a positive value indicates a profitable project.
24. Below, review the **Capital Expense Summary** and **Operating Expense Summary** modules. These are summaries of what has been entered through the separate process step modules in the Summary and Process Tabs. If something appears unsatisfactory, review the associated process step settings accordingly.

1.2 Key Inputs:

Information for each process step is viewed and controlled in two locations:

- Summary Tab
 - Here, process steps are separated into modules under the **Model Control Panel**
 - All essential parameters for each step are located in these modules, including:
 - Switching the step on/off (i.e., selecting Yes/No on “Use this step?”)
 - Process conditions
 - Equipment capacity
 - Additional chemical species employed
- Process Tab
 - Here, process steps are horizontally separated into sections across the screen.
 - Parameters less essential to the mass balance calculation are controlled here, including:
 - Time duration for each step
 - Equipment pressure (most cases are non-pressurized, so atmospheric pressure is entered by default)
 - Further, calculations are made for energy and material usage, and equipment may be selected for each step. These are found to the right of each process step section.

1.3 Key Outputs:

The primary outputs for this model are related to process economics, and are found in the Summary Tab under **MODEL OUTPUTS** (Cell M1)

- Net CO₂ Sequestration
 - This value is found in bold under CO2 Sequestration within the **Process Summary** module (Cell M11).
 - The energy requirements of some processes may result in significant CO₂ emissions, leading to low overall net sequestration. The method to increase the CO₂ net sequestered is explained in the **MODEL OUTPUTS** section of this manual.
- Net Present Value
 - This value is found in bold under Process Economics within the **Process Summary** module (Cell M16).
 - This value indicates the profitability of the CM project under evaluation. A positive value indicates that the project is profitable over its full life, while a negative value indicates the project is not profitable.
 - This value is based on the project life, discount rate, capital, operating, and transport expenses, and revenue from products and tax credits.
- Capital Expense
 - The capital expense of each process step is summarized in the **Capital Expense Summary** module (Cell M18).
 - The capital equipment employed for each process step may be edited in the Process Tab within its respective process step section.
- Operating Expense
 - The material and energy use may be found with their associated operating expense in the **Operating Expense Summary** module (Cell M45).
 - Here, the source of electric and thermal energy may be selected.
 - The amount of each species is not easily edited, as they are generated by the model mass balance.
 - To edit costs associated with chemical species, see Species Data Tab.

1.4 Key Assumptions:

- It is assumed that a batch process is used, rather than a continuous one.
 - Mass balance calculations are made based on running a single batch with a time duration.
 - Using this duration and the user-specified annual operating time of the process, the model calculates how many batches can be run per year.
 - The target annual CO₂ sequestration rate is divided by the number of batches per year to determine the quantity of CO₂ to sequester in each batch.
 - The time duration of each process step may be manually edited in the Process Tab.
- It is assumed that only one cation (Mg or Ca) present in the feedstock is targeted for extraction and carbonation. This avoids accounting for competitive reaction and precipitation between the two cations.
 - The amount of the non-targeted cation that is neglected due to this assumption is shown near the top of the Process Tab (Cell A21). This is in addition to the amount of the target cation that is not reacted due to efficiency assumptions input within the Summary Tab.

- Due to the high variability of reaction schemes and feedstock, reaction kinetics are not employed in this tool’s model. Instead, efficiency assumptions are used to govern each point of the process where a reaction would take place.
 - These efficiency values are input in the Efficiency Assumptions module under **Other Model Parameters** in the Summary Tab.

1.5 General Flow of Mass Balance

The general flow of the mass balance is shown in Figure 4, where “X” indicates the target cation. Text in each box is precisely as written within the model cells. A bottom-up approach has been taken with this model, where the amount of CO₂ sequestered is the primary input. Based on the desired CO₂ sequestered amount, material and energy requirements are calculated.

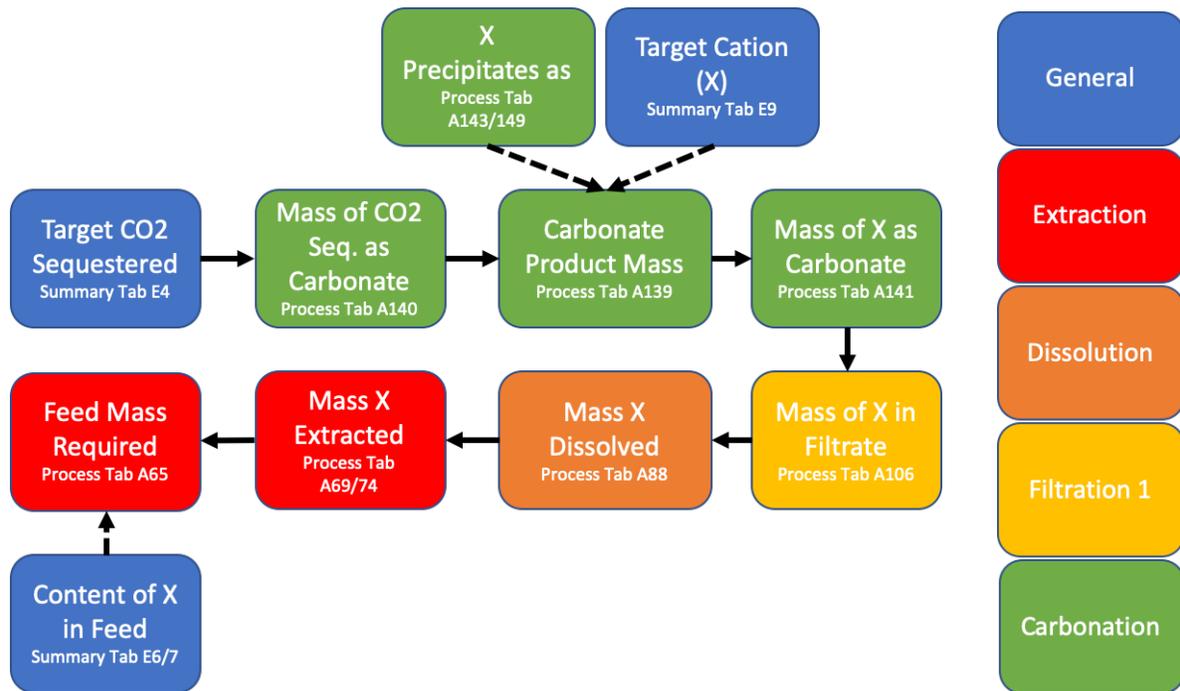


Figure 4: Diagram of important steps in the model’s mass balance
 X indicates the target cation (Mg or Ca)
 Colors indicate process step section, with key to the right

2. Explanation of Process Steps

This section of the manual explains the purpose of each process step shown in Figure 1 and in the Summary and Process Tabs of the tool.

0. Feed Preparation

This involves preliminary steps taken to prepare the alkaline feed for processing, and is not included within the process diagram. The options within this step include:

“Mix feed with water and/or other species”

Description:

- This would be useful in the case of producing alternate cement or concrete. By default, this option is selected as “No.” Selection of “Yes” will activate the cell below, asking for a mass ratio of water or other species to feed.

Impact on Key Outputs:

- Information entered within these options is used to calculate the material requirements of the Feed Preparation step, ultimately impacting Operating Expense and the project’s NPV. These selections have no impact on reaction progress or reactivity.

“Size Reduction”

Description:

This is a follow up to the “Size Reduction Suggestion” within the **Model Control Panel**. By default, this option is selected as “No.” Selection of “Yes” will activate the cells below, asking if a mill, crusher, or both will be used, along with the desired particle sizes to be produced by the mill and/or crusher. Specific equipment may be chosen in the 0. Feed Preparation section of the Process Tab (Section 5).

- A crusher would be used to reduce particle size to the order of 5,000-250,000 μm .
- A mill would be used after a crusher to further reduce the particle size to sizes of 3-100 μm .
- The recommended particle size is 75-125 μm , where the additional energy used to reduce the size below this range is greater than the added reactivity.

Impact on Key Outputs:

- Use of size reduction activates energy calculations, impacting Operating Expense and the project’s NPV.
- Energy used here will result in additional CO₂ emissions, impacting the Net CO₂ Sequestered.

1. Extraction

This is the first step included in the process flow diagram. It involves extracting the alkaline cations from the feed and converting them to a more reactive form via a thermal reaction. If no thermal reaction is employed by the process under evaluation, select “No” for this step.

Assumptions:

- It is assumed that this is carried out via a thermal cation exchange reaction, where an ammonium salt is reacted with the alkaline feed to produce an alkaline salt.
- Reaction kinetics are not employed in this model. Instead, the efficiency of the extraction reaction should be input in the Efficiency Assumptions module under **Other Model Parameters**.
- It is assumed that the reaction takes place at a constant temperature.
- The energy required for this reaction is modeled by heating silica and air within a furnace. For a more rigorous calculation, use the dHrxn Calculator Tab.

Impact on Key Outputs:

- The Extraction step involves an energy-intensive thermal reaction, impacting Net CO₂ Sequestered, Operating Expense, and the project's NPV.
- Most of the reagents come with a high economic cost, heavily affecting Operating Expense and the project's NPV.
- Equipment in this step is modeled by a selection of reactors, heaters, and furnaces. The costing of the reactors is affected by the reactor volume, while the heater and furnace costing are affected by the heat duty. Selection of equipment affects Capital Expense and the project's NPV.

2. Dissolution

This step is likely to take place for any indirect mineralization process. Here, you may choose whether dissolution occurs in water or a diluted acid solution. If neither of these are employed by the process under evaluation, select “No” for this step.

Assumptions:

- Dissolution is assumed to occur at ambient temperature (25 °C).
- Dissolution is assumed to occur at ambient pressure (1.013 bar). If you want pressurized dissolution, the pressure may be edited in the 2. Dissolution section of the Process Tab.
- In the case of using alkaline salts, the tool calculates the amount of water required to dissolve X% of the salt alkaline salt, where X is the Mg/Ca Dissolution Efficiency input under Efficiency Assumptions module in the Summary Tab.
- If selecting “Diluted Acid”, it is assumed the acid is mixed with water. In this case, no kinetics or acid solubility are used to determine the required solution volume. Instead, you must input a ratio of acid solution to feed. The Mg/Ca Dissolution Efficiency input is used here to determine the X% of feed that dissolves in the diluted acid solution.

Impact on Key Outputs:

- Use of acid and/or water for dissolution comes with economic cost, impacting the Operating Expense and the project's NPV.
- Equipment for this step is tooled by options for standard vessels, the costing of which is dictated by the volume required. Hence, the “Dissolution Volume Required” output of the dissolution step impacts Capital Cost and the project's NPV.

3. Filtration 1

This step is used to separate aqueous alkaline solution from any unwanted material. In this tool, this step is essentially an extension of the 2. Dissolution step. The amount of the target alkaline cation that remains in the liquid filtrate is calculated based on the alkaline salt's solubility and the dissolution efficiency.

Assumptions:

- No considerations are taken for particle size distribution or its role in filtration. It is assumed all liquid passes through the filter as “filtrate,” while all solid remains as “residue”.
- It is assumed that this step only takes place if 2. Dissolution precedes it.
 - i.e., if 2. Dissolution is deactivated, 3. Filtration 1 should also be deactivated.

Impact on Key Outputs:

- Equipment for this is modeled by a gravity filter, the costing of which is affected by the filter area. This affects Capital Cost and the project's NPV.

4. Carbonation

This step is essential to the tool's calculations. Carbonation may be performed in aqueous solution (“Wet”) or as a gas-solid reaction (“Dry”).

Within this step is the option to select Preliminary Curing. This would likely be employed for production of alternate cement, where reactants may need to settle, mold, or cure at a specified temperature without the presence of CO₂. In this case, additional settings should be input within the 4. Carbonation section of the Process Tab.

Assumptions:

- It is assumed that pure CO₂ is used for carbonation. There are no measures for competitive adsorption of different gaseous species.
- Reaction kinetics are not employed for the carbonation reaction. Instead, input a Mg/Ca Carbonation efficiency within the Efficiency Assumptions module in the Summary Tab.
 - Similarly, there is no measure for pH. The option to include a base is merely for accounting for material usage.
- For Wet carbonation, there are two efficiency assumptions involved:
 - Mg/Ca Carbonation efficiency means X% of the Mg/Ca available in solution reacts with CO₂ to form the specified mineral product.
 - Carbonation [Wet] efficiency means X% of the CO₂ entering the system is bound to an alkaline cation rather than leaving the system unbound.
- For Dry carbonation, the efficiency means X% of the CO₂ entering the system is absorbed rather than leaving the chamber/reaction unbound.

Impact on Key Outputs:

- Selection of efficiencies for this step affects the materials and energy required in all upstream steps, ultimately affecting Operating Expense and the project's NPV.

- Equipment for this step involves a curing chamber (if Preliminary Curing is employed) and a carbonation vessel. These are modeled by autoclaves, the costing of which is affected by the volume. This impacts Capital Expense and the project's NPV.
- Energy requirements are calculated for the separate cases of Preliminary Curing, Dry carbonation, and Wet carbonation. This affects the Operating Expense and the project's NPV. This also results in additional CO₂ emissions, affecting the project's Net CO₂ Sequestered.

5. Filtration 2

This step would be employed in the case of Wet carbonation to separate the solid carbonate products from the liquid filtrate. No calculations are performed here, and it is merely used to account for time and capital equipment.

Assumptions:

- No considerations are taken for particle size distribution or its role in filtration. It is assumed that the solid carbonate product is perfectly separated from the liquid filtrate.
- It is assumed that this step only occurs if wet carbonation is performed in 4. Carbonation.
 - i.e., if 4. Carbonation uses dry carbonation, 5. Filtration 2 should be deactivated.

Impact on Key Outputs:

- Equipment for this step is modeled by a gravity filter, the costing of which is affected by the filter area. This impacts Capital Expense and the project's NPV.

6. Recovery

This step is placed at the end of the process as a means to recover the extraction reagent, acid, base, water, and CO₂.

Assumptions:

- The recovery percentage (e.g. "Reagent Recovered (%)") input in the Summary Tab is multiplied by the amount of material (e.g., reagent) used within the initial process batch. This calculates an amount of material that can be recycled in the subsequent batch.
- The recovery percentage is assumed to apply to every batch after the initial batch for the entire year.
 - If you desire to model a gradual decline in recovery, they should input a value that is averaged over the entire year.
- It is assumed that no energy is required for material recovery. However, boxes were left green in the Operating Expense box within the 6. Recovery section of the Process Tab so energy may be input manually.

Impact on Key Outputs:

- Use of this step has a major impact on the material requirements over the full year of the project's operation. This affects Operating Expense and the project's NPV.
- Options are given for using equipment for recovery steps. This is modeled by various vessels, the costing of which are affected by volume. This impacts Capital Expense and the project's NPV.

3. Summary Tab

The Summary Tab summarizes all of the tool's primary input and output values. These values are categorized into separate "modules" within thick rectangular borders. There are three columns of modules: **Model Control Panel**, **Other Model Parameters**, and **MODEL OUTPUTS**.

Most parameters within the Summary Tab have comments that give explanation as needed. In this section of the manual, additional explanation is given for the more complex parameters.

Model Control Panel

- Target CO₂ Sequestered (Cell E4)
 - This parameter is very important for the entire mass balance of the tool's model. This value is the "Target" sequestration rate (i.e., not net-sequestered). CO₂ net-sequestered is explained in under Other Model Parameters
- Efficiency Assumptions (Cell I2)
 - Based on the inputs of the Selected Target Cation and the process step modules, efficiency assumption options relevant to the process under evaluation will appear green. Explanation of all efficiency options:
 - Mg/Ca Extraction (Cell I4/I8)
 - X% of Mg/Ca within the alkaline feed is extracted and available for the next process step.
 - Mg/Ca Dissolution (Cell I5/I9)
 - X% of Mg/Ca available for dissolution (either from the raw feed or after thermal extraction) is dissolved and available for next process step.
 - Mg/Ca Carbonation [Wet] (Cell I6/I10)
 - X% of Mg/Ca available for carbonation reacts with CO₂ and is carbonated to the form of the Target Carbonate Product.
 - Carbonation [Wet] (Cell I12)
 - X% of CO₂ entering the aqueous carbonation system reacts and binds with the available alkaline cations rather than leaving the system unbound.
 - (if this step is an enclosed system, use 100% here)
 - If the CO₂ leaving the system unbound is recycled, indicate this using Unbound CO₂ Recovered (%) (Cell E90)
 - Carbonation [Dry] (Cell I13)
 - X% of CO₂ entering the solid-gas carbonation system reacts and binds with the feed rather than leaving the system unbound.
 - (if this step is an enclosed system, use 100% here)
 - If the CO₂ leaving the system unbound is recycled, indicate this using Unbound CO₂ Recovered (%) (Cell E90)
- Economics (Cell I15)
 - The parameters in this module either directly or indirectly affect the project's NPV.
 - Discount Rate
 - This value is directly used in the NPV calculations. It is the rate of return expected on the investment (i.e., the cost of borrowing money).
 - Tax Credit

- This value is directly input in the NPV calculations.
 - It is assumed that the tax credit applies to all CO₂ sequestered within the product.
 - (this is NOT the net-CO₂ sequestered. Rather it is the TOTAL CO₂ sequestered)
 - Current CEPCI Value
 - CEPCI – Chemical Engineering Plant Cost Index. This is a value used in the bare module costing method of estimating the cost of chemical engineering plant equipment.
 - The bare module costing method uses parameters specific to various types of equipment. These parameters are developed and published in textbooks, and have a CEPCI value associated with the date that the parameters are published. By using the current CEPCI value, the cost estimations of the equipment may be normalized to the current month and year.
 - At the time of developing this tool, the current CEPCI value was 596. This changes monthly and may be found here:
 - <https://www.chemengonline.com/pci>
 - Equipment Costing Model
 - The bare module cost generated for each equipment type does not include contingency and auxiliary fees for installation. This option allows you to select three different costing options:
 - Bare Module Cost – sum of direct and indirect costs for equipment.
 - Total Module Cost – Bare Module Cost, plus costs for contingency and fees and auxiliary facilities (i.e., installation and purchase costs) for equipment added to existing facility.
 - Grassroots Cost – installation on completely new facility that’s being started on undeveloped land.
- Transport (Cell I22)
 - This module allows you to account for costs and emissions associated with transporting the feed and/or product.
 - For each option (feed and product transport), selecting “Yes” will activate green input cells for the distance traveled and method of transport.
 - Calculations are performed in the Transport Tab, and the results are displayed in this module (Transport Expense, Transport Emissions)
 - Data and calculations further explained in the Transport Tab section of this manual.
- CO₂ Curing Comparison (Cell I35)
 - Carbon mineralization may be applied by injecting CO₂ into concrete to enhance the curing process, create a stronger concrete product, and store CO₂. This module estimates the amount of concrete that could be made with the same target CO₂ sequestered input in **Model Control Panel**.
 - In this module, select the Concrete Product to produce (Cell I38)
 - Publication data differs among producing concrete in bulk and producing concrete blocks. Hence, an option among the two was given here.
 - Select the process type (Cell I29)

- This is a drop-down menu to select either Mg or Ca as the cation to target. A third option is to select “N/A (cement)”, used in the case of a CM process to make alternate cement.
- The selected target cation determines the amount of alkalinity available per kilogram of feed. This ultimately affects the amount of feed required to sequester the target amount of CO₂.
- As discussed in Key Assumptions (Section 1.4) the tool does not account for competition between Mg and Ca, and only considers the carbonation of the selected target cation.
- Feed Particle Size (Cell E10)
 - This parameter is used to determine whether the alkaline feed should undergo size reduction. The size must be entered in micrometers (i.e., microns, μm).
 - This cell alone does not force size reduction to be undertaken through the process, and hence does not force additional capital or operating expenses. Size reduction is selected in the controls of the 0. Feed Preparation step.
 - Based on the size input, the cell below will suggest if a crusher and/or mill should be used, informing you on what to select in 0. Feed Preparation.
 - A crusher would be used to reduce particle size to the order of 5,000-250,000 μm.
 - A mill would be used after a crusher to further reduce the particle size to sizes of 3-100 μm.
 - The recommended particle size is 75-125 μm, where the additional energy used to reduce the size below this range is greater than the added reactivity.
- Cost of CO₂ supply (Cell E14)
 - This cell affects operating expenses and ultimately the project’s net-present value.
 - In the case of tax credits that involve incentives per tonne CO₂ sequestered, do not enter a negative value here. Tax credits should be input in the Economics module under **Other Model Parameters**. If the CO₂ is acquired at no cost, type 0.
- Target Market Product (Cell E16)
 - This cell gives a drop-down menu of different product options:
 - Carbonate Product
 - This assumes a standard carbonate mineral product, which may be selected in a different drop-down menu in the cell below.
 - For aggregate production, select this product option.
 - Bulk Cement
 - This involves producing a material that replaces portland cement within concrete mixtures.
 - This does not involve curing cement with CO₂.
 - Bulk Concrete
 - This involves producing a material that fully replaces conventional concrete.
 - This does not involve curing concrete with CO₂.
- Process steps (Cell E37)
 - All process step modules are explained in Section 2 of this manual.

Other Model Parameters

- Efficiency Assumptions (Cell I2)
 - Based on the inputs of the Selected Target Cation and the process step modules, efficiency assumption options relevant to the process under evaluation will appear green. Explanation of all efficiency options:
 - Mg/Ca Extraction (Cell I4/I8)
 - X% of Mg/Ca within the alkaline feed is extracted and available for the next process step.
 - Mg/Ca Dissolution (Cell I5/I9)
 - X% of Mg/Ca available for dissolution (either from the raw feed or after thermal extraction) is dissolved and available for next process step.
 - Mg/Ca Carbonation [Wet] (Cell I6/I10)
 - X% of Mg/Ca available for carbonation reacts with CO₂ and is carbonated to the form of the Target Carbonate Product.
 - Carbonation [Wet] (Cell I12)
 - X% of CO₂ entering the aqueous carbonation system reacts and binds with the available alkaline cations rather than leaving the system unbound.
 - (if this step is an enclosed system, use 100% here)
 - If the CO₂ leaving the system unbound is recycled, indicate this using Unbound CO₂ Recovered (%) (Cell E90)
 - Carbonation [Dry] (Cell I13)
 - X% of CO₂ entering the solid-gas carbonation system reacts and binds with the feed rather than leaving the system unbound.
 - (if this step is an enclosed system, use 100% here)
 - If the CO₂ leaving the system unbound is recycled, indicate this using Unbound CO₂ Recovered (%) (Cell E90)
- Economics (Cell I15)
 - The parameters in this module either directly or indirectly affect the project's NPV.
 - Discount Rate
 - This value is directly used in the NPV calculations. It is the rate of return expected on the investment (i.e., the cost of borrowing money).
 - Tax Credit
 - This value is directly input in the NPV calculations.
 - It is assumed that the tax credit applies to all CO₂ sequestered within the product.
 - (this is NOT the net-CO₂ sequestered. Rather it is the TOTAL CO₂ sequestered)
 - Current CEPCI Value
 - CEPCI – Chemical Engineering Plant Cost Index. This is a value used in the bare module costing method of estimating the cost of chemical engineering plant equipment.
 - The bare module costing method uses parameters specific to various types of equipment. These parameters are developed and published in textbooks, and have a CEPCI value associated with the date that the parameters are

published. By using the current CEPCI value, the cost estimations of the equipment may be normalized to the current month and year.

- At the time of developing this tool, the current CEPCI value was 596. This changes monthly and may be found here:
 - <https://www.chemengonline.com/pci>
- Equipment Costing Model
 - The bare module cost generated for each equipment type does not include contingency and auxiliary fees for installation. This option allows you to select three different costing options:
 - Bare Module Cost – sum of direct and indirect costs for equipment.
 - Total Module Cost – Bare Module Cost, plus costs for contingency and fees and auxiliary facilities (i.e., installation and purchase costs) for equipment added to existing facility.
 - Grassroots Cost – installation on completely new facility that’s being started on undeveloped land.
- Transport (Cell I22)
 - This module allows you to account for costs and emissions associated with transporting the feed and/or product.
 - For each option (feed and product transport), selecting “Yes” will activate green input cells for the distance traveled and method of transport.
 - Calculations are performed in the Transport Tab, and the results are displayed in this module (Transport Expense, Transport Emissions)
 - Data and calculations further explained in the Transport Tab section of this manual.
- CO2 Curing Comparison (Cell I35)
 - Carbon mineralization may be applied by injecting CO₂ into concrete to enhance the curing process, create a stronger concrete product, and store CO₂. This module estimates the amount of concrete that could be made with the same target CO₂ sequestered input in **Model Control Panel**.
 - In this module, select the Concrete Product to produce (Cell I38)
 - Publication data differs among producing concrete in bulk and producing concrete blocks. Hence, an option among the two was given here.
 - Select the process type (Cell I29)
 - There are primarily two different methods of approaching curing concrete with CO₂:
 - “Portland Cement Curing” - uses ordinary portland cement for the concrete (e.g., CarbonCure)
 - “Ca-Silicate Cement Curing” – alters the proportions of the ordinary portland cement mixture (e.g., Solidia)
 - These two technologies have published different results, so both options are given in this estimation module.
 - Due to lack of data on energy demand of CO₂-curing processes, an “Assumed Energy Demand” should be specified (Cell I40)
 - This is to calculate the overall CO₂ avoided by the process. If no energy demand is known, leave this value as “0”. This will result in a less accurate estimation of the CO₂ emissions avoided by the process.

- It is also difficult to acquire economic data for the CO₂-curing processes. Hence, this is omitted from this estimation module.
- The calculation is performed in the CO₂ Curing Tab (Section 0 of the manual).
 - Data is used from various publications as noted within the Tab. Cells are left green in the case you have proprietary data that more accurately describes the technology being assessed.
- Outputs of this estimation module are:
 - Product Yield – the amount of bulk concrete or concrete blocks produced during a full year with the target CO₂ sequestered.
 - Process Emissions – the CO₂ emitted by the process based on the Assumed Energy Demand.
 - Net CO₂ Avoidance – the CO₂ emissions avoided due to this process. This accounts for the CO₂ sequestered within the concrete product, the Process Emissions, and the avoided CO₂ that would otherwise have been emitted from production of conventional concrete products.
 - This value could be compared to the Net Sequestered value in **MODEL OUTPUTS**

MODEL OUTPUTS

Process Summary module (Cell M2)

- **CO₂ Sequestration** (Cell M7)
 - The CO₂ “Sequestered as Carbonate” is identical to the “Target CO₂ Sequestered” input under **Model Control Panel**
 - The CO₂ “Emitted from Process” is calculated based on the process’ energy demand and the source of electricity and heat.
 - Energy demand and sources are viewed below in **Operating Expense Summary**
 - The CO₂ “Emitted from Transport” is based on the **Transport** module and the selected energy source.
 - The CO₂ “**Net Sequestered**” is the difference of the CO₂ sequestered as carbonate and the CO₂ emitted from the process and transportation. To mitigate process emissions and maximize climate impact, it may be desired to change the CO₂ “Net Sequestered” to the full amount desired.
- To change the CO₂ “**Net Sequestered**” to the value actually desired, use the Excel Goal Seek function:
 - Click on the cell with the CO₂ “**Net Sequestered**” value (Cell M11).
 - i.e., this cell should have a number value, not text.
 - In the Excel ribbon menu, navigate to Data → What-If Analysis → Goal Seek
 - On “Set cell:” the cell should be the cell selected of CO₂ “**Net Sequestered**” (Cell M11).
 - On “To value:” enter the desired CO₂ annual sequestration rate. This may be the value initially input in “Target CO₂ Sequestered” (Cell E4).
 - On “By changing cell:” enter the cell column and row of the initially entered “Target CO₂ Sequestered” (e.g., for Process 1 - Cell “F4”)
 - Click “OK”

- Excel will iteratively change the “Target CO2 Sequestered” value until the desired “**Net Sequestered**” value is reached.
 - This will result in changes to several parameters calculated throughout the tool, essentially increasing/decreasing the capacity of the proposed process in order to achieve the desired “**Net Sequestered**” value. The main parameters likely to change include the required alkaline feed and dissolution volume
- Process Economics (Cell M12)
 - The “Total Transport Expense” is a sum of the expenses generated in the Transport module.
 - The “Total Capital Expense” is a sum of the capital expense incurred due to all equipment required by the process. This value is elaborated upon in the Capital Expense Summary module.
 - The “Total Operating Expense” is sum of the operating expense incurred due to all material and energy process requirements. Here, a negative value means the product revenue is greater than the cost of materials and energy.
- The “**Project Net Present Value**” (i.e., NPV) is an indication of the profitability of the process under evaluation. Here, a positive value indicates a profitable project, while a negative value indicates the project is not profitable.
 - This value is based on the project life, discount rate, capital, operating, and transport expenses, and the tax credit.
 - The calculation is performed in the NPV Tab. This tab is only for reference, and there are no green cells for user inputs.

Capital Expense Summary module (Cell M18)

- This module summarizes all equipment specified in each process step section in the Process Tab (Section 5 of this manual).
- No edits can be made here. Equipment can be edited on the far right of each process step section in the Process Tab. (Column T)

Operating Expense Summary modules (Cell M45)

- This module summarizes all material and energy requirements of the process due to the various user inputs throughout all process steps.
- No edits can be made here. The operating expense of each process step is summarized in each process step section within the Process Tab.

4. Analysis Tab

This tab is dedicated to performing various analyses on the model outputs. By default, five analyses have been performed:

- Net Present Value Profile
 - This plot is generated based on values in the NPV Tab.
 - At the point where the curve crosses the x-axis (NPV = \$0), the project becomes profitable.
 - If the curve never crosses above the x-axis, the project is estimated to take longer than 50 years to become profitable, and is likely a poor investment.
- CAPEX and OPEX Distribution
 - These pie charts are generated to display how the capital/operating expense is distributed amongst all process step inputs.
 - By default, all possible equipment types are included in the legend, even if they are not used in the process under evaluation.
- Sensitivity Analysis: Mg and Ca Efficiency
 - A plot is generated for each process depicting the tool's sensitivity to individual changes of Mg and Ca efficiency on the NPV calculation.
 - For example, the curve of "Ca Extraction" indicates how the project NPV changes due to changes in the Ca Extraction efficiency input value. This assumes that all model input values remain constant aside from the Ca Extraction efficiency input value.
 - This applies to the other two curves, "Ca Dissolution" and "Ca Carbonation"
 - Only the plot corresponding to the target cation will be valid.
 - E.g., if Ca is the target cation for Process 1, the Mg Efficiency plot for process 1 will be invalid and can be ignored.
 - Additionally, two-variable analyses are performed for the combination of extraction and dissolution efficiency. These are located in the Summary Tab, beginning in Cell AF2. A color scale is used, where the green cells indicate the efficiency combinations that result in the most profitable project.
- Sensitivity Analysis: Expense and Revenue
 - A plot is generated for each process depicting the sensitivity of the project's NPV to changes in the price of alkaline feed, CO₂, product, and tax credit.
 - All relationships are linear. The price where a line crosses the x-axis (i.e., NPV value of \$0) indicates the minimum price (for tax credit and product) or maximum price (for alkaline feed and CO₂) required for a profitable CM project.
- Sensitivity analysis is performed with Excel's built-in iterative "What-if Analysis Data Table".
 - Due to the programming of this Excel function, the data tables must be generated in the same tab as the manipulated parameters.
 - In this case, efficiency inputs are in the Summary Tab, so the data tables are also located in the Summary Tab to the right of **MODEL OUTPUTS**.
 - This type of analysis could be performed for various other model parameters. For more information, visit [here](#).

5. Process Tab

This tab is divided horizontally into eight sections. The top section summarizes all outputs of the other seven sections, which correspond to each process step. Each of the seven process step sections consist of four parts, as shown in Figure 5. Some process step sections are not associated with energy demands, and thus the column of “Energy Parameters and Calculations” is blank.

		Mass Balance Parameters and Calculations	Energy Parameters and Calculations	OPEX Manual Inputs and Calculations	Equipment Selection and CAPEX Calculations
Process Step Section	0. Feed Preparation				
	1. Extraction				
	2. Dissolution				
	3. Filtration 1				
	4. Carbonation				
	5. Filtration 2				
	6. Recovery				

Figure 5: Organization of Process Step Sections within Process Tab

Equipment for each process step may be selected from drop-down menus in the far-right column of each process step section. The costing of the equipment is performed in the Equipment Tabs.

The Process Tab primarily consists of calculations and model outputs. However, there are some light green input cells that are less essential to the tool’s calculations. Blue cells host calculations or references to the Summary Tab, and should not be changed. In this section of the manual, some of the more complicated calculations performed in the Process Tab will be explained.

Summary Section

- Batch time (Cell A16)
 - The batch time is calculated based on the “Assumed Time” input in each of the process step sections. Only the process steps that are activated with “Yes” are included in this calculation.
 - Time duration of each process step is written as default in the respective process step section. This may be changed by the user
 - The batch time dictates the amount of CO₂ that may be sequestered in one batch, impacting the capacity required for all equipment and ultimately the Capital Expense and the project’s NPV.
- Cation Neglected (Amount and CCS *potential*) (Cells A22-24)
 - These values have no impact on the primary model calculations, and are used for your reference.
 - The amount of the non-targeted cation that is neglected within the feedstock is calculated based on the composition of the alkaline feed (Cell A23)
 - The maximum amount of CO₂ that could be sequestered with the neglected cation is calculated based on a mass ratio of CO₂ to the neglected cation (Cell A24)
- Amount of target cation unused (Cell A26)
 - This value is based on the carbonation efficiency for the target cation. There is currently no recycle option for the target cation in the model.
- **Materials Summary** (Cell K7)
 - The cells calculating material amounts (Columns M and P) use “array” formulas to add all material amounts from each of the process step sections below.

- After clicking on one of these cells, [control+shift+enter] must be pressed for the formula to work. Otherwise, the cell will return “#Value”.
- The cost associated with the material amounts (Columns N and Q) is calculated by referencing the costs input in the Species Data Tab.
 - Costs for most of the species used in the model are already input by default within the Species Data Tab.
- If no cost is shown for a certain species, the data in the Species Data Tab is likely incomplete. Navigate to the Species Data Tab and manually input a cost value.

6. Data Input Tabs (Yellow)

Yellow-colored tabs host data that is referenced within the Summary and Process Tabs, and are referred to here as Data Input Tabs. While the data entered by default is cited within cell comments or at the bottom of the spreadsheet, it may not apply to all situations. If you have more accurate data for the information within the Data Input Tabs, the default data within light green cells may be manually over-written.

As noted within the tabs, the Excel formula “vlookup” is used to reference these Data Input Tabs, and the syntax requires a column number. At the top of the columns, there are column numbers, shown in Figure 6 below. These numbers should not be removed or interfered with. Doing so would likely result in errors in the model calculations.



Figure 6: Example of Column Numbers in Data Input Tabs

Below are descriptions and information pertaining to the four Data Input Tabs.

Species Data Tab

This tab is used as a data reference throughout the excel file. Several anions, cations, solids, salts, minerals, etc. are listed with corresponding relevant data, like molecular weight, price, and solubility. Due to limitations on data availability or time constraints, data is incomplete for some species, especially for the species price. To ensure accurate calculation of operating expense, confirm that all raw materials used within the process under evaluation have a price value entered in this tab.

Parameters under the **Model Control Panel** in the Summary Tab offer drop-down menus for choices of species. If a material used in the process is not available in the menu, it may be manually added to the Species Data Tab:

1. Determine the type of species to be added (gas, liquid, salt, acid, etc)
 - a. In this example, Hydrobromic Acid (HBr) will be added
2. In the Species Data Tab Column A, find set of species type that matches your new species
 - a. Acids are located in A46-A50
3. Navigate to the bottom-most row for the desired species type
 - a. This would be row A50, shown in the screenshot:

46	Acid	Acetic Acid (CH ₃ COOH)
47	Acid	Hydrochloric Acid (HCl)
48	Acid	Sulfuric Acid (H ₂ SO ₄)
49	Acid	Oxalic Acid (C ₂ H ₂ O ₄)
50	Acid	Citric Acid (C ₆ H ₈ O ₇)

4. Right-click on the row number and click insert
 - a. This would be the number “50”, shown in the screenshot:

4	Paste Special	CH ₃ COOH)
4		Acid (HCl)
4	Insert	(H ₂ SO ₄)
4	Delete	(C ₂ H ₂ O ₄)
5	Clear Contents	(C ₆ H ₈ O ₇)

5. Now, fill in all relevant information for the newly added species. A good rule of thumb would be to mimic the data that is already input for the other species of the same type.
 - a. For acids, this includes the Name, Molecular Weight, Price, and Density.

Feed Tab

This tab is used as a reference for the drop-down menu of alkaline feeds within the **Model Control Panel** in the Summary Tab. Data within this tab pertains to the magnesium and calcium contents of the alkaline feeds. For most feeds, data was collected as MgO and CaO percent by mass (Columns D and E). In columns F and G, this is converted to Mg and Ca percent by mass, which are the values output in the **Model Control Panel**.

For industrial wastes, literature data is input by default and cited within cell comments and at the bottom of the tab. For mined material, composition data was collected from the [Mineralogy Database](#). (If the default data does not reflect your feed, simply overwrite the data)

If your feed is not already in the Feed Tab, input it in the green cells starting at Cell A30. The essential data is the name and the Mg/Ca contents (columns B, F, G, respectively).

CO2 Curing Tab

This tab contains data for the CO₂ Curing Comparison module in the Summary Tab. Data that may be changed here includes:

- Conversion factor of the amount of product produced per tonne of CO₂ sequestered.
- The ratio of ordinary concrete that can be replaced by the CO₂-cured concrete (i.e., the Replacement Ratio).

This data was previously generated in a review and analysis of Carbon Capture and Utilization systems using mineral carbonation, as cited in the CO₂ Curing Tab (Woodall et al, 2019).

Energy Tab

This tab used data from the DAC TEA Tool generated by N. McQueen. This data includes the cost and emissions associated with various sources of electric and thermal energy. If you have different data for a particular energy source, simply replace it within one of the green cells.

7. Reference Tabs (Red)

Red-colored tabs host calculations and generate data that is referenced throughout the tool. With the exception of the Transport Tab, Reference Tabs do not have green input cells, and should not be altered. Below is information about the calculations performed in each tab:

NPV Tab

The NPV Tab uses all expense data generated throughout the tool to calculate the project's Net Present Value (NPV). Expense data includes capital, material, energy, and transport. Also included are revenue generated by products and tax credit. These values are expanded to 50 years, and are summed to produce a cash flow for each year (Column 9 of each Process NPV table). In Column 10, present cash flow ($CF_{\text{present},n}$) is calculated using the equation:

$$CF_{\text{present},n} = \frac{CF_n}{(1+i)^n}$$

where CF_n is the cash flow for year n , and i is the discount rate. Finally, the NPV is calculated for each possible year in Column 11 by adding capital expense to the CF_{present} for every year of the project life,

$$NPV = -CAPEX + \sum_{i=1}^{n=PL} CF_{\text{present},n}$$

where PL is the Project Life specified in the Summary Tab under **Model Control Panel**.

Equipment Tabs

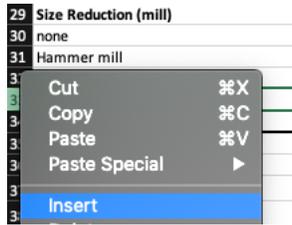
There are two Equipment Tabs, corresponding to the two processes that may be evaluated by the tool. Within these tabs is bare module costing data for various equipment options from two textbooks, cited in the orange box at the top of each tab. While multiple equipment options were provided for most process steps, some only have one (Mixers, Filters). If you would like to add another equipment option:

1. Determine the type of equipment to be added (Extraction Reactor, Filter 1, etc)
 - a. For this example, we will add a new mill
2. In the relevant Equipment Tab (1 or 2) column A, find set of equipment type that matches your new equipment
 - a. Size Reduction (mill) is located A29-A33
3. Navigate to the bottom-most row for the desired equipment type
 - a. This would be row A33, shown in the screenshot:

29	Size Reduction (mill)
30	none
31	Hammer mill
32	Ball mill
33	Jet mill
34	

4. Right-click on the row number and click insert

- a. This would be the number “33”, shown in the screenshot:



- Now, fill in all relevant information for the newly added equipment. A good rule of thumb would be to mimic the data that is already input for the other equipment of the same type. Alternatively, insert estimates for the Bare Module Cost (Column H) with a given CEPCI value (Column G).
- For cells containing equations, drag the above cell down to the newly inserted row to copy the equation:

Size Reduction (mill)				
none	\$	-	\$	-
Hammer mill	\$	56,139.41	\$	40,010.67
Ball mill	\$	734,794.53	\$	523,689.47
Jet mill	\$	278,429.26	\$	198,437.07

- Now, the newly added equipment should appear in the drop-down menu in the relevant process step section of the Process Tab.

Transport Tab

This tab hosts calculations for the cost and emissions associated with transporting the alkaline feed and/or the process’s products. Data is primarily used from the most recent Transportation Energy Data Book published by Oak Ridge National Lab.

Values for diesel price and energy density are entered here by default, but may be changed.

Data is given for three freight modes: rail, water, and truck. As emphasized in the Transportation Energy Data Book, it is very difficult to compare modal energy intensity data due to inherent differences in nature of service, routes available, etc. This is illustrated in Rows 15-17 of the Transport Tab. Energy use is on the same order of magnitude for rail and water, and data is provided in the same format (BTU/ton-mile). However, for a heavy-unit truck, data is only provided in BTU/mile for one truck. A truck capacity of 39,500 lb/truck is assumed. This results in a three- to four-fold increase in transport costs for truck relative to rail and water.

BWI Tab

This tab has reference values for the Bond Work Index (BWI) of various minerals. These values are not used in any formulas, and only exist for your reference.

In the 0. Feed Preparation section of the Process Tab, the calculation for size reduction energy requires a Bond’s Work Index value. By default, an average value is entered. You may choose a different value from the BWI Tab and manually input it into the Process Tab.

8. dHrxn Calculator Tab

This tab is available to perform a more rigorous calculation of process energy requirements for chemical reactions based on the heat of reaction. By inserting each species involved in the reaction and their associated stoichiometric coefficients, a Reaction Energy is generated. An example for the thermal reaction is loaded as default and shown for the reaction below:



Thermal Extraction Reaction							
Process 1				Process 2			
	Species	n	Hf	Species	n	Hf	
Feed	Forsterite (Mg ₂ SiO ₄)	1	-2170.37	Forsterite (Mg ₂ SiO ₄)	1	-2170.37	
Reagent	(NH ₄) ₂ SO ₄	2	-2361.80	(NH ₄) ₂ SO ₄	2	-2361.80	
Reactant 3			0.00			0.00	
Reactant 4			0.00			0.00	
Reactant 5			0.00			0.00	
Product 1	MgSO ₄	2	-2556.40	MgSO ₄	2	-2556.40	
Product 2	NH ₃	4	-184.80	NH ₃	4	-184.80	
Product 3	SiO ₂	1	-910.70	SiO ₂	1	-910.70	
Product 4	H ₂ O (vap)	2	-483.64	H ₂ O (vap)	2	-483.64	
Product 5			0.00			0.00	
dHrxn (kJ)			396.63			396.63	

As shown in the screenshot, each species involved in the reaction is input into the Heat of Reaction module, and the net heat of reaction is calculated. The value is positive, indicating an endothermic reaction (i.e., it requires heat to proceed).

The value generated in the screenshot above is on the basis of one mole of feed. To the right of this module in the dHrxn Calculator Tab, the energy required per reaction batch is calculated using the full feed rate per batch.

Reaction energy values must be manually input into the Process Tab:

- For thermal extraction reaction, input the reaction energy into the green cells of the energy calculation of 1. Extraction section.
- For acid dissolution reaction, input the reaction energy into the green cells of the operating expense box.
- The carbonation reaction is exothermic, indicating that some energy could be recovered in this step. Input the reaction energy into the energy calculation of 4. Carbonation section as “Assumed Recovered Energy”.