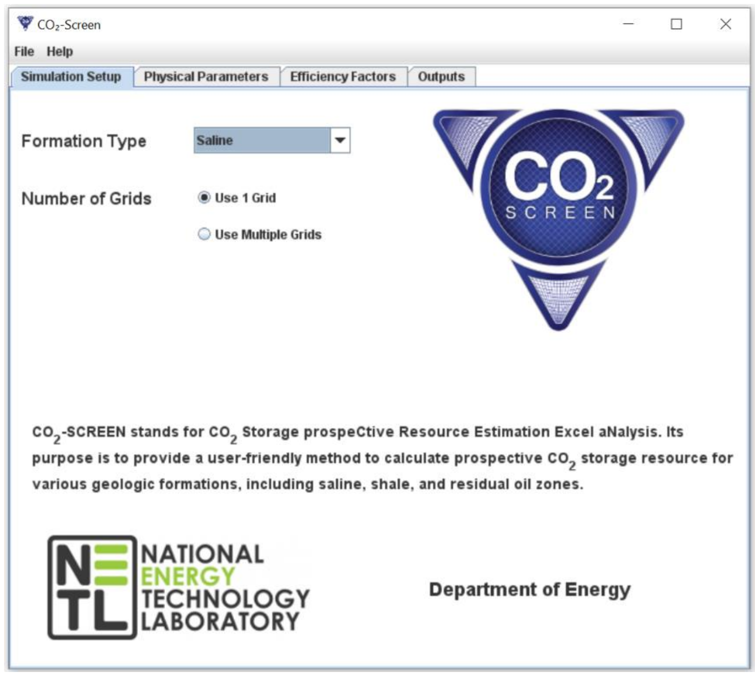
NATIONAL ENERGY TECHNOLOGY LABORATORY



CO_2 Storage prospeCtive Resource Estimation Excel aNalysis (CO_2-SCREEN) User's Manual

8 May 2020

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Cover Illustration: CO_2-SCREEN Splash Page.

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CO_2 Storage prospeCtive Resource Estimation Excel aNalysis (CO_2-SCREEN) User's Manual

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DOE/NETL-2020/2133

8 May 2020

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Acronyms, Abbreviations, and Symbols

Term	Description
ρ	Density
ρ_{sCO_2}	Maximum mass of CO_2 sorbed per unit volume solid rock, e.g. the asymptotic value of an appropriate isotherm
ϕ	Porosity
A_t	Area
CO_2	Carbon dioxide
CO_2-SCREEN	Storage prospeCtive Resource Estimation Excel aNalysis
DOE	U.S. Department of Energy
E_ϕ	Effective-to-total porosity
E_A	Net-to-total area
E_d	Microscopic displacement
E_{Ds}	Fraction of CO_2 mass dissolved in the oil phase
EDX	Energy Data eXchange
E_h	Net-to-gross thickness
E_s	Sorption efficiency
E_{saline}	Saline efficiency
E_V	Volumetric displacement
Gt	Gigatons
GUI	Graphical user interface
h_g	Thickness
Mt	Million metric tons
NETL	National Energy Technology Laboratory
	CO_2 concentration
S_{wirr}	Irreducible water saturation
S_{or}	Residual oil saturation with respect to water
TDS	Total dissolved solids
TOC	Total organic content

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Glossary

Term	Symbol	Units	Description
Area	A_t	km^2	Total area (map view) of the formation being assessed for CO_2 storage
CO_2 Concentration	$R_{c/o}$		Concentration of CO_2 in 1 m^3 of oil at the (averaged) pressure (P) and (averaged) temperature (T) of a reservoir prior to injection
CO_2 Density	ρ_{CO_2}	kg/m^3	Density of CO_2 at the (averaged) pressure (P) and (averaged) temperature (T) of formation being assessed for CO_2 storage prior to injection
CO_2 Storage	G_{CO_2}		CO_2 storage resource (mass)
Depositional Environment			The combination of physical, chemical, and biological processes under which sediment accumulates
Effective-to-Total Porosity	E_ϕ		Fraction of formation porosity available for CO_2 storage
Formation			The fundamental unit of lithostratigraphy. A body of rock that is sufficiently distinctive and continuous that it can be mapped
Microscopic Displacement	E_d		The fraction of pore space unavailable due to immobile in-situ fluids
Net-to-Gross Thickness	E_h		Fraction of formation thickness available for CO_2 storage
Net-to-Total Area	E_A		Fraction of formation area available for CO_2 storage
Oil Displacement	E_{Ds}		Fraction of CO_2 mass dissolved in the oil phase
Physical Parameters			The parameters required to calculate the potential CO_2 storage resource (i.e. area, thickness, porosity)
Porosity	ϕ_{tot}	%	Average total porosity of formation being assessed for CO_2 storage
Reservoir Pressure	P	MPa	The pressure of the formation defined by A and h at storage conditions
Residual Oil Zone Formations	*ROZ*		Reservoir rock containing immobile oil, with respect to water, at oil saturation levels generally less than 40 percent
Saline Efficiency	E_{saline}		CO_2 storage efficiency factor that reflects a fraction of the total pore volume that is filled by CO_2
Saline Formations			Subsurface geographically extensive sedimentary rock layers saturated with waters or brines that have a high total dissolved solids (TDS) content (i.e. over 10,000 mg/L TDS)
Storage Efficiency Values			Values defining the fraction of storage likely for each storage parameter
S_{wirr}	S_{wirr}		Irreducible water saturation

Glossary (cont.)

Term	Symbol	Units	Description
S_{or}	S_{or}		Residual oil saturation with respect to water
Sorbed CO_2	ρ_{sCO_2}		Maximum mass of CO_2 sorbed per unit volume solid rock, e.g. the asymptotic value of an appropriate isotherm
Sorbed CO_2 Efficiency	E_s		Fraction of the total potential sorbed volume of CO_2 within the net effective volume of the formation
Temperature	T	°C	The temperature of the formation defined by *A* and *h* at storage conditions
Thickness	h_g	*m*	Average gross thickness of formation being assessed for CO_2 storage
Volumetric Displacement	E_V		The combined fraction of immediate volume surrounding an injection well that can be contacted by CO_2 and the fraction of net thickness that is contacted by CO_2 as a consequence of the density difference between CO_2 and in-situ water

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ABSTRACT

This user's manual guides the use of the National Energy Technology Laboratory's (NETL) CO_2 Storage prospeCtive Resource Estimation Excel aNalysis (CO_2-SCREEN) tool, which was developed to aid users screening geologic formations for prospective CO_2 storage resources. This manual is specific to the CO_2-SCREEN 4.0 version which is based in Python. CO_2-SCREEN applies U.S. Department of Energy (DOE) methods and equations for estimating prospective CO_2 storage resources for saline formations, shale formations, and residual oil zones (ROZ). CO_2-SCREEN was developed to be substantive and user-friendly and provide a consistent method for calculating prospective CO_2 storage resources. CO_2-SCREEN uses a Java based graphical user interface for data inputs and uses Python to calculate prospective CO_2 storage resources.

1. INTRODUCTION

Since 2011, the U.S. Department of Energy, National Energy Technology Laboratory (DOE-NETL) Carbon Storage Program has developed methods and equations for assessing the prospective storage resource of carbon dioxide (CO_2) in various geologic formations (Goodman et al., 2011; Goodman et al., 2013; NETL, 2015; Goodman et al., 2016; Levine et al., 2016; Sanguinito et al., 2020). In order to make high-level, energy-related government policy and business decisions the ability to accurately predict the CO_2 storage resource is needed. NETL's Best Practice manual (NETL, 2013) defines prospective CO_2 storage resource as a mass estimate of CO_2 that can be stored in a geologic reservoir at the primary stage of a CO_2 storage project. This definition comes from the CO_2 geologic storage classification system which was modified from the petroleum industry classification system (Oil and Gas Reserves Committee, 2011). This system outlines how to identify and characterize potential CO_2 storage locations at regional and site scales.

This user's manual describes version 4.0 of the CO_2 Storage prospeCtive Resource Estimation Excel aNalysis (CO_2-SCREEN) tool and provides instructions for use. CO_2-SCREEN is available on the Energy Data eXchange (EDX) and can be downloaded here: https://edx.netl.doe.gov/dataset/co2-screen.

2. INSTALLING CO_2-SCREEN

2.1 SYSTEM REQUIREMENTS

The following computer capabilities are recommended for using CO_2-SCREEN:

- **Personal computer (PC) with 64-bit operating system and operating system of Microsoft Windows 7 or later**
- **Mac with operating system of Mojave or later**

The tool may be able to operate on computers with fewer capabilities, but the user may experience lengthy simulation run times.

2.2 INSTALLATION

CO_2-SCREEN can be downloaded off the Energy Data eXchange (EDX) from the following link: https://edx.netl.doe.gov/dataset/co2-screen.

Download the zipped folder named "co2-screen-v4_python.zip" seen in Figure 1.

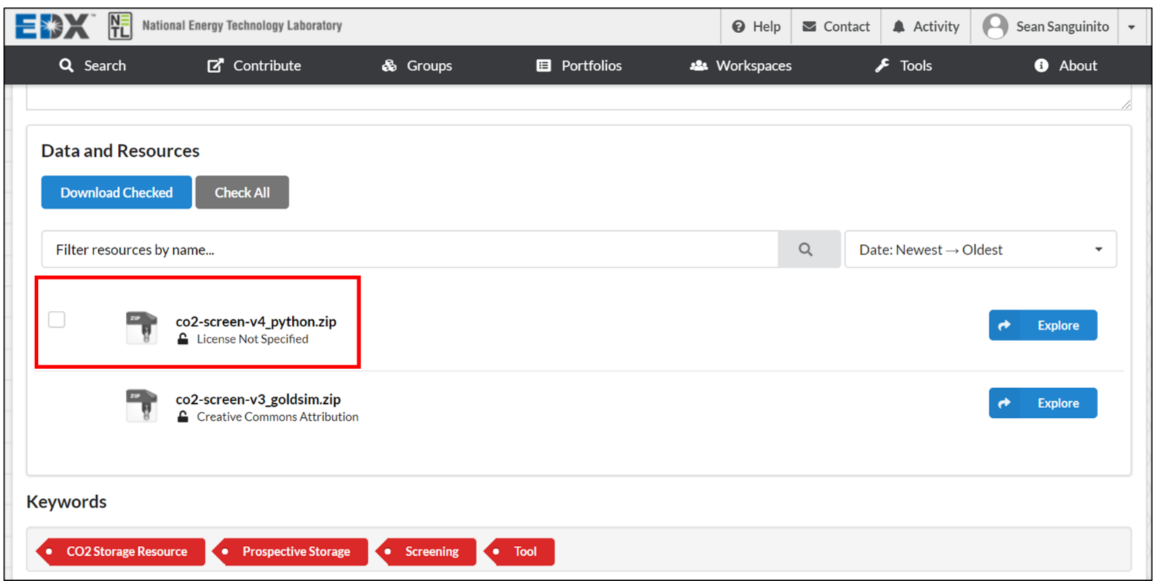

Figure 1: Screenshot of the download file for CO_2-SCREEN.

After the zipped folder is downloaded, extract the folder contents and place them in any directory on your computer. Keep all files associated with CO_2-SCREEN in the same directory (i.e. do not move input or output files around). Windows users can simply double click on the CO2SCREEN.jar file to run the tool. Mac users may need to user Terminal to open the tool (see Section 3.3 below).

3. GETTING STARTED

3.1 WINDOWS USERS

To run CO_2-SCREEN, simply double click on the "CO2SCREEN.jar" file. This will open the CO_2-SCREEN splash page seen in Figure 2.

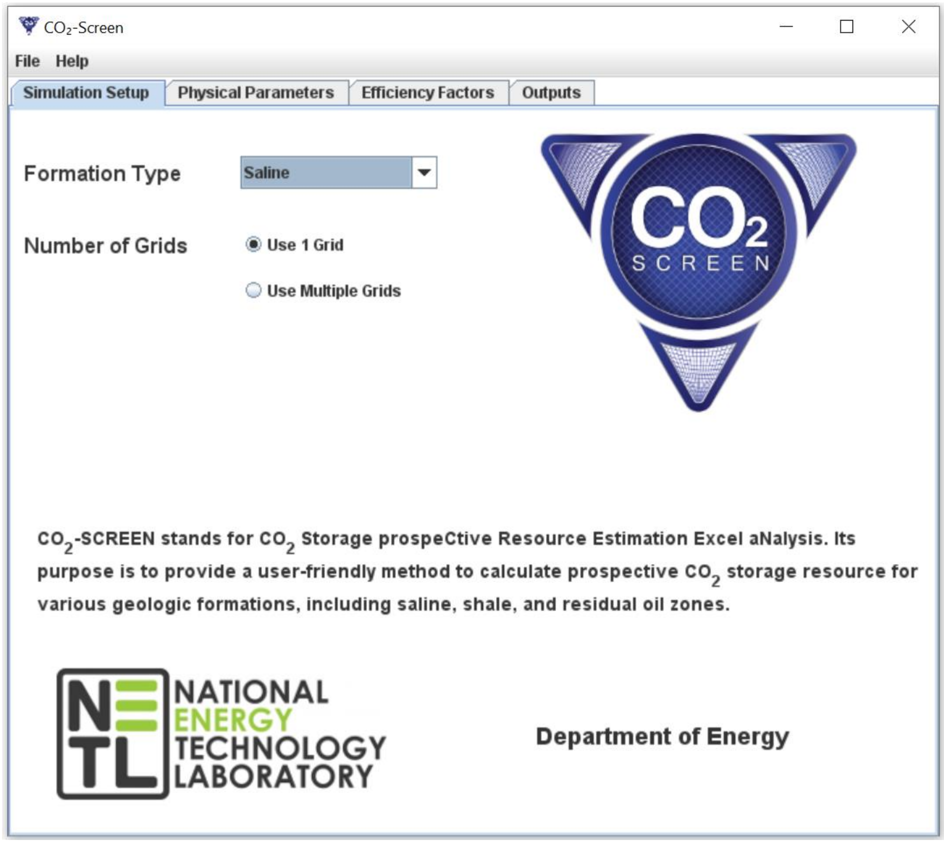

Figure 2: CO_2-SCREEN splash page.

3.2 LINUX USERS

To run CO_2-SCREEN, open a console/terminal and execute the "CO2SCREEN.jar" file using 'java -jar CO2SCREEN.jar' (without the apostrophes). This will open the CO_2-SCREEN splash page seen in Figure 2.

3.3 MAC USERS

To run CO_2-SCREEN on newer versions of MacOS (Catalina and newer) you need to ensure the files have permission to execute and write on your system. To do this, open Terminal and navigate to the directory that contains the CO_2-SCREEN files, specifically the FormationApps folder. Execute 'chmod +x *Mac'. Then execute './SalineMac', './ShaleMac', and './ROZMac'. Navigate back to the CO_2-SCREEN folder and execute 'java -jar CO2SCREEN.jar'. This will open the CO_2-SCREEN splash page seen in Figure 2. The permissions to write will remain for future uses of CO_2-SCREEN but it may still need to be opened using terminal for each use.

4. INSTRUCTIONS FOR USE

4.1 SIMULATION SETUP

CO_2-SCREEN is organized into 4 tabs: Simulation Setup, Physical Parameters, Efficiency Factors, and Outputs. The Simulation Setup tab is automatically opened when CO_2-SCREEN is first launched (see Figure 2). The first choice a user must make is deciding what geologic formation they would like to estimate prospective CO_2 resource for. The user can choose their formation type from a dropdown list (Figure 3) which includes: Saline, Shale, or ROZ (residual oil zones).

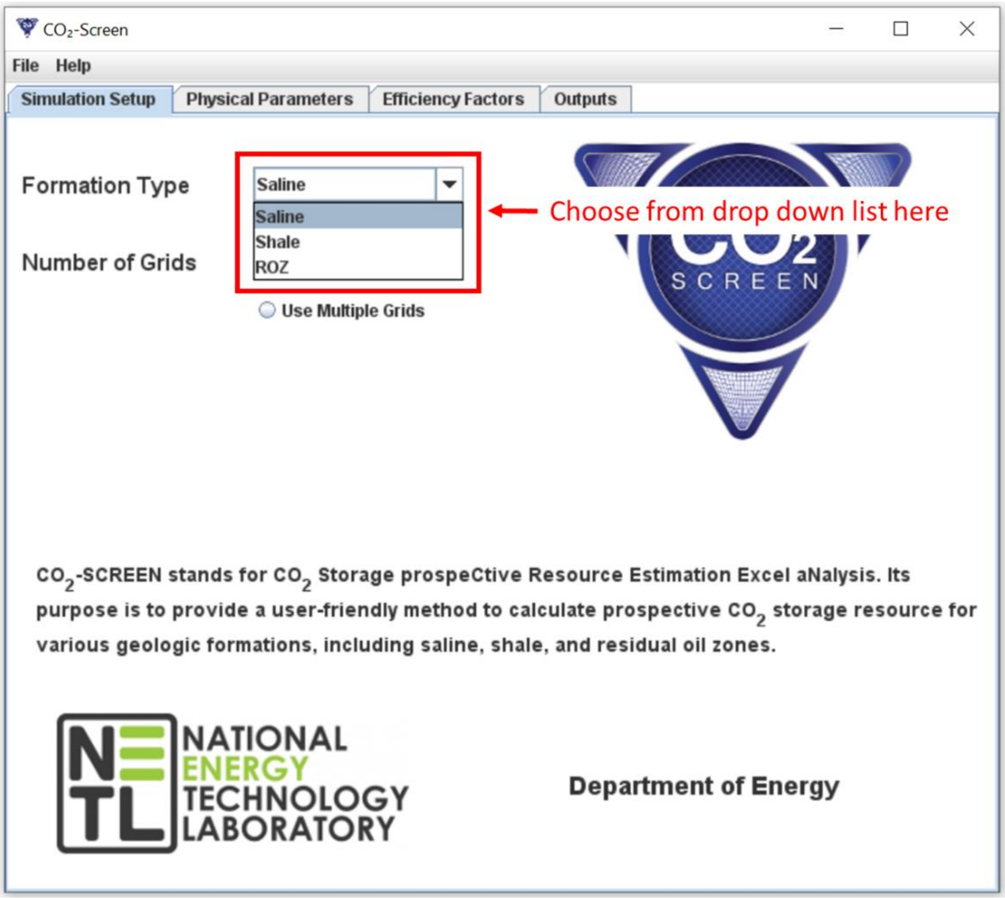

Figure 3: Formation Type drop down options on Simulation Setup Tab.

The next choice is deciding how many grids to divide the formation or region of interest into. A user can use a single grid, which will calculate CO_2 storage and efficiency values based on a single region. Or the user can use multiple grids which allows the user to enter different data values on a grid by grid basis which can be useful to account for geologic heterogeneity. If a user chooses a single grid, they can move onto the Physical Parameters tab (see section 4.2) to begin entering geologic data. If a user chooses to use multiple grids, they will need to enter their

Physical Parameter and Storage Efficiency Factor data into provided Excel files (see Section 4.5 for details on multiple grid use).

4.2 PHYSICAL PARAMETERS

After selecting formation type and single grid, navigate to the Physical Parameters tab. Depending on what formation type was chosen previously, you will see various geologic parameters (Figure 4). Enter a mean and standard deviation value for each parameter. Values entered here must be positive.

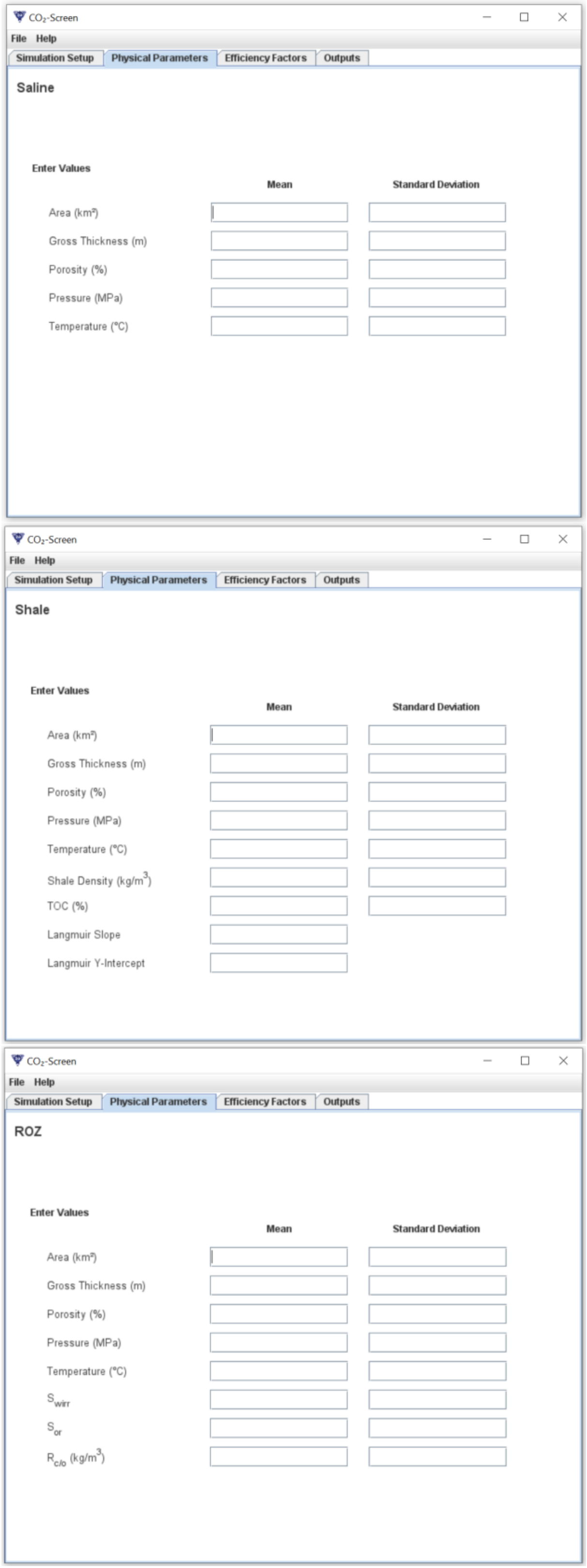

Figure 4: Screenshot of the Physical Parameters tab for each formation type.

For saline formations, there are five physical parameters including Area, Gross Thickness, Porosity, Pressure, and Temperature. These five terms are used for shale and ROZ formations as well. To account for CO_2 storage as a sorbed phase, shale also requires inputs for Shale Density, Total Organic Content (TOC), Langmuir Slope, and Langmuir Y-intercept (see Section 5.2). To account for residual oil reducing free phase storage but also increasing storage via CO_2 dissolution in oil, ROZ formations require inputs for irreducible water saturation (S_{wirr}), residual oil saturation (with respect to water) (S_{or}), and the concentration of CO_2 in oil ($R_{c/o}$). After entering all required formation data on the Physical Parameters tab, navigate to the Efficiency Factors tab.

4.3 EFFICIENCY FACTORS

Once again, based on the formation originally chosen, you will see different options for entering efficiency factor values (Figure 5). All efficiency factors are entered as P_{10} and P_{90} values and must range between 0 and 1 (i.e. 0 = 0% efficiency and 1 = 100% efficiency).

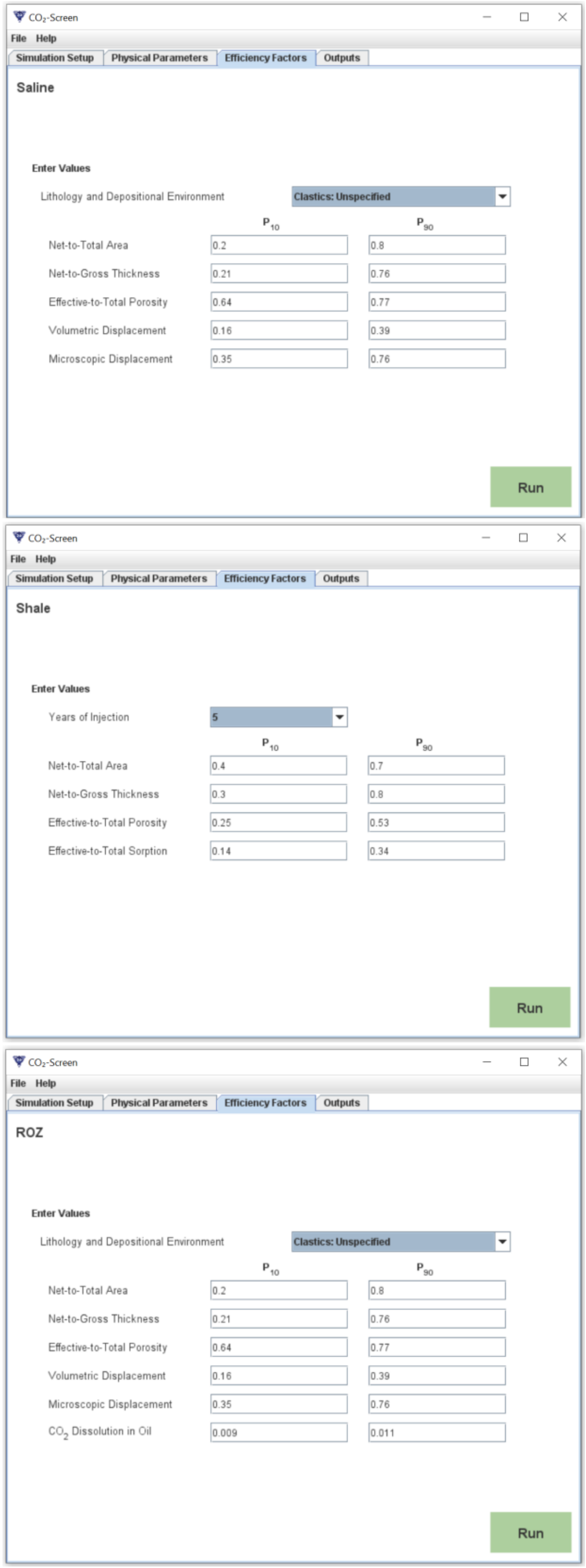

Figure 5: Screenshot of Efficiency Factors tab for Saline, Shale, and ROZ formations.

Ideally, efficiency factor ranges should be based on geologic parameters specific to the formation being assessed but in the absence of detailed geologic data, users have the option to auto-populate P_{10} and P_{90} ranges for all five saline efficiency terms (Net-to-Total Area, Net-to-Gross Thickness, Effective-to-Total Porosity, Volumetric Displacement, and Microscopic Displacement). These auto-populated values were developed by the International Energy Agency Greenhouse Gas R&D Programme (IEA GHG, 2009) and are a function of lithology and depositional environment (Table 1).

Table 1: Lithology and Depositional Environment Options

Lithology	Depositional Environment
Clastics	Unspecified
Dolomite	Unspecified
Limestone	Unspecified
Clastics	Alluvial Fan
Clastics	Delta
Clastics	Eolian
Clastics	Fluvial
Clastics	Peritidal
Clastics	Shallow Shelf
Clastics	Shelf
Clastics	Slope Basin
Clastics	Strand Plain
Limestone	Peritidal
Limestone	Reef
Limestone	Shallow Shelf

If a dataset does not require an efficiency term, a user can enter a 1 (100 percent efficiency) for the P_{10} and P_{90} range. An example of this situation would be if a dataset was using net area instead of gross area. In this case, the user would enter a 1 for the P_{10} and P_{90} range for Net-to-Gross Area to avoid double discounting. In large datasets, that may have varying degrees of uncertainty in the data, it is encouraged to use the multiple grid system to account for this uncertainty using varying ranges for efficiency factors.

For shale formations, there are only four efficiency factor terms (Net-to-Total Area, Net-to-Gross Thickness, Effective-to-Total Porosity, and Effective-to-Total Sorption). Again, users are encouraged to enter P_{10} and P_{90} ranges based on their geologic formation specific data, but they have the option here to auto-populate the Effective-to-Total Porosity and Effective-to-Total Sorption efficiency factors based on years of injection. These auto-populated values are derived from Myshakin et al. (2018) which used numerical modeling to study the efficiency of free phase and sorbed phase storage of CO_2 in shale.

Residual Oil Zone formations are geologically similar to saline formations except they contain some amount of residual oil. Because of this, they utilize the same five storage efficiency factors with an additional factor to account for oil, CO_2 Dissolution in Oil. Users once again have the option to manually enter values or they can auto-populate values for the same efficiency factors as saline based on lithology and depositional environment. The efficiency factor for CO_2 Dissolution in Oil defaults to a P_{10} and P_{90} range of 0.009 to 0.011 sourced from Sanguinito et al. (2020) which used numerical simulations to analyze this term.

As a final reiteration, users should enter P_{10} and P_{90} efficiency factor ranges based on the geologic data of the formation they are assessing and only rely on auto-populated values when necessary. When values for all terms are entered, click the green Run button (Figure 6). A "Running" animation should be displayed as the tool works. When it finishes, users can navigate to the Output tab.

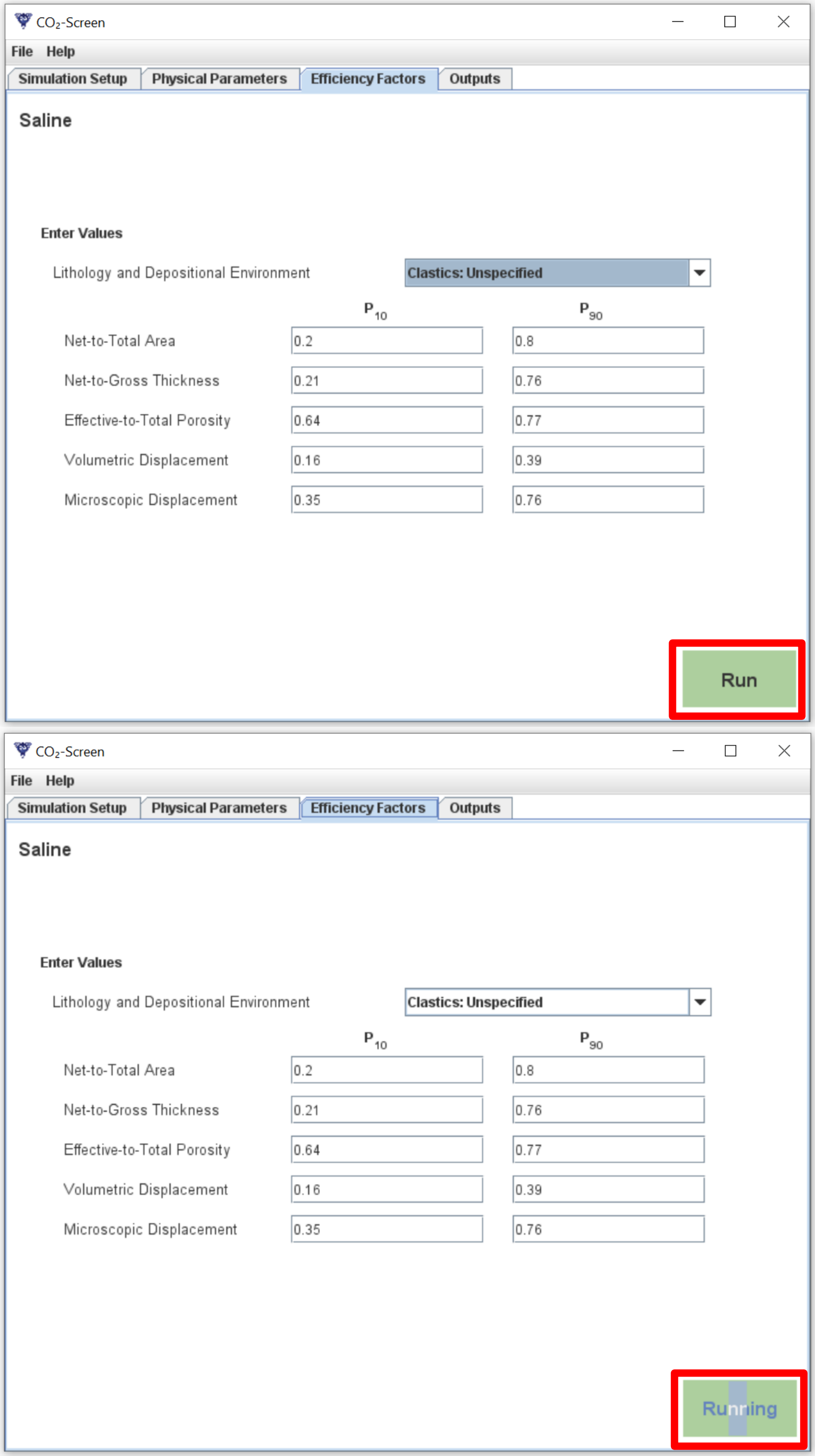

Figure 6: Screenshot displaying the green Run button as well as the "Running" animation.

4.4 OUTPUTS

The Outputs tab (Figure 7) will display different information depending on the formation being assessed while all outputs are presented as a P_{10}, P_{50}, and P_{90} value. Saline formations will display the Total CO_2 storage resource, the Total Efficiency, and the Lithology and Depositional Environment chosen. Shale formations will display the Total CO_2 storage resource, Total Efficiency, Free Phase CO_2 storage resource, Free Phase Efficiency, Sorbed Phase CO_2 Storage, and Sorption Efficiency. ROZ formations will display the Total CO_2 storage resource, Total Efficiency, Free Phase CO_2 storage resource, Free Phase Efficiency, Dissolved in Oil CO_2 storage resource, Dissolved in Oil Efficiency, and Lithology and Depositional Environment chosen.

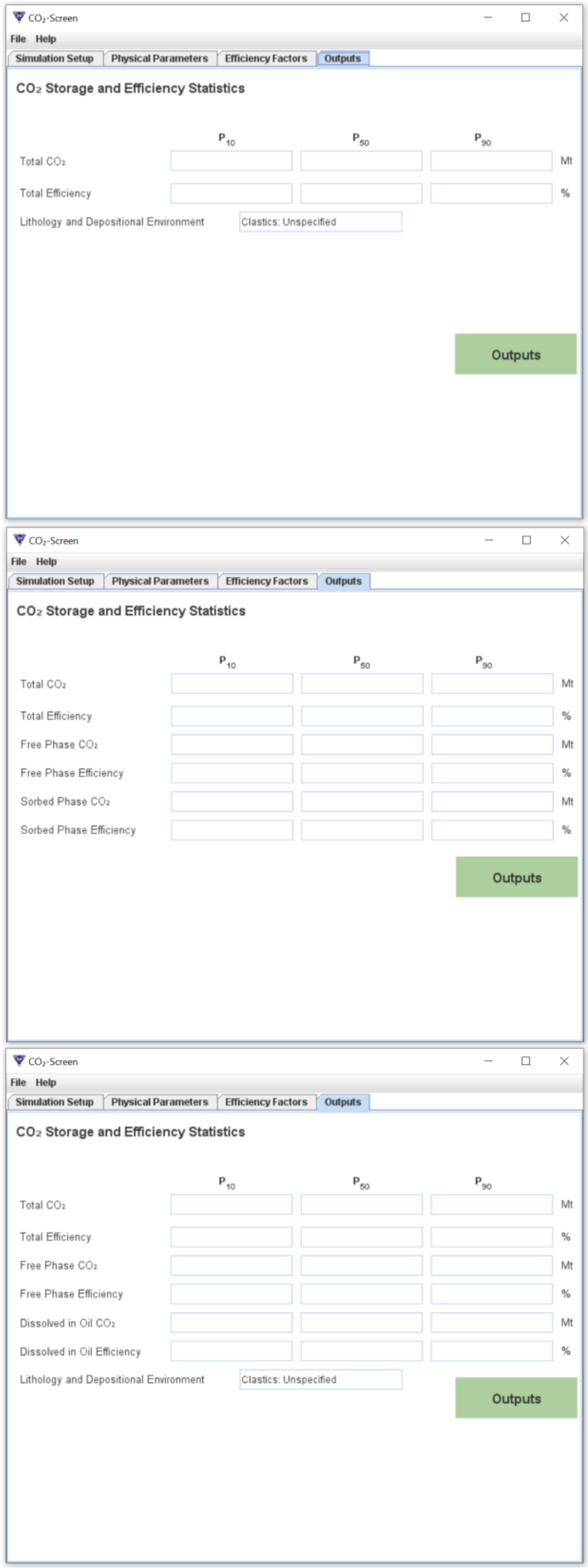

Figure 7: Screenshot of Outputs tab showing results displayed for each formation type.

Clicking on the green Outputs button will open up an Excel spreadsheet (Figure 8) with this same information. It can easily be copied, printed, or exported for external use.

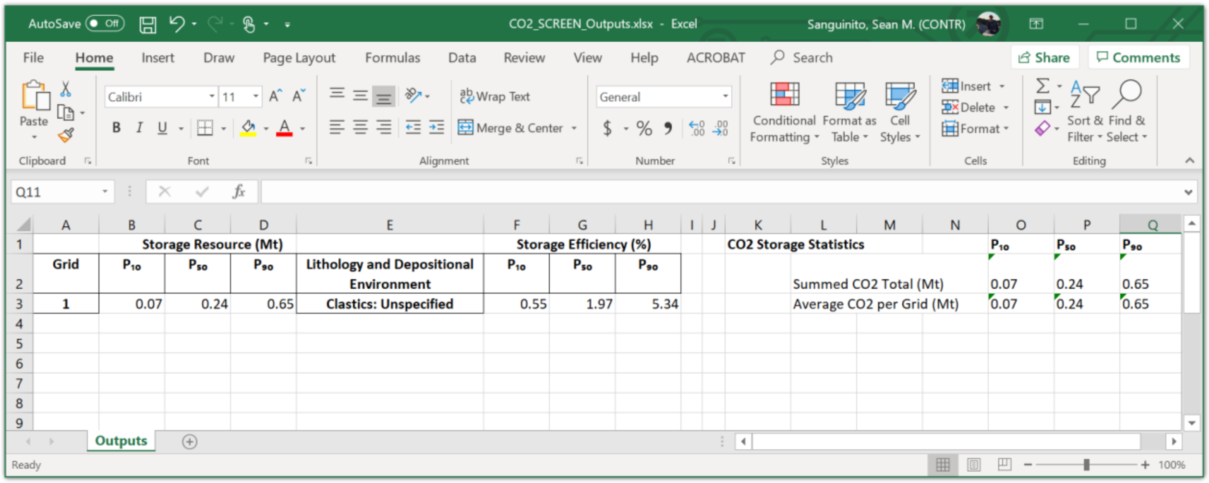

Figure 8: Screenshot of the Excel Outputs sheet generated by CO_2-SCREEN.

4.5 MULTIPLE GRID SYSTEM

Using the multiple grid system can be very helpful to handle geologic heterogeneity as well as variable data uncertainty. Entering data for multiple grids requires using Excel input files. These files are located in the FormationApps folder that is part of the downloaded zip file. In the FormationApps Folder, open the Inputs folder. Here the user will find six input files; PhysicalParametersSaline.xlsx, PhysicalParametersShale.xlsx, PhysicalParametersROZ.xlsx, StorageEfficiencyFactorsSaline.xlsx, StorageEfficiencyFactorsShale.xlsx, and StorageEfficiencyFactorsROZ.xlsx. The user should open up the PhysicalParameters and StorageEfficiency files for the formation they are assessing (See Figure 9 for a Saline Example).

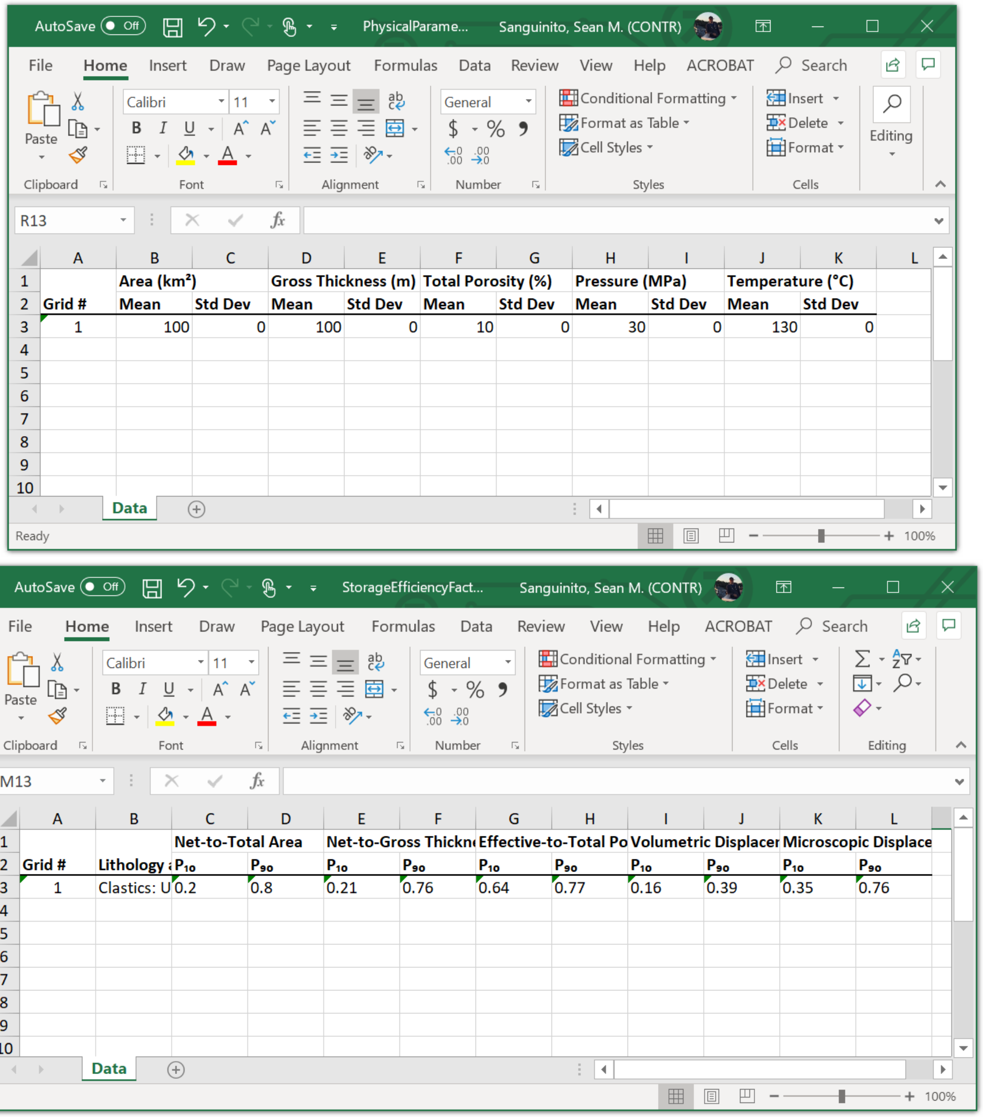

Figure 9: Screenshot showing what the PhysicalParametersSaline.xlsx and StorageEfficiencySaline.xlsx files look like.

Users should note that their files may look different than Figure 9 because every time CO_2-SCREEN is run, the input files are overwritten with the current input data. To avoid confusion, example files for all six input files are provided in the FormationApps>Examples folder. Add data for as many grids as needed to each file. Make sure you provide data for the same number of grids for Physical Parameters as well as Efficiency Factors. When all data are entered, save and close the Excel files. Now choose your formation type and select the "Use Multiple Grids" option on the Simulation Setup tab. Then navigate to the Efficiency Factors tab and click the green Run button. When utilizing the multiple grid system, the results displayed on the Outputs tab will be limited to the summed total CO_2 storage resource of all the grids. Saline will have Total CO_2, shale will have Total CO_2, Free Phase CO_2, and Sorbed Phase CO_2, and ROZ will have Total CO_2, Free Phase CO_2, and Dissolved in Oil CO_2. The Excel spreadsheet of outputs will have each grid's individual CO_2 storage and efficiency estimates.

5. CO_2-SCREEN CALCULATIONS

CO_2-SCREEN uses embedded DOE-NETL equations and methods to provide a method for calculating prospective CO_2 storage resources. These equations are described below.

5.1 SALINE FORMATIONS

CO_2-SCREEN calculates CO_2 storage resource for saline formations following the methodology detailed in Goodman et al. (2011) and refined in Goodman et al. (2016). This method uses the following equation:

$$G_{CO_2} = A_t h_g \phi_{tot} \rho_{CO_2} E_{saline} \tag{1}$$

where,

$$E_{saline} = E_A E_h E_\phi E_V E_d \tag{2}$$

All variables are described in the glossary. These terms are treated stochastically, and a log odds approach is used for distribution transformation (Goodman et al., 2011). See Appendix A for details on the log odds approach. Monte Carlo sampling from these distributions is performed using the following equation:

$$G_{CO_2} = A_t h_g \phi_{tot} \rho_{CO_2} \frac{1}{\left(1+e^{(-X_A)}\right)} * \frac{1}{\left(1+e^{(-X_h)}\right)} * \frac{1}{\left(1+e^{\left(-X_\phi\right)}\right)} * \frac{1}{\left(1+e^{(-X_V)}\right)} * \frac{1}{\left(1+e^{(-X_D)}\right)} \tag{3}$$

where, X_A, X_h, X_ϕ, X_V, and X_D, are log-odds transformed efficiency factors for the area, thickness, porosity, volumetric displacement, and microscopic displacement, respectively. Monte Carlo sampling is simulated 10,000 times and the P_{10}, P_{50}, and P_{90} values of the volumetric CO_2 mass storage resource are calculated.

5.2 SHALE FORMATIONS

CO_2-SCREEN calculates CO_2 storage resource for shale formations following the methodology detailed in Levine et al. (2016). This method uses the following equation:

$$G_{CO_2} = A_t E_A h_g E_h \left[\rho_{CO_2} \phi_{tot} E_\phi + \rho_{sCO_2} (1-\phi) E_S\right] \tag{4}$$

Again, all variables are defined in the glossary above. Once again, these terms are treated stochastically, and Monte Carlo sampling is performed using the following equation:

$$G_{CO_2} = \left[A_t h_g \phi_{tot} \rho_{CO_2} \frac{1}{\left(1+e^{(-X_A)}\right)} * \frac{1}{\left(1+e^{(-X_h)}\right)} * \frac{1}{\left(1+e^{\left(-X_\phi\right)}\right)}\right] + \left[A_t h_g \rho_{sCO_2} \rho_{shale} (LV)(1-\phi) \frac{1}{\left(1+e^{(-X_A)}\right)} * \frac{1}{\left(1+e^{(-X_h)}\right)} * \frac{1}{\left(1+e^{(-X_S)}\right)}\right] \tag{5}$$

where, ρ_{shale} is the density of shale and LV is the Langmuir volume. CO_2-SCREEN calculates Langmuir volume as:

$$LV = TOC * L_s * L_{y-int} \tag{6}$$

where, TOC is the total organic content as a percent, L_s is the Langmuir slope, and L_{y-int} is the Langmuir y-intercept. As always, using region/formation specific data are encouraged for all input parameters. However, if data are not available for Langmuir slope or y-intercept, it is recommended that users use values of 27 and 73 respectively. These values were calculated based on data from 10 different Marcellus Shale samples and thus only act as a proxy to other shale formations. Geographic information on these samples is provided in Table 2. Langmuir adsorption capacity data were plotted against total organic carbon percentage to calculate the slope and y-intercept seen in Figure 10.

Table 2: Geographic Information

Sample Suffix	Sample ID (Lat:Long:Suffix)	Formation	Type	Geographic Location
F5	390011790800F5	Marcellus	Bulk	Petersburg, WV
F3	390041790754F3	Marcellus	Bulk	Petersburg, WV
F4	391610790358F4	Marcellus	Bulk	Whip Gap, WV
F1	392005785407F1	Marcellus	Bulk	Burlington, WV
F2	392005785407F2	Marcellus	Bulk	Burlington, WV
Bedford	400817783501BD	Marcellus	Bulk	Bedford, PA
OCSC	425120764726OC	Oatka Crk	Bulk	Canoga, NY
USSC	425120764726US	Union Spr	Bulk	Canoga, NY
Type	425828762002TS	Marcellus	Bulk	Marcellus, NY
Oatka	425843775918OC	Oatka Crk	Bulk	Le Roy, NY

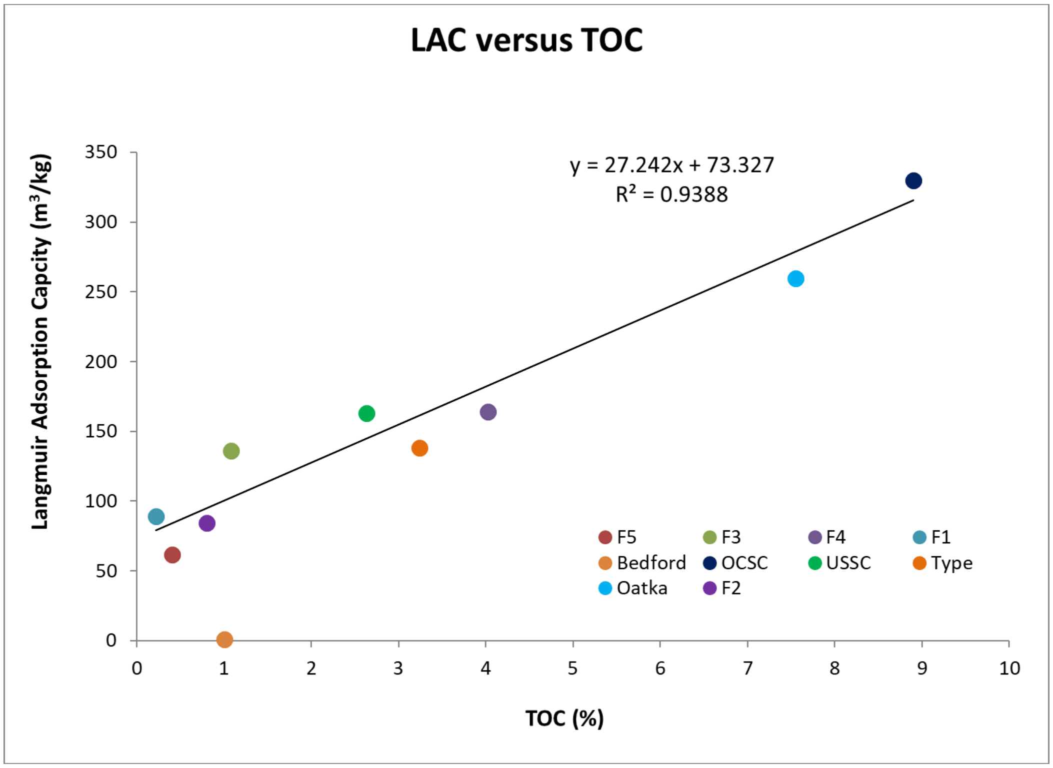

Figure 10: Langmuir adsorption capacity plotted as a function of TOC (%) to calculate Langmuir slope and y-intercept.

5.3 RESIDUAL OIL ZONE FORMATIONS

CO_2-SCREEN calculates CO_2 storage resource for shale formations following the methodology detailed in Sanguinito et al. (2020). This method uses the following equation:

$$G_{CO_2} = A_t E_A h_g E_h \phi_{tot} E_\phi \left[(1 - S_{wirr} - S_{or})\, \rho_{CO_2} E_v + S_{or} Rc_{/o}\, E_{Ds}\right] \tag{7}$$

Again, all terms are described in the glossary above and the terms are treated stochastically performing Monte Carlo sampling using the following equation:

$$G_{CO_2} = \left[A_t h_g \phi_{tot} \rho_{CO_2} (1 - S_{wirr} - S_{or}) \frac{1}{(1+e^{(-X_A)})} * \frac{1}{(1+e^{(-X_h)})} * \frac{1}{\left(1+e^{(-X_\phi)}\right)} * \frac{1}{(1+e^{(-X_v)})}\right] + \left[A_t h_g \phi_{tot} S_{or} Rc_{/o} \frac{1}{(1+e^{(-X_A)})} * \frac{1}{(1+e^{(-X_h)})} * \frac{1}{(1+e^{(-X_{Ds})})}\right] \tag{8}$$

It is recommended that values for $Rc_{/o}$ and E_{Ds} be based on region/formation specific data but if none exists users may wish to utilize a range of values, Table 3, which were generated using numerical modeling based on practical values in the literature (Sanguinito et al., 2020).

Table 3: Recommended ROZ Values for Data Limited Scenarios

Parameter	Low Value	High Value
$R_{c/o}$	679.23	741.44
E_{Ds}	0.009	0.011

6. TROUBLE SHOOTING

6.1 CO_2-SCREEN KEEPS "RUNNING" FOREVER

If the CO_2-SCREEN tool keeps running for longer than expected (i.e. longer than several minutes) it is likely having an issue with reading input files or writing output files.

- **Write Permissions**
  - If you are a Mac user, you may need to add write permissions depending on your operating system. See Section 3.3 for details on how to do this.
  - If you are a Windows user, make sure any anti-virus software (i.e. Windows Defender) is not blocking Java write permissions.
- **Numbering Multiple Grids**
  - When inputting data for multiple grids, make sure the grids are labeled sequentially and the number of grids matches between the StorageParameters file and StorageEfficiencyFactors file.

6.2 "SHARING VIOLATION" ERROR

Sometimes, a user may experience a "sharing violation" error when trying to save a StorageEfficiencyFactors input file. This can happen in certain cases as a function of how anti-virus software interacts with Microsoft Office. Typically, the file the user is attempting to edit/save is being used by the CO_2-SCREEN tool and thus cannot be changed while the tool is in use. To avoid this, simply exit the CO_2-SCREEN tool, edit the input files and save them, then reopen CO_2-SCREEN and run it.

6.3 OTHER

If users experience other issues with executing this tool, they should contact the following individuals for extra troubleshooting help.

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APPENDIX A: STORAGE EFFICIENCY FACTORS

The auto-populated storage efficiency values associated with the various lithologies and depositional environments were sourced from International Energy Agency Greenhouse Gas R&D Programme (IEA GHG, 2009). These values were developed using numerical modeling and simulation on data from over 20,000 reservoirs.

When a user selects a lithology and depositional environment, P_{10} and P_{90} values, calculated by IEA GHG (2009), are auto-populated. P_{10} and P_{90} values are the 10^{th} and 90^{th} percent probability based on a Gaussian function (Figure A1).

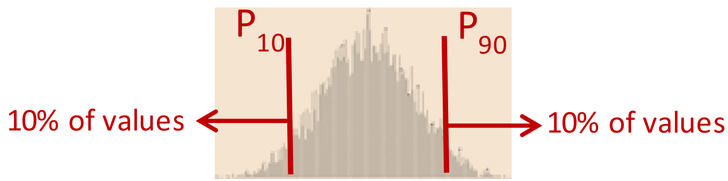

Figure A1: Gaussian function showing P_{10} and P_{90} range.

These values are then transformed using a log-odds normal distribution (Aitchison and Shen, 1980):

$$X = ln\left(\frac{p}{1-p}\right). \quad \text{(A1)}$$

X_{10} and X_{90} values are calculated using Equation A1. Then the mean (μ_X) and standard deviation (σ_X) are calculated from the X_{10} and X_{90} values using standard Gaussian distribution relationships for a log-odds distribution:

$$\sigma_X = \frac{X_{90}-X_{10}}{Z_{90}-Z_{10}} \quad \text{(A2)}$$

and

$$\mu_X = X_{10} - \sigma_x Z_{10}, \quad \text{(A3)}$$

where Z_p is the P^{th} percentile value of the standard normal distribution. Here, Z_{10} equals -1.28 and Z_{90} equals 1.28.

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APPENDIX B: SENSITIVITY ANALYSIS

Monte Carlo methods are commonly used to quantify uncertainty within complex systems such as the storage of CO_2 in geologic media (see Goodman et al., 2011). Models requiring probabilistic interpretations benefit from Monte Carlo methods through the optimization achieved by simulating a large number of realizations. Monte Carlo results will begin to converge on the most probable result with increasing number of realizations. A sensitivity analysis of CO_2-SCREEN (Figure B1) shows how Monte Carlo convergence occurs (Ballio and Guadagnini, 2004). Probabilistic CO_2 storage resource results are normalized to one million realizations and indicate a reasonable convergence by 10,000 realizations.

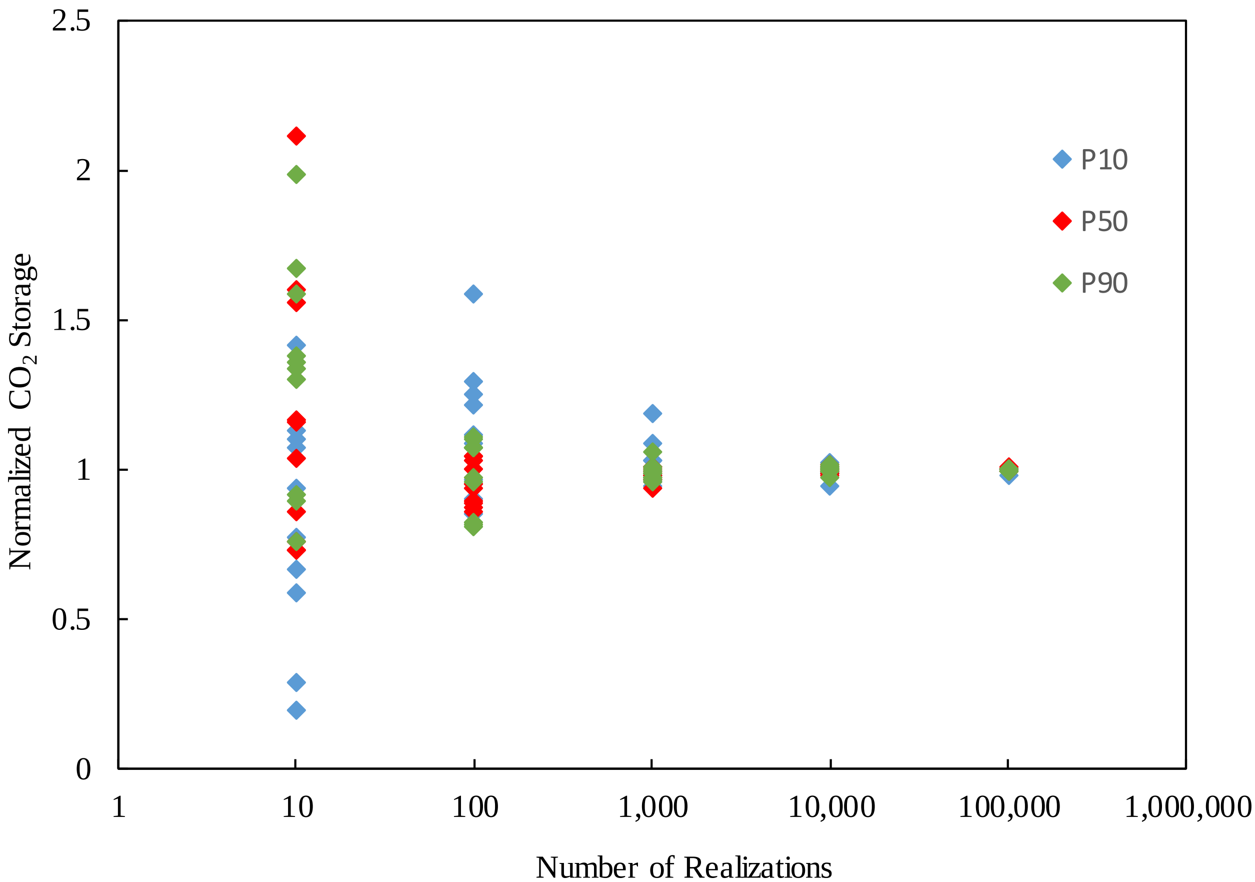

Figure B1: Sensitivity analysis showing probabilistic CO_2 storage resource values normalized to one million realizations plotted against the number of realizations for that simulation.

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