# NATIONAL ENERGY TECHNOLOGY LABORATORY



# CO<sub>2</sub> <u>Storage prospeCtive Resource</u> <u>Estimation Excel aNalysis (CO<sub>2</sub>-SCREEN)</u> User's Manual

8 May 2020





**Office of Fossil Energy** 

DOE/NETL-2020/2133

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Cover Illustration: CO<sub>2</sub>-SCREEN Splash Page.

**Suggested Citation:** Sanguinito, S.; Goodman, A.; Haeri, F. *CO*<sub>2</sub> *Storage prospeCtive Resource Estimation Excel aNalysis (CO*<sub>2</sub>*-SCREEN) User's Manual*; DOE/NETL-2020/2133; NETL Technical Report Series; U.S. Department of Energy, National Energy Technology Laboratory: Pittsburgh, PA, 2020; p 36. DOI: 10.2172/1617640.

An electronic version of this report can be found at: https://edx.netl.doe.gov/carbonstorage

# CO<sub>2</sub> Storage prospeCtive Resource Estimation Excel aNalysis (CO<sub>2</sub>-SCREEN) User's Manual

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#### DOE/NETL-2020/2133

8 May 2020

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# **Table of Contents**

ABST	RACT	1
1. I	NTRODUCTION	2
2. I	NSTALLING CO <sub>2</sub> -SCREEN	3
2.1	SYSTEM REQUIREMENTS	3
2.2	INSTALLATION	3
3. (	ETTING STARTED	4
3.1	WINDOWS USERS	4
3.2	LINUX USERS	4
3.3	MAC USERS	4
4. I	NSTRUCTIONS FOR USE	5
4.1	SIMULATION SETUP	5
4.2	PHYSICAL PARAMETERS	6
4.3	EFFICIENCY FACTORS	8
4.4	OUTPUTS	13
4.5	MULTIPLE GRID SYSTEM	15
5. (	CO2-SCREEN CALCULATIONS	17
5.1	SALINE FORMATIONS	17
5.2	SHALE FORMATIONS	17
5.3	RESIDUAL OIL ZONE FORMATIONS	19
<b>6.</b> 7	ROUBLE SHOOTING	21
6.1	CO2-SCREEN KEEPS "RUNNING" FOREVER	21
6.2	"SHARING VIOLATION" ERROR	21
6.3	OTHER	21
7. I	EFERENCES	22
а ррг	NDIX A. STORAGE EFFICIENCY FACTORS	.1
	NDIX A. GIURAUE EFFICIENCI FACIURO	1-T
APP	INDIA D; JEINJIIIVII Y AINALYJIJ	)-1

# **List of Figures**

Figure 1: Screenshot of the download file for CO <sub>2</sub> -SCREEN	3
Figure 2: CO <sub>2</sub> -SCREEN splash page	4
Figure 3: Formation Type drop down options on Simulation Setup Tab.	5
Figure 4: Screenshot of the Physical Parameters tab for each formation type	7
Figure 5: Screenshot of Efficiency Factors tab for Saline, Shale, and ROZ formations	9
Figure 6: Screenshot displaying the green Run button as well as the "Running" animation	12
Figure 7: Screenshot of Outputs tab showing results displayed for each formation type	14
Figure 8: Screenshot of the Excel Outputs sheet generated by CO <sub>2</sub> -SCREEN	15
Figure 9: Screenshot showing what the PhysicalParametersSaline.xlsx and	
StorageEfficiencySaline.xlsx files look like	16
Figure 10: Langmuir adsorption capacity plotted as a function of TOC (%) to calculate Langm	uir
slope and y-intercept	19

# **List of Tables**

Table 1: Lithology and Depositional Environment Options	10
Table 2: Geographic Information	18
Table 3: Recommended ROZ Values for Data Limited Scenarios	20

# Acronyms, Abbreviations, and Symbols

Term	Description
ρ	Density
$\rho_{sCO_2}$	Maximum mass of $CO_2$ sorbed per unit volume solid rock, e.g. the asymptotic value of an appropriate isotherm
$\phi$	Porosity
A <sub>t</sub>	Area
CO <sub>2</sub>	Carbon dioxide
CO <sub>2</sub> -SCREEN	Storage prospeCtive Resource Estimation Excel aNalysis
DOE	U.S. Department of Energy
$E_{\phi}$	Effective-to-total porosity
E <sub>A</sub>	Net-to-total area
E <sub>d</sub>	Microscopic displacement
E <sub>Ds</sub>	Fraction of $CO_2$ mass dissolved in the oil phase
EDX	Energy Data eXchange
E <sub>h</sub>	Net-to-gross thickness
Es	Sorption efficiency
Esaline	Saline efficiency
Ev	Volumetric displacement
Gt	Gigatons
GUI	Graphical user interface
$h_g$	Thickness
Mt	Million metric tons
NETL	National Energy Technology Laboratory
	CO <sub>2</sub> concentration
Swirr	Irreducible water saturation
Sor	Residual oil saturation with respect to water
TDS	Total dissolved solids
тос	Total organic content

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# Glossary

Term	Symbol	Units	Description
Area	A <sub>t</sub>	km²	Total area (map view) of the formation being assessed for CO $_{\rm 2}$ storage
CO <sub>2</sub> Concentration	R <sub>c/o</sub>		Concentration of $CO_2$ in 1 m <sup>3</sup> of oil at the (averaged) pressure (P) and (averaged) temperature (T) of a reservoir prior to injection
CO <sub>2</sub> Density	$ ho_{CO_2}$	kg/m³	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 <sub>2</sub> Storage	$G_{CO_2}$		CO <sub>2</sub> storage resource (mass)
Depositional Environment			The combination of physical, chemical, and biological processes under which sediment accumulates
Effective-to-Total Porosity	$E_{\phi}$		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 <sub>d</sub>		The fraction of pore space unavailable due to immobile in-situ fluids
Net-to-Gross Thickness	E <sub>h</sub>		Fraction of formation thickness available for CO $_2$ storage
Net-to-Total Area	E <sub>A</sub>		Fraction of formation area available for CO $_2$ storage
Oil Displacement	E <sub>Ds</sub>		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	$oldsymbol{\phi}_{tot}$	%	Average total porosity of formation being assessed for $\text{CO}_2$ storage
Reservoir Pressure	Р	МРа	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 <sub>saline</sub>		$CO_2$ 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
Swirr	Swirr		Irreducible water saturation

Term	Symbol	Units	Description
S <sub>or</sub>	Sor		Residual oil saturation with respect to water
Sorbed CO <sub>2</sub>	$ ho_{sCO_2}$		Maximum mass of CO $_2$ sorbed per unit volume solid rock, e.g. the asymptotic value of an appropriate isotherm
Sorbed CO <sub>2</sub> Efficiency	Es		Fraction of the total potential sorbed volume of CO $_2$ within the net effective volume of the formation
Temperature	Т	°C	The temperature of the formation defined by <i>A</i> and <i>h</i> at storage conditions
Thickness	$h_g$	т	Average gross thickness of formation being assessed for $CO_2$ storage
Volumetric Displacement	Ev		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

# **Glossary (cont.)**

# Acknowledgments

This work was completed as part of National Energy Technology Laboratory (NETL) research for the U.S. Department of Energy's (DOE) Carbon Storage Program. The authors wish to acknowledge Bryan Morreale (NETL Research & Innovation Center), and Traci Rodosta and Andrea McNemar, (NETL Technology Development and Integration Center).

The authors wish to acknowledge Timothy Jones and Joel Chittum from MATRIC for their work building the graphical user interface (GUI) in Java. This research was supported in part by appointments from the NETL Research Participation Program, sponsored by the U.S. DOE and administered by the Oak Ridge Institute for Science and Education (ORISE).

Research performed by Leidos Research Support Team staff was conducted under the RSS Contract 89243318CFE000003.

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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<sub>2</sub>) 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<sub>2</sub> storage resource is needed. NETL's Best Practice manual (NETL, 2013) defines prospective CO<sub>2</sub> storage resource as a mass estimate of CO<sub>2</sub> that can be stored in a geologic reservoir at the primary stage of a CO<sub>2</sub> storage project. This definition comes from the CO<sub>2</sub> 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<sub>2</sub> storage locations at regional and site scales.

This user's manual describes version 4.0 of the CO<sub>2</sub> Storage prospeCtive Resource Estimation Excel aNalysis (CO<sub>2</sub>-SCREEN) tool and provides instructions for use. CO<sub>2</sub>-SCREEN is available on the Energy Data eXchange (EDX) and can be downloaded here: <u>https://edx.netl.doe.gov/dataset/co2-screen</u>.

# 2. <u>INSTALLING CO<sub>2</sub>-SCREEN</u>

# 2.1 SYSTEM REQUIREMENTS

The following computer capabilities are recommended for using CO<sub>2</sub>-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: <u>https://edx.netl.doe.gov/dataset/co2-screen</u>.

Download the zipped folder named "co2-screen-v4\_python.zip" seen in Figure 1.



 $Figure 1: Screen shot of the download file for CO_2 - SCREEN.$ 

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. <u>GETTING STARTED</u>

# 3.1 WINDOWS USERS

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



Figure 2: CO<sub>2</sub>-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<sub>2</sub>-SCREEN splash page seen in Figure 2.

# 3.3 MAC USERS

To run CO<sub>2</sub>-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<sub>2</sub>-SCREEN files, specifically the FormationApps folder. Execute 'chmod +x \*Mac'. Then execute './SalineMac', './ShaleMac', and './ROZMac'. Navigate back to the CO<sub>2</sub>-SCREEN folder and execute 'java -jar CO2SCREEN.jar'. This will open the CO<sub>2</sub>-SCREEN splash page seen in Figure 2. The permissions to write will remain for future uses of CO<sub>2</sub>-SCREEN but it may still need to be opened using terminal for each use.

# 4. <u>INSTRUCTIONS FOR USE</u>

# 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).

🖤 CO₂-Screen		-		×
File Help				
Simulation Setup Physic	cal Parameters Efficiency Factors Outputs			
Formation Type Number of Grids	Saline Shale ROZ O Use Multiple Grids	arop down li	st her	e
CO <sub>2</sub> -SCREEN stands purpose is to provid various geologic fo	for CO <sub>2</sub> Storage prospeCtive Resource Estimation le a user-friendly method to calculate prospective mations, including saline, shale, and residual oil z	n Excel aNalysi CO <sub>2</sub> storage r ones.	s. Its esource	e for
NE TL IEC	FIONAL RGY CHNOLOGY Department CORATORY	of Energy		

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.

no nop			
Simulation Setup Physical Parameters	Efficiency Factors Outputs	]	_
Saline			
Enter Values	Mean	Standard Deviation	
Area (km²)	1		
Gross Thickness (m)			
Porosity (%)			
Praesura (MPa)			
Temperature (VC)			
Temperature ( C)			
<b>9</b> CO. Secon		_	
ile Help			
Simulation Setup Physical Parameters	Efficiency Factors Outputs	1	
Shale			
Enter Values			
	Mean	Standard Deviation	
Area (km²)			
Gross Thickness (m)			
Porosity (%)			
Pressure (MPa)			
Temperature (°C)			
Shale Density (kg/m <sup>3</sup> )			
TOC (%)			
( )			
Langmuir Slong			
Langmuir Slope			
Langmuir Slope Langmuir Y-Intercept		-	
Langmuir Slope Langmuir Y-Intercept CO <sub>2</sub> -Screen ite Help Simulation Setup   Physical Parameters	Efficiency Factors Cutputs	-	
Langmuir Slope Langmuir Y-Intercept CO <sub>2</sub> -Screen ite Help Simulation Setup   Physical Parameters ROZ	Efficiency Factors Culture	-	
Langmuir Slope Langmuir Y-Intercept CO <sub>2</sub> -Screen ite Help Simulation Setup   Physical Parameters ROZ	Efficiency Factors Outputs	-	
Langmuir Slope Langmuir Y-Intercept CO <sub>2</sub> -Screen ite Help Simulation Setup   Physical Parameters ROZ	Efficiency Factors Outputs	-	
Langmuir Slope Langmuir Y-Intercept CO <sub>2</sub> -Screen ie Help Simulation Setup Physical Parameters ROZ Enter Values	Efficiency Factors Outputs	-	
Langmuir Slope Langmuir Y-Intercept CO2-Screen ie Help Simulation Setup Physical Parameters ROZ Enter Values	Efficiency Factors Outputs Mean		
Langmuir Slope Langmuir Y-Intercept CO <sub>2</sub> -Screen ite Help Simulation Setup Physical Parameters ROZ Enter Values Area (km <sup>2</sup> )	Efficiency Factors Outputs Mean	Standard Deviation	
Langmuir Slope Langmuir Y-Intercept CO2-Screen ite Help Simulation Setup Physical Parameters ROZ Enter Values Area (km <sup>2</sup> ) Gross Thickness (m)	Efficiency Factors Outputs Mean	Standard Deviation	
Langmuir Slope Langmuir Y-Intercept © CO <sub>2</sub> -Screen ite Help Simulation Setup Physical Parameters ROZ Enter Values Area (km <sup>2</sup> ) Gross Thickness (m) Porosity (%)	Efficiency Factors Outputs Mean	Standard Deviation	
Langmuir Slope Langmuir Y-Intercept CO2-Screen ite Help Simulation Setup Physical Parameters ROZ Enter Values Area (km?) Gross Thickness (m) Porosity (%) Pressure (MPa)		Standard Deviation	
Langmuir Slope Langmuir Y-Intercept © CO <sub>2</sub> -Screen Te Help Simulation Setup Physical Parameters ROZ Enter Values Area (km <sup>2</sup> ) Gross Thickness (m) Porosity (%) Pressure (MPa) Temperature (*C)		Standard Deviation	
Langmuir Slope Langmuir Y-Intercept © CO <sub>2</sub> -Screen Te Help Simulation Setup Physical Parameters ROZ Enter Values Area (km <sup>2</sup> ) Gross Thickness (m) Porosity (%) Pressure (MPa) Temperature (*C) S <sub>wirr</sub>		Standard Deviation	
Langmuir Slope Langmuir Y-Intercept  CO <sub>2</sub> -Screen  te Help  Simulation Setup Physical Parameters  ROZ  Enter Values  Area (km <sup>2</sup> ) Gross Thickness (m) Porosity (%) Pressure (MPa) Temperature (*C) S <sub>wirr</sub> S <sub>or</sub>		Standard Deviation	
Langmuir Slope Langmuir Y-Intercept CO <sub>2</sub> -Screen ite Help Simulation Setup Physical Parameters ROZ Enter Values Area (km <sup>2</sup> ) Gross Thickness (m) Porosity (%) Pressure (MPa) Temperature (*C) S <sub>wirr</sub> S <sub>or</sub> R <sub>-m</sub> (kg/m <sup>3</sup> )		Standard Deviation	

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<sub>2</sub> 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<sub>2</sub> dissolution in oil, ROZ formations require inputs for irreducible water saturation (S<sub>wirr</sub>), residual oil saturation (with respect to water) (S<sub>or</sub>), and the concentration of CO<sub>2</sub> 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).

imulation Setup Physical Parame						
	ters Efficiency Fa	ctors Outpu	ıts			
Saline						
Enter Values						
Lithology and Depositional Envir	onment	Clastics: Un	specified		-	1
	P 10			P <sub>90</sub>		1
Net-to-Total Area	0.2		0.8			
Net-to-Gross Thickness	0.21		0.76			
Effective-to-Total Porosity	0.64		0.77			
Volumetric Displacement	0.16		0.39			
Microscopic Displacement	0.35		0.76			
						Run
CO2-Screen					-	
e Help		V	_			
imulation Setup   Physical Parame	ers Efficiency Fa	ctors Outpu	its			
Enter Values						
Years of Injection	5	•				
	- P <sub>10</sub>			P		
Net-to-Total Area	0.4		0.7	30		
Net-to-Gross Thickness	0.3		0.8			
Effective-to-Total Porosity	0.25		0.53			
Effective-to-Total Sorption	0.14					
			0.34			
			0.34			
			0.34			
			0.34			
			0.34			
			0.34			
			0.34			
			0.34			Run
			0.34			Run
CO2-Screen			0.34			Run
CO2-Screen e Help mulation Setup   Physical Parame	ters Ffficiency Fa	ctors Output	0.34		_	Run
CO2-Screen e Help imrulation Setup   Physical Parame 2027	ters Fafficiency Fa	ctors Output	0.34 fts		_	Run
<sup>®</sup> CO₂-Screen e Help imulation Setup   Physical Parame ROZ	ers Éfficiency Fa	ctors Output	U.34		-	Run
<sup>®</sup> CO₂-Screen e Help imulation Setup   <sup>°</sup> Physical Parame ROZ	ters Fafficiency Fa	ctors / Outpu	0.34 fts		_	Run
CO2-Screen e Help mulation Setup Physical Parame ROZ	ters Fafficiency Fa	ctors  ´ Outpu	U.34		-	Run
CO2-Screen e Holp imulation Setup Physical Parame ROZ Enter Values	iers Efficiency Fa	ctors <sup>^</sup> Outpu	0.34		_	Run
CO2-Screen Holp Imulation Setup Physical Parame ROZ Enter Values Lithology and Depositional Envir	ters Efficiency Fa	ctors Outpu	ts specified		-	Run
Co2-Screen     Holp     imulation Setup     Physical Parame  ROZ  Enter Values Lithology and Depositional Envir Net-to-Total Area	ters Efficiency Fa	ctors Outpu	tts	P <sub>50</sub>	-	Run
Co2-Screen Holp Physical Parame ROZ Enter Values Lithology and Depositional Envir Net-to-Total Area	ters Efficiency Fa	ctors Outpu	ts	P <sub>30</sub>	-	Run
Co2-Screen     Hotp     Translation Setup      Physical Parame  ROZ  Enter Values Lithology and Depositional Envir Net-to-Total Area Net-to-Gross Thickness	ters Efficiency Fa	ctors <sup>(</sup> Outpu Clastics: Un	rs specified 0.9 0.76	P <sub>50</sub>	-	Run
Co <sub>2</sub> -Screen     Help     Translation Setup     Physical Parame  ROZ  Enter Values Lithology and Depositional Envir Net-to-Total Area Net-to-Gross Thickness Effective-to-Total Porosity	ers Efficiency Fa onment 0.2 0.64	ctors <sup>1</sup> Outpu Clastics: Um	rs 0.8 0.7 0.77	P <sub>90</sub>	-	Run
Co <sub>2</sub> -Screen Help Translation Setup Physical Parame ROZ Enter Values Lithology and Depositional Envir Net-to-Total Area Net-to-Gross Thickness Effective-to-Total Porosity Volumetric Displacement	ers Efficiency Fa onment 0.2 0.64 0.16	Clastics: Un	rs 0.4 0.4 0.8 0.7 0.7 0.39	P <sub>50</sub>	-	Run
Co-Screen Help Frouduation Setup Physical Parame RCZ Enter Values Lithology and Depositional Envir Net-to-Total Area Net-to-Gross Thickness Effective-to-Total Porosity Volumetric Displacement Microscopic Displacement	ers Efficiency Fa onment 0.2 0.64 0.16 0.35	Clastics: Un	rs 0.34	P <sub>50</sub>	-	Run
Co <sub>2</sub> -Screen Holp Truttation Setup Physical Parame COZ Enter Values Lithology and Depositional Envir Net-to-Total Area Net-to-Gross Thickness Effective-to-Total Porosity Volumetric Displacement Microscopic Displacement CO <sub>2</sub> Dissolution in Oil	ters Efficiency Fa onment 0.2 0.21 0.64 0.16 0.35 0.009	Clastics: Un	specified           0.34           0.8           0.76           0.76	P <sub>50</sub>	-	Run
CO <sub>2</sub> -Screen  Holp  Imutation Setup Physical Parame  ROZ  Enter Values  Lithology and Depositional Envir Net-to-Total Area Net-to-Gross Thickness Effective-to-Total Porosity Volumetric Displacement Microscopic Displacement CO <sub>2</sub> Dissolution in Oil	ers Efficiency Fa	Clastics: Un	specified 0.8 0.77 0.39 0.76 0.77 0.39 0.76 0.011	P <sub>30</sub>	-	Run
CO <sub>2</sub> -Screen Help Innulation Setup Physical Parame ROZ Enter Values Lithology and Depositional Envir Net-to-Total Area Net-to-Total Area Net-to-Gross Thickness Effective-to-Total Porosity Volumetric Displacement Microscopic Displacement CO <sub>2</sub> Dissolution in Oil	ers Efficiency Fa	Clastics: Un	specified 0.9 0.9 0.7 0.39 0.76 0.77 0.39 0.76 0.011	P <sub>30</sub>	-	Run
CO <sub>2</sub> -Screen Help Insulation Setup Physical Parame ROZ Enter Values Lithology and Depositional Envir Net-to-Total Area Net-to-Gross Thickness Effective-to-Total Porosity Volumetric Displacement Microscopic Displacement CO <sub>2</sub> Dissolution in Oil	ers Efficiency Fa onment 0.2 0.64 0.35 0.009	Clastics: Un	specified	P <sub>30</sub>		Run

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 autopopulate  $P_{10}$  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).

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

#### Table 1: Lithology and Depositional Environment Options

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<sub>2</sub> 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.

ile Help Simulation Setup Physical Parameters Efficiency Factors Outputs Saline Enter Values Lithology and Depositional Environment Clastics: Unspecified  P <sub>10</sub> P <sub>30</sub> Net-to-Total Area 0.2 0.8 Net-to-Total Area 0.2 0.8 Net-to-Gross Thickness 0.21 0.76 Effective-to-Total Porosity 0.64 0.77 Volumetric Displacement 0.16 0.39 Microscopic Displacement 0.35 0.76 Run V CO <sub>2</sub> -Screen – • • • • • • • • • • • • • • • • • •	Filep   mutation Setup Physical Parameters Efficiency Factors Outputs   Enter Values   Lithology and Depositional Environment Clastics: Unspecified     P10 P30 P30   Net-to-Total Area 0.2 0.8   Net-to-Total Area 0.21 0.76   Effective-to-Total Porosity 0.84 0.77   Volumetric Displacement 0.16 0.39   Microscopic Displacement 0.35 0.76     CO2-Screen -      Help     mutation Setup Physical Parameters   Efficiency Factors Outputs     aline           Enter Values   Lithology and Depositional Environment   Clastics: Unspecified   P10   P20   P30								
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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<sub>2</sub> storage resource, the Total Efficiency, and the Lithology and Depositional Environment chosen. Shale formations will display the Total CO<sub>2</sub> storage resource, Total Efficiency, Free Phase CO<sub>2</sub> storage resource, Free Phase Efficiency, Sorbed Phase CO<sub>2</sub> Storage, and Sorption Efficiency. ROZ formations will display the Total CO<sub>2</sub> storage resource, Total Efficiency, Free Phase CO<sub>2</sub> storage resource, Free Phase Efficiency, Dissolved in Oil CO<sub>2</sub> storage resource, Dissolved in Oil Efficiency, and Lithology and Depositional Environment chosen.

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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.

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Figure 8: Screenshot of the Excel Outputs sheet generated by CO<sub>2</sub>-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  $CO_2$ , 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. <u>CO<sub>2</sub>-SCREEN CALCULATIONS</u>

 $CO_2$ -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:

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

where,  $X_A$ ,  $X_h$ ,  $X_\phi$ ,  $X_V$ , 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<sub>10</sub>, P<sub>50</sub>, and P<sub>90</sub> values of the volumetric CO<sub>2</sub> 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:

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

$$G_{CO_{2}} = \left[ A_{t}h_{g}\phi_{tot}\rho_{CO_{2}} \frac{1}{(1+e^{(-X_{A})})} * \frac{1}{(1+e^{(-X_{h})})} * \frac{1}{(1+e^{(-X_{h})})} \right] + \left[ A_{t}h_{g}\rho_{sCO_{2}}\rho_{shale}(LV)(1-\phi) \frac{1}{(1+e^{(-X_{A})})} * \frac{1}{(1+e^{(-X_{h})})} * \frac{1}{(1+e^{(-X_{h})})} \right]$$
(5)

where,  $\rho_{shale}$  is the density of shale and LV is the Langmuir volume. CO<sub>2</sub>-SCREEN calculates Langmuir volume as:

$$LV = TOC * L_s * L_{y-int}$$
(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.

Sample Suffix	Sample ID (Lat:Long:Suffix)	Formation	Туре	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
Туре	425828762002TS	Marcellus	Bulk	Marcellus, NY
Oatka	425843775918OC	Oatka Crk	Bulk	Le Roy, NY

Table 2: Geographic Information



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:

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

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

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

Parameter	Low Value	High Value			
Rc <sub>/o</sub>	679.23	741.44			
E <sub>Ds</sub>	0.009	0.011			

#### Table 3: Recommended ROZ Values for Data Limited Scenarios

## 6. TROUBLE SHOOTING

### 6.1 CO<sub>2</sub>-SCREEN KEEPS "RUNNING" FOREVER

If the CO<sub>2</sub>-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 antivirus 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<sup>th</sup> and 90<sup>th</sup> 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):

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

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

$$\sigma_X = \frac{X_{90} - X_{10}}{Z_{90} - Z_{10}} \tag{A2}$$

and

$$\mu_X = X_{10} - \sigma_x Z_{10}, \tag{A3}$$

where  $Z_p$  is the P<sup>th</sup> 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<sub>2</sub> storage resource values normalized to one million realizations plotted against the number of realizations for that simulation.

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