

# **Technoeconomic Assessment Tool for Direct Air Capture**

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User Manual

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Additional writing on the development of this model and output analysis will be available in:

Noah McQueen, Jennifer Wilcox. (2020) “Model-Based Approach to Energy and Economic Analyses for Direct Air Capture (DAC) Technologies” *Frontiers in Energy Research*, forthcoming.

Disclaimer:

This is an open source Direct Air Capture (DAC) Technoeconomic Assessment (TEA tool). The results and analysis given by this tool are to be used as a relative estimation of economic performance by prospective DAC projects. Hence, results should not be taken as a definitive solution. Use of this model is done at the user’s risk. The authors are not liable for damage resulting from use of the model.

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## 1. Introduction:

Compared to capturing carbon dioxide (CO<sub>2</sub>) from point-source emitters such as industrial facilities, removing CO<sub>2</sub> directly from the atmosphere carries additional energetic and economic challenges due to the dilute concentration of CO<sub>2</sub> in the air. Direct Air Capture (DAC) technologies thus must perform with lower thermodynamic efficiencies and with higher capital expenses than point source capture systems.

Cost projections for DAC technologies within published literature vary significantly across scope of analysis and performance assumptions. This tool was developed to provide a standardized model to evaluate the economic feasibility of novel proposed systems and innovations against an existing-technology baseline.

This tool produces two key cost projections for modeling novel technologies and systems: Estimated energy requirements per ton of CO<sub>2</sub> captured as the dominant operating expense, and estimated adsorbent material costs, as a significant capital expense. The driving factors behind these costs are transparent to the user, and the tool includes sensitivity analysis to inform users as to which technical parameters can most significantly affect final costs of capture.

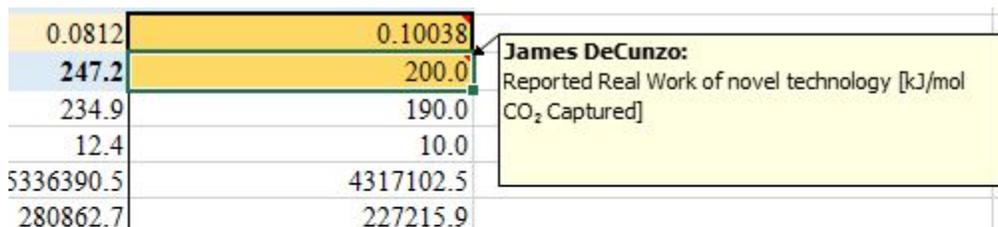
### 1.1 Navigating the Model: A Quick Guide

This section provides a generalized guide to navigate the DAC TEA Workbook (“the tool”) and each of its 6 Worksheet tabs. At the bottom of the Excel Workbook there are 5 green tabs: DAC Model, Adsorbent Cost Model, Typical CAPEX Breakdown, Typical OPEX Breakdown, and Process Flow Diagrams. These green tabs are user facing and include all inputs, outputs, performance calculations, and analysis. The 1 red tab Lookup Tables is used for reference by formulas and care should be taken not to unintentionally modify any cells or values.

Overviews of each of these 6 tabs are presented in subsections 1.2 – 1.7 of this guide. Instruction on using the two primary modeling functions of the tool, DAC Model and Adsorbent Cost Model, and narrative descriptions of the simpler functions and reference tabs, Typical CAPEX Breakdown, Typical OPEX Breakdown, and Process Flow Diagrams, are provided in their respective overview subsections.

Explanation of specific model process steps and calculations within the tabs are given in section 2 of this manual, Explanation and Rationale of Results and Calculations.

In addition to the step-by-step instructions and narrative descriptions in this guide, additional guidance is included in the tool as comments, visible when hovering the cursor over a cell with a red marker in the top right corner, as seen in Figure 1. If the full comment is not visible, right click on the cell and select “edit comment”, and then resize the cell until contents are visible.



The image shows a portion of an Excel spreadsheet with two columns of numerical data. The first column contains values: 0.0812, 247.2, 234.9, 12.4, 5336390.5, and 280862.7. The second column contains values: 0.10038, 200.0, 190.0, 10.0, 4317102.5, and 227215.9. A yellow tooltip box is overlaid on the cell containing 0.10038, displaying the text: "James DeCunzo: Reported Real Work of novel technology [kJ/mol CO<sub>2</sub> Captured]".

0.0812	0.10038
247.2	200.0
234.9	190.0
12.4	10.0
5336390.5	4317102.5
280862.7	227215.9

Figure 1: Example of a cell comment

Generally cells within the workbook are color coded based on intended interaction with the user, seen in Figure 2. Yellow cells are inputs that can be modified by a user to affect results, white cells are formulas and constants that should not be modified, and blue, red, and grey cells indicate results.

Color Key
Process specific, must be defined
You can change me if you want/need
I'm a formula/constant, let me be
Important OPEX Results
Important CAPEX Results
Important Overall Results

Figure 2: Color coding key indicating which cells should be modified

## 1.2 DAC Model

This first tab models Direct Air Capture systems based on user inputs and calculated process chemistry, generating theoretical operating expenses (OPEX) and capital expenses (CAPEX). It provides 1 baseline system based on published literature values, 1 theoretical technology-agnostic system based on averages of published literature values to represent how conventional systems might be expected to perform given different operating conditions, and 1 custom system representing a novel system or technology dependent on user inputs of operating performance. These 3 systems are described in further detail below.

The model is organized to facilitate comparisons across the 3 systems along four-sections of calculations leading to the Total Cost of captured CO<sub>2</sub>. These four sections are: Input Parameters and Calculations, OPEX, CAPEX, and Total Cost.

The 3 modeled systems are:

- Column C: **NASEM 2019 Sorbent Mid-Range**: a theoretical solid sorbent system using performance values averaged from literature, published in <sup>1</sup>NASEM 2019 and used here as a baseline example of demonstrated costs of DAC.
- Column D: **New Technology: Theoretical**: a theoretical, technology agnostic system where input parameters are proposed operating conditions of the system. The tool uses established performance values in literature to model how a conventional system would perform energetically under these inputs by calculating Theoretical Real Work [kJ/mol CO<sub>2</sub> Captured], and relating associated operating expenses (“OPEX”) of energy consumption. Theoretical capital expenses (“CAPEX”) are also calculated using a regression relating published capital expenses of systems to the reported Real Work of Capture of those systems. *See Section 2 for detailed explanations of these calculations.*

- **Column E: New Technology: Reported:** This system allows direct comparison of the New Technology: Theoretical system outputs with independent data, such as might be reported by a DAC lab group or company. Users can hold the input parameters of this column equal to the New Technology: Theoretical system, except for inputs of specific Real Work of Capture [kJ/mol CO<sub>2</sub> Captured] in the OPEX section, as well as the CAPEX in dollars per ton from company projections, or the outputs of the Adsorbent Cost Model tab. This column does not contain theoretical OPEX calculations or CAPEX calculations, but incorporates the emissions factors of energy sources to help reach Total Cost of capture.

### 1.2.1 Step-by-step use of the DAC Model

See Section 2 for detailed explanations of these calculations.

1. Save the model template for your new analysis: File → Save as → (name your file).
2. Open the model to the DAC Model tab and navigate to the top left section, Input Parameters and Calculations, as in seen in Figure 3.

Input Parameters and Calculations				
	NASEM 2019 Sorbent Mid-Range	New Technology: Theoretical	New Technology: Reported	
CO <sub>2</sub> Captured [tonnes/year]	1.00E+06	1.00E+06	1.00E+06	1.00E+06
CO <sub>2</sub> Captured [moles/year]	2.27E+10	2.27E+10	2.27E+10	2.27E+10
Air Flow Rate [moles/year]	8.11E+13	8.11E+13	8.11E+13	8.11E+13
Air Flow Rate [tonnes/year]	2.35E+09	2.35E+09	2.35E+09	2.35E+09
CO <sub>2</sub> Concentration in Inlet	0.0004	0.0004	0.0004	0.0004
Percent Capture [%]	70%	70%	70%	70%
Final Purity [%]	95.0%	95.0%	95.0%	95.0%
Separation Temperature [°C]	25	25	25	25
Temperature [K]	298.15	298.15	298.15	298.15
Gas Constant [kJ/mol*K]	0.008314	0.008314	0.008314	0.008314
Molecular Weight of CO <sub>2</sub> [g/mole]	44.011	44.011	44.011	44.011
Molecular Weight of Air [g/mole]	29	29	29	29
Electricity Source	Wind (Onshore)	Wind (Onshore)	Wind (Onshore)	
Cost of Electricity [\$/GJ]	17.90	17.90	17.90	17.90
Electricity Emissions [kgCO <sub>2</sub> /GJ]	3	3	3	3
Thermal Energy Source	Natural Gas	Natural Gas	Natural Gas	
Cost of Thermal Energy [\$/GJ]	3.23	3.23	3.23	3.23
Thermal Energy Emissions [kgCO <sub>2</sub> /GJ]	63	63	63	63
Percent Electricity [%]	20%	20%	20%	20%
Percent Thermal Energy [%]	80%	80%	80%	80%
Plant Lifetime	20	20	20	20
Discount Rate	4%	4%	4%	4%
Capital Recovery Factor	7.35818%	7.35818%	7.35818%	7.35818%
Maintenance [% of OPEX]	30%	30%	30%	30%
Labor [% of Maintenance]	30%	30%	30%	30%

Figure 3: Input Parameters and Calculations section. Input variables for the three modeled systems can be modified in this section.

3. Modify the CO<sub>2</sub> Captured [tonnes/year] for the three systems to establish the scale of DAC plant you would like to model. The default value is 1 Megaton per year.
4. Modify the **New Technology: Theoretical** and **New Technology: Demonstrated** process specific input parameters (Percent Capture, Final Purity, and Separation Temperature) according to the novel process you are evaluating.
5. Optionally modify secondary input parameters

6. Navigate down the spreadsheet to reach the OPEX section. The Material Flows subsection is background processing, but the Theoretical Energy subsection seen in Figure 4 introduces the first model outputs.

<b>Theoretical Energy</b>			
<b>Minimum Work Requirements [kJ/mol CO<sub>2</sub> Captured]</b>	<b>20.1</b>	<b>20.1</b>	<b>20.1</b>
Theoretical Minimum Electricity [kJ/mol CO <sub>2</sub> Captured]	4.02	4.02	4.02
Theoretical Minimum Thermal [kJ/mol CO <sub>2</sub> Captured]	16.1	16.1	16.1
Minimum Real Electricity [GJ]	91231.1	91231.1	91231.1
Minimum Real Thermal [GJ]	364924.4	364924.4	364924.4
Minimum Cost of Electricity [\$/mole CO <sub>2</sub> Captured]	0.00007	0.00007	0.00007
Minimum Cost of Thermal [\$/mole CO <sub>2</sub> Captured]	0.00029	0.00029	0.00029
Minimum Cost of Electricity [\$/tonne CO <sub>2</sub> Captured]	1.63	1.63	1.63
Minimum Cost of Thermal [\$/tonne CO <sub>2</sub> Captured]	1.18	1.18	1.18
<b>Total Minimum Energy OPEX [\$/tonne CO<sub>2</sub> Captured]</b>	<b>\$ 2.81</b>	<b>\$ 2.81</b>	<b>\$ 2.81</b>
Minimum CO <sub>2</sub> Emissions from Electricity [tonne CO <sub>2</sub> /tonne CO <sub>2</sub> Captured]	0.00	0.00	0.00
Minimum CO <sub>2</sub> Emissions from Thermal [tonne CO <sub>2</sub> /tonne CO <sub>2</sub> Captured]	0.02	0.02	0.02
Minimum Total CO <sub>2</sub> Emissions [tonne CO <sub>2</sub> /tonne CO <sub>2</sub> Captured]	0.02	0.02	0.02
<b>Total Minimum Energy OPEX [\$/tonne CO<sub>2</sub> Net Removed]</b>	<b>\$ 2.88</b>	<b>\$ 2.88</b>	<b>\$ 2.88</b>
Theoretical Thermodynamic Efficiency (Established via Correlation)	0.0812	0.0812	<b>0.1004</b>
<b>Theoretical Real Work [kJ/mol CO<sub>2</sub> Captured]</b>	<b>247.2</b>	<b>247.2</b>	<b>200.0</b>
Theoretical Real Electricity [kJ/mol CO <sub>2</sub> Captured]	49.4	49.4	40.0
Theoretical Real Thermal [kJ/mol CO <sub>2</sub> Captured]	197.8	197.8	160.0
Theoretical Real Electricity [GJ]	1123450.6	1123450.6	908863.7
Theoretical Real Thermal [GJ]	4493802.5	4493802.5	3635454.8
Theoretical Cost of Electricity [\$/mole CO <sub>2</sub> Captured]	0.00089	0.00089	0.00072
Theoretical Cost of Thermal [\$/mole CO <sub>2</sub> Captured]	0.00064	0.00064	0.00052
Theoretical Cost of Electricity [\$/tonne CO <sub>2</sub> Captured]	20.11	20.11	16.27
Theoretical Cost of Thermal [\$/tonne CO <sub>2</sub> Captured]	14.51	14.51	11.74
<b>Theoretical Energy OPEX [\$/tonne CO<sub>2</sub> Captured]</b>	<b>\$ 34.62</b>	<b>\$ 34.62</b>	<b>\$ 28.01</b>
Maintenance [\$/tonne CO <sub>2</sub> Captured]	\$ 14.84	\$ 14.84	\$ 12.00
Labor [\$/tonne CO <sub>2</sub> Captured]	\$ 4.45	\$ 4.45	\$ 3.60
<b>Total Theoretical OPEX [\$/tonne CO<sub>2</sub> Captured]</b>	<b>\$ 53.92</b>	<b>\$ 53.92</b>	<b>\$ 43.62</b>
Theoretical CO <sub>2</sub> Emissions from Electricity [tonne CO <sub>2</sub> /tonne CO <sub>2</sub> Captured]	0.00	0.00	0.00
Theoretical CO <sub>2</sub> Emissions from Thermal [tonne CO <sub>2</sub> /tonne CO <sub>2</sub> Captured]	0.28	0.28	0.23
Theoretical Total CO <sub>2</sub> Emissions [tonne CO <sub>2</sub> /tonne CO <sub>2</sub> Captured]	0.29	0.29	0.23
<b>Total Theoretical Energy OPEX [\$/tonne CO<sub>2</sub> Net Removed]</b>	<b>\$ 75.60</b>	<b>\$ 75.60</b>	<b>\$ 56.79</b>
Note: Electricity and thermal breakdowns assume 20% electricity and 80% thermal energy consistent with many pilot scale processes. This could deviate for new technologies, specifically those claiming to reduce thermal requirements.			

Figure 4: OPEX section, Theoretical Energy Subsection

7. Review the first important OPEX output, the Minimum Work Requirement [kJ/mol CO<sub>2</sub> Captured]. Using each systems inputs of breakdown of energy between electricity and thermal and the selected sources of electricity and thermal energy, a Total Minimum Energy OPEX [\$/tonne CO<sub>2</sub> Captured] is then generated. After incorporating emissions from energy sources, a Total Minimum Energy OPEX [\$/tonne CO<sub>2</sub> Net-removed] is also created.
- This analysis can be helpful to compare company reported Real Work of capture against this technical baseline, given the company provides process specific input parameters of their technology or system (Percent Capture, Final Purity, and Separation Temperature).
8. Optionally modify the Theoretical Thermodynamic Efficiency for the **New Technology: Theoretical**, producing a Theoretical Real Work [kJ/mol CO<sub>2</sub> Captured] of the new technology.
9. The model then follows the same procedure incorporating energy mix, price, and emissions as with the Minimum Work Requirement to generate Theoretical Energy OPEX [\$/tonne CO<sub>2</sub> Captured], and Total Theoretical Energy OPEX [\$/tonne CO<sub>2</sub> Net Removed].

10. For the **New Technology: Reported**, input the Reported Real Work of CO<sub>2</sub> capture for the novel system in the golden outlined cell aligned with Theoretical Real Work. This will update the Thermodynamic Efficiency for comparisons with the theoretical projection based on other demonstrated technologies. Energy related OPEX and CAPEX for **New Technology: Reported** will now be calculated using the reported value.
11. Navigate down the spreadsheet to reach the CAPEX section and Total Cost section as visualized in Figure 5.

CAPEX				
<b>Regression Parameters</b>				
CAPEX = 16.771*[Total Energy]				
Intercept		0		0
Total Energy Coefficient		16.771		16.771
<b>Regression</b>				
CAPEX [\$/tonne CO <sub>2</sub> Captured]	\$	94.21	\$	94.21
CAPEX [\$/tonne CO <sub>2</sub> Net Removed]	\$	132.09	\$	132.09
Capital Investment [\$/tonne CO <sub>2</sub> /yr]	\$	1,280.30	\$	1,280.30
Total Capital Investment for Scale [\$]	\$	1,280,303,221.09	\$	1,280,303,221.09
Total Capital Investment for Scale [Million \$]	\$	1,280.30	\$	1,280.30
<b>Total Cost</b>				
Total Cost [\$/tonne CO <sub>2</sub> Captured]	\$	148.12	\$	148.12
Total Cost [\$/tonne CO <sub>2</sub> Net Removed]	\$	207.69	\$	207.69

Figure 5: CAPEX and Total Cost sections

12. Review the output CAPEX [\$/tonne CO<sub>2</sub> Captured], CAPEX [\$/tonne CO<sub>2</sub> Net Removed], and Total Capital Investment for Scale. For the **New Technology: Reported**, the user may input a company reported value, or the output of the Adsorbent Cost Model tab (see below).
13. Finally, review the Total Cost [\$/tonne CO<sub>2</sub> Captured] and Total Cost [\$/tonne CO<sub>2</sub> Net Removed].
14. Navigate to the Sensitivity Analysis table on the upper right of the DAC Model tab, Figure 6. In addition to the baseline Percent Electricity vs Real Work [kJ/mol], users can select other variables to be visualized.

Sensitivity Analysis																			
Sensitivity of Cost [\$/tCO <sub>2</sub> ] of New Reported Technology to Real Work Requirements and Percent Electricity																			
\$	95.40	25	50	75	100	125	150	175	200	225	250	275	300	325	350	375	400	425	
5%	\$ 55.29	\$ 58.79	\$ 62.30	\$ 65.81	\$ 69.31	\$ 72.82	\$ 76.32	\$ 79.83	\$ 83.33	\$ 86.84	\$ 90.35	\$ 93.85	\$ 97.36	\$ 100.86	\$ 104.37	\$ 107.88	\$ 111.38		
10%	\$ 55.94	\$ 60.09	\$ 64.25	\$ 68.40	\$ 72.56	\$ 76.71	\$ 80.86	\$ 85.02	\$ 89.17	\$ 93.33	\$ 97.48	\$ 101.64	\$ 105.79	\$ 109.95	\$ 114.10	\$ 118.26	\$ 122.41		
15%	\$ 56.59	\$ 61.39	\$ 66.19	\$ 71.00	\$ 75.80	\$ 80.60	\$ 85.41	\$ 90.21	\$ 95.01	\$ 99.82	\$ 104.62	\$ 109.42	\$ 114.23	\$ 119.03	\$ 123.83	\$ 128.64	\$ 133.44		
20%	\$ 57.23	\$ 62.69	\$ 68.14	\$ 73.59	\$ 79.04	\$ 84.50	\$ 89.95	\$ 95.40	\$ 100.85	\$ 106.30	\$ 111.76	\$ 117.21	\$ 122.66	\$ 128.11	\$ 133.57	\$ 139.02	\$ 144.47		
25%	\$ 57.88	\$ 63.98	\$ 70.09	\$ 76.19	\$ 82.29	\$ 88.39	\$ 94.49	\$ 100.59	\$ 106.69	\$ 112.79	\$ 118.89	\$ 124.99	\$ 131.10	\$ 137.20	\$ 143.30	\$ 149.40	\$ 155.50		

Figure 6: Sensitivity Analysis Table

15. To modify the variables visualized in the Sensitivity Analysis table:
  - Select the entire table area, including headers
  - In the Excel Quick Access Toolbar, open the Data tab

- In the Forecast section on the right, click What If Analysis, then Data table

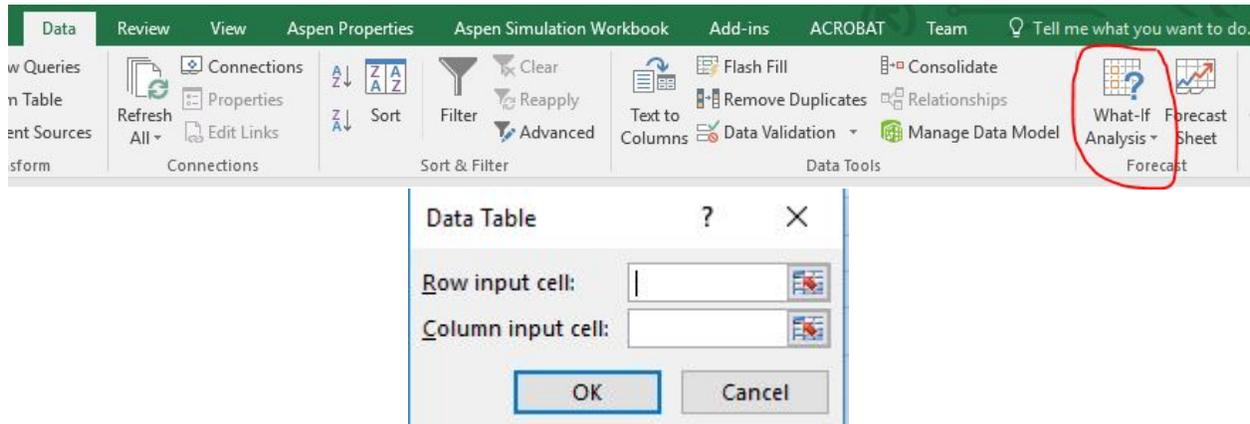


Figure 8: Sensitivity Analysis modification procedure screenshots

- A window with two input cells will appear
- Row input cell: Select the variable in the workbook that corresponds to the variable you would like to be changed in the left column of the table – in the default table, this is Percent Electricity (%)
- Column input cell: Select the variable in the workbook that corresponds to the variable you would like to be changed across the top row of the table – in the default table, this is Real Work (kJ/mol)
- Click ‘Okay’ and the table should populate automatically

### 1.3 Adsorbent Cost Model

The second tab of the tool breaks down the key performance and cost drivers of adsorbent materials in DAC systems. The tool produces a final Cost of Adsorbent [\$/tCO<sub>2</sub>] based on user inputted performance parameters of a proposed adsorbent, and compares the economic outcome of that **New Technology: Reported** to a baseline **NASEM Sorbent Mid-Range** as seen in Figure 9. This functionality can be used to evaluate and validate the cost-saving potential of new adsorbent materials relative to existing technology.

DAC Plant Calibration Assumptions				
	CO2 Capture [tonnes/year]	1,000,000	You can change me in the 'DAC Model' Tab	
	CO2Capture [moles/year]	2.27E+10		
	Plant Lifetime	20	You can change me in the 'DAC Model' Tab	
	Discount Rate	4%	You can change me in the 'DAC Model' Tab	
	Capital Recovery Factor	7.35818%	You can change me by changing the discount rate	
	Molecular Weight of CO <sub>2</sub> [g/mole]	44.011		
Sensitivity Analysis (Variable : Cost of Adsorbent)	Adsorbent Properties		NASEM 2019 Sorbent Mid-Range	New Technology: Reported
		CO2 Capture [tonnes/year]	1.00E+06	1.00E+06
		CO2Capture [moles/year]	2.27E+10	2.27E+10
	1:1	Adsorbent Cost [\$ /kg]	\$ 50.00	\$ 100.00
	2:0.5	Adsorbent Capacity [mol CO <sub>2</sub> /kg Sorbent]	1.00	2.00
	2:0.5	Sorbent Lifetime [years]	0.50	1.00
Process Operation				
	Days operating [days/year]	340	340	
	Plant Lifetime [years]	20	20	
1:1	Cycle Time [min]	20	10.00	
1:1	Cycles [cycles/year]	24,480	48,960	
1:1	Desorption Swing Capacity [mol/mol]	0.8	0.9	
	Capital Recovery Factor	7.36%	7.36%	
Process Calculations				
	Adsorbent Required [kg/yr]	2,320,424	257,825	
	Adsorbent Cost [\$ /yr]	\$ 116,021,202.66	\$ 25,782,489.48	
	Cost of Adsorbent [M\$/yr]	\$ 116.0	\$ 25.8	
	Cost of Adsorbent [\$ /tCO <sub>2</sub> ]	\$ 116.02	\$ 25.78	

Note: this is an estimate for the sorbent only

Figure 9: Adsorbent Cost Model

The DAC Plant Calibration Assumptions are all pulled in to the tab from the DAC Model tab, so modifications to those variables should be made in the Input Parameters and Calculations section of that tab.

Sensitivity analysis of the key performance variables (Adsorbent Cost [\$ /kg], Adsorbent Capacity [mol CO<sub>2</sub>/kg Sorbent], Sorbent Lifetime [years], Cycle Time [min], and Desorption Swing Capacity [mol/mol]) can help inform users as to which performance improvements to focus on. Visualized sensitivity analysis is in the upper right side of the tab, and can be modified by following the procedure laid out in the above DAC Model section.

In addition, the final Cost of Adsorbent [\$ /tCO<sub>2</sub>] can be incorporated into a full CAPEX breakdown at the bottom of the tab as visualized in Figure 10. This result can be compared against existing published CAPEX of other systems in the Typical CAPEX Breakdown tab, as well as used as an input in the CAPEX section of the DAC Model tab.

#### 1.4 Typical CAPEX Breakdown

This tab contains a bar graph and table outlining the CAPEX for the upper and lower bounds for liquid solvent from the <sup>1</sup>NASEM 2019 study, as well as the CAPEX for a typical solid sorbent system. Company provided CAPEX data, as well as outputs from the Adsorbent Cost Model, can be added to the table and graph for visual comparison.

The upper two tables “Liquid Solvent” and “Solid Sorbent” contain baseline literature values so that costs of individual CAPEX components can be modified in the “For Bar Graph” table without losing the original literature values. The Liquid Solvent values seeded in “For Bar Graph” have been annualized.

It is important to note that novel technologies and systems may have other major capital equipment costs not represented as columns in this table.

### 1.5 Typical OPEX Breakdown

This tab contains a bar graph and table outlining the OPEX upper and lower bounds for liquid solvent systems from the <sup>1</sup>NASEM 2019 study, as well as the OPEX for typical solid sorbent system. Company provided OPEX data can be added to the table and graph for visual comparison.

The upper two tables “Liquid Solvent” and “Solid Sorbent” contain baseline literature values so that costs of individual CAPEX components can be modified in the “For Bar Graph” table without losing the original literature values.

### 1.6 Process Flow Diagrams

This tab contains reference process flow diagrams for:

- Solvent-based DAC – based on <sup>1</sup>NASEM 2019
- Sorbent-based DAC – based on <sup>1</sup>NASEM 2019
- Moisture Swing DAC – based on <sup>5</sup>Lackner, 2009
- Electrochemically Mediated DAC – based on <sup>6</sup>Hatton et al, 2019

### 1.7 Lookup Tables

The data in this tab is referenced by various formulas in the user-facing tabs.

- Columns B – U contain the Correlation Table for Second Law Efficiencies and formula - see Theoretical Thermodynamic Efficiency section below for explanation.
- Columns X – AB contain energy cost and emissions intensities, as well as data citations.

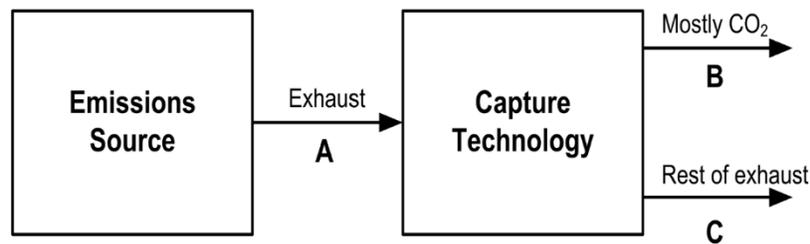
## 2. Explanation and Rationale Results and Calculations

This section of the guide provides additional detail on the process steps and calculations in this tool. More extensive provision of formulae, data used in development, and analysis of results will be available in: Noah McQueen, Jennifer Wilcox. (2020) “Model-Based Approach to Energy and Economic Analyses for Direct Air Capture (DAC) Technologies” *Frontiers in Energy Research*, forthcoming.

### 2.1 DAC Model

#### 2.1.1 Minimum Work Requirements [kJ/mol CO<sub>2</sub> Captured]

This is the calculated absolute minimum amount of energy required to separate CO<sub>2</sub> from the air given the systems input parameters. The minimum work calculation is based on the theoretical minimum energy required to separate a mixture at a given composition. It is based on the following model and formula (Figure 3):



$$W_{\min} = RT \left[ n_B^{CO_2} \ln(y_B^{CO_2}) + n_B^{B-CO_2} \ln(y_B^{B-CO_2}) \right] + RT \left[ n_C^{CO_2} \ln(y_C^{CO_2}) + n_C^{C-CO_2} \ln(y_C^{C-CO_2}) \right] - RT \left[ n_A^{CO_2} \ln(y_A^{CO_2}) + n_A^{A-CO_2} \ln(y_A^{A-CO_2}) \right]$$

Figure 3: Process model and formula for calculation of minimum work, used to establish Minimum Work Requirements [kJ/mol CO<sub>2</sub> Captured]. <sup>2</sup>Wilcox, 2012.

In this equation R is the gas constant [0.008314 kJ/mol\*K], T is the temperature of the separation [K], n is the molar flows, and y is the mole fractions of the components in that stream. The equation relies on the mass balance around the DAC separation unit and gives the absolute thermodynamic minimum work of separation. In short, the minimum work is technology agnostic, and provides the ultimate baseline to crosscheck any system or company performance claim – it is impossible to separate CO<sub>2</sub> with energy inputs below the minimum work.

The Minimum Work Requirement output in this model is based on the user defined inputs Percent Capture [%] of CO<sub>2</sub> from the inlet stream, Final Purity [%] of captured CO<sub>2</sub>, and separation temperature [°C]. The results of the calculation were consistent with <sup>3</sup>Wilcox et al, 2017.

#### 2.1.2 Total Minimum Energy OPEX [\$/tonne CO<sub>2</sub> Captured]

Based on the Minimum Work Requirement and the inputs Percent Electricity [%], Percent Thermal Energy [%], Electricity Source, and Thermal Energy Source, an absolute minimum operating cost of energy is produced. Costs of electricity and thermal energy are relative to the selected source, and are located in column Y of the Lookup Tables tab.

### 2.1.3 Total Minimum Energy OPEX [\$/tonne CO<sub>2</sub> Net Removed]

This calculation subtracts projected emissions from thermal and electrical energy requirements from the CO<sub>2</sub> captured, providing a cost for CO<sub>2</sub> net-removed. Emissions factors for energy sources are located in column Z of the Lookup Tables tab.

### 2.1.4 Theoretical Thermodynamic Efficiency (Established via Correlation)

The baseline Theoretical Thermodynamic Efficiency value is based on a correlation between published literature values of the reported Real Work and the Minimum Work Requirement of those systems. It effectively discounts the Minimum Work Requirement of the new technology to match the efficiencies that other DAC systems have demonstrated.

### 2.1.5 Theoretical Real Work [kJ/mol CO<sub>2</sub> Captured]

This is the result of the modification of the Minimum Work Requirement by the Theoretical Thermodynamic Efficiency, representing how a conventional system would be expected to perform.

### 2.1.6 Theoretical Energy OPEX [\$/tonne CO<sub>2</sub> Captured]

This factors in the inputs Percent Electricity [%], Percent Thermal Energy [%], Electricity Source, and Thermal Energy Source to the theoretical real work to produce a cost.

### 2.1.7 Total Theoretical OPEX [\$/tonne CO<sub>2</sub> Captured]

This calculation incorporates not just energy consumption and cost, but also Maintenance and Labor OPEX. These costs are high level assumptions seen at the bottom of the Input Parameters tab – Maintenance 30% of OPEX, Labor 30% of maintenance.

### 2.1.8 Total Theoretical Energy OPEX [\$/tonne CO<sub>2</sub> Net Removed]

This output is the result of discounting the Total Theoretical OPEX [\$/tonne CO<sub>2</sub> Captured] by the energy related emissions from thermal and electrical energy requirements and sources.\

### 2.1.9 CAPEX [\$/tonne CO<sub>2</sub> Captured]

The calculation uses a relationship between CAPEX and total energy based on published literature values of the CAPEX costs of a system and the systems Theoretical Real Work. This CAPEX is thus a rough estimate of how much a conventional system would cost at this level of performance.

### 2.1.10 CAPEX [\$/tonne CO<sub>2</sub> Net Removed]

This calculation incorporates the emissions from energy consumption to discount the CAPEX [\$/tonne CO<sub>2</sub> Captured].

### 2.1.11 Total Capital Investment for Scale [\$]

This calculation simply multiplies the CAPEX [\$/tonne CO<sub>2</sub> Net Removed] against the input CO<sub>2</sub> Captured [tonnes/year].

### 2.1.12 Total Cost [\$/tonne CO<sub>2</sub> Captured]

This calculation adds up the OPEX and CAPEX values to indicate the total cost to capture 1 ton of CO<sub>2</sub> from the atmosphere.

### 2.1.1 Total Cost [\$/tonne CO<sub>2</sub> Net Removed]

This calculation adds up the OPEX and CAPEX values but also incorporates emissions from energy consumption using the defined energy sources to indicate the cost to remove one net ton of CO<sub>2</sub> from the atmosphere.

## 3. References

This includes literature cited in this user guide. An extensive list of literature and prior work used in the design and data of this tool will be available in: Noah McQueen, Jennifer Wilcox. (2020) “Model-Based Approach to Energy and Economic Analyses for Direct Air Capture (DAC) Technologies” *Frontiers in Energy Research*, forthcoming.

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