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Cover Illustration: Inputs, GoldSim Model Structure, and Outputs of CO₂-SCREEN.

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NETL CO₂ Storage prospective Resource Estimation Excel aNalysis (CO₂-SCREEN) User's Manual

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Acronyms, Abbreviations, and Symbols

Term	Description
ρ	Density
ϕ	Porosity
A	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_h	Net-to-Gross Thickness
E_{saline}	Saline Efficiency
E_V	Volumetric Displacement
Gt	Gigatons
h	Thickness
LUT	Lookup table
Mt	Million metric tons
NETL	National Energy Technology Laboratory
RSCP	Regional Carbon Sequestration Partnerships
TDS	Total dissolved solids

Glossary

Term	Symbol	Units	Description
Area	A	km^2	Area (map view) that defines the formation being assessed for CO ₂ storage
Basin			A depression in the crust of the Earth, caused by plate tectonic activity and subsidence, in which sediments accumulate
Density	ρ	kg/m^3	Density of CO ₂ evaluated at the pressure and temperature that represents storage conditions defined by A and h
Depositional Environment			The combination of physical, chemical, and biological processes under which sediment accumulates
Effective-to-Total Porosity	E_{ϕ}		Fraction of the pore space that can store CO ₂
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		The fraction of the thickness available for CO ₂ storage
Net-to-Total Area	E_A		The fraction of the area (map view) available for CO ₂ storage
Physical Parameters			The parameters required to calculate the potential CO ₂ storage resource (i.e. area, thickness, porosity)
Porosity	ϕ	%	The volume of void space per volume of rock
Reservoir Pressure		MPa	The pressure of the formation defined by A and h at storage conditions
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
Temperature		$^{\circ}C$	The temperature of the formation defined by A and h at storage conditions
Thickness	h	m	The thickness of the formation for which CO ₂ storage is assessed as defined by A
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) CO₂ Storage prospective Resource Estimation Excel aNalysis (CO₂-SCREEN) tool, which was developed to aid users screening saline formations for prospective CO₂ storage resources. CO₂-SCREEN applies U.S. Department of Energy (DOE) methods and equations for estimating prospective CO₂ storage resources for saline formations. CO₂-SCREEN was developed to be substantive and user-friendly. It also provides a consistent method for calculating prospective CO₂ storage resources that allows for consistent comparison of results between different research efforts, such as the Regional Carbon Sequestration Partnerships (RCSP). CO₂-SCREEN consists of an Excel spreadsheet containing geologic inputs and outputs, linked to a GoldSim Player model that calculates prospective CO₂ storage resources via Monte Carlo simulation.

1. INTRODUCTION

Since 2007, the U.S. Department of Energy, National Energy Technology Laboratory (DOE-NETL) Carbon Storage Program and Regional Carbon Sequestration Partnership (RCSP) has cooperated with the goal of assessing the prospective storage resource of carbon dioxide (CO₂) in the United States and Canada (NETL, 2015; Goodman et al., 2011; Popova et al., 2012; Goodman et al., 2013; Popova et al., 2014; Goodman et al., 2016; Levine et al., 2016). In order to make high-level, energy-related government policy and business decisions the ability to accurately predict the CO₂ storage resource is needed. NETL's Best Practice manual (NETL, 2013) defines prospective CO₂ storage resource as a mass estimate of CO₂ that can be stored in a geologic reservoir at the primary stage of a CO₂ storage project. This definition comes from the CO₂ 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 CO₂ storage locations at regional and site scales.

This user's manual describes CO₂ Storage prospective Resource Estimation Excel aNalysis (CO₂-SCREEN) tool: a tool which was developed by the DOE-NETL to screen saline formations for prospective CO₂ storage resources.

CO₂-SCREEN is available on the [Energy Data eXchange \(EDX\)](#). This manual describes CO₂-SCREEN, explains the organization and structure of the software files, and provides instructions for use.

2. TOOL DESCRIPTION

The NETL CO₂-SCREEN tool was developed to provide a substantive, user-friendly, and consistent mechanism to calculate CO₂ storage resources. CO₂-SCREEN is composed of three files: this User's Manual with background information and instructions for use, an Excel file used for data inputs and outputs, and a GoldSim Player file used to run Monte Carlo simulations. The Excel file, NETL-CO₂-SCREEN.xlsx, allows a user to input subsurface geological physical parameter values and establish ranges for storage efficiency factors. The GoldSim Player file, NETL-CO₂-SCREEN.gsp, accesses the input data saved in the Excel file, calculates probability estimates for CO₂ storage resources using Monte Carlo methods, and outputs these values back into the Excel file in a separate tab.

CO₂-SCREEN includes the input of five storage efficiency factors (Table 1) which represent the fraction of formation volume accessible for CO₂ storage. These efficiency factors are entered as P₁₀ and P₉₀ probability values and range from 0 to 1.

Table 1: Definitions of efficiency factors

Storage Efficiency Term	Symbol	Definition
Net-to-Total Area	E_A	Fraction of the area (map view) available for CO ₂ storage
Net-to-Gross Thickness	E_h	Fraction of the thickness available for CO ₂ storage
Effective-to-Total Porosity	E_ϕ	Fraction of the pore space that can store CO ₂
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
Microscopic Displacement	E_d	The fraction of pore space unavailable due to immobile in-situ fluids

Ideally, efficiency factor ranges should be based on the geologic properties of the formation being assessed. In CO₂-SCREEN, efficiency factor ranges can be manually entered by the user based upon geologic properties. In the absence of detailed geologic information, CO₂-SCREEN can auto-populate efficiency ranges based on the user's choice of lithology and depositional environment (Table 2), as provided by the International Energy Agency Greenhouse Gas (IEA GHG, 2009). Efficiency factors may also be removed by manually setting the factor to equal 1 (100 percent efficiency) if the user determines the efficiency factor is not needed. CO₂-SCREEN allows storage efficiency ranges to be separately constrained to allow for varying data availability.

Table 2: Lithology and depositional environment options (IEA GHG, 2009; NETL, 2015)

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

3. EXCEL FILE

The CO₂-SCREEN Excel file is used as both the input and output file and also contains several informational tabs (Table 3). Operational details can be found in section 5. The Excel file is linked to the GoldSim Player file, NETL-CO₂-SCREEN.gsp, and is required for CO₂-SCREEN to function properly. Inputs and outputs are designated by two separate tabs in Excel.

Table 3: CO₂-SCREEN Excel file tab descriptions

Tab	Description
Read Me	Foreword and general instructions
Saline (Inputs)	Enter background information, storage efficiency factors, and geologic storage parameters for saline formations here
Saline (Outputs)	GoldSim results for saline inputs are populated here
Calculations	Calculations related to grid specific storage efficiency factors
Depositional Environments	Calculations of storage efficiency factors based upon lithology and depositional environment
Glossary	Brief description of terms used throughout CO ₂ -SCREEN
References	References used throughout CO ₂ -SCREEN
Contact	Contact information

3.1 INPUTS

The Saline (Inputs) tab (Figure 1) contains instructions, information, and reference values on the left side and an input area on the right side. Here, the user will enter general information, storage efficiency values, and physical geologic parameters.

NETL CO₂-SCREEN

Instructions:

- Type general information into cells B6:B9
- Storage Efficiency Factors
 - Option One: Choose the lithology and depositional environment using the drop-down list in cell I17 (yellow). This will auto-populate storage efficiency P_{18} and P_{19} values in cells J21:J25 and J21:J25 (yellow)
 - Option Two: Enter user specific P_{18} and P_{19} values in cells K21:K25 and L21:L25 (green)
- Physical Parameters
 - Enter formation data for each grid
 - Any grids not being used require 2's in all cells in that row
 - Grid Specific Efficiency
 - Choose grid specific efficiency factor ranges
 - Can choose different lithology and depositional environments or set user specified ranges on a grid to grid basis
 - Do not alter spreadsheet cell layout as this may cause errors when syncing with GoldSim Player
 - After data are input, save and close spreadsheet before running GoldSim Player
 - Each simulation using GoldSim will overwrite output values

*** (Area, Thickness, Porosity)**
These will be treated as gross estimates requiring application of efficiency terms. To use "net" values manually enter 1 for respective P_{18} and P_{19} efficiency terms.

† (Pressure, Temperature)
Ranges are limited by the book up table in GoldSim Player
Pressure must range between 0.1 and 60 MPa
Temperature must range between 1 and 180°C

Reference Values

Tag	Tag	Tag
1.24	1.25	1.26

Data Inputs

General Information

Researcher Name	Jane Smith
Formation Name	Example Formation
Date	1/1/2017
Run ID	123-Clastics

Storage Efficiency Factors

Auto-populate: Choose lithology and depositional environment
User Specified: Directly enter P_{18} and P_{19} values

Lithology and Depositional Environment

Classics: Unspecified

	Auto-populated		User Specified					
	P_{18}	P_{19}	P_{18}	P_{19}	X_{18}	X_{19}	H_1	H_2
Net-to-Total Area	0.20	0.80	0	0	-1.39	1.39	0.00	1.00
Net-to-Gross Thickness	0.21	0.79	0	0	-1.32	1.15	-0.08	0.97
Effective-to-Total Porosity	0.64	0.77	0	0	0.58	1.21	0.89	0.10
Volumetric Displacement	0.16	0.39	0	0	-1.66	-0.45	-1.05	0.47
Microscopic Displacement	0.35	0.75	0	0	-0.62	1.15	0.27	0.88

Physical Parameters

Mean and standard deviation values for each grid

Grid #	Area* (km ²)		Gross Thickness* (m)		Total Porosity* (%)		Pressure* (MPa)		Temperature* (°C)	
	Mean	Std Dev	Mean	Std Dev	Mean	Std Dev	Mean	Std Dev	Mean	Std Dev
1	1	1	1	1	1	1	1	1	1	1
2	1	1	1	1	1	1	1	1	1	1
3	1	1	1	1	1	1	1	1	1	1
4	1	1	1	1	1	1	1	1	1	1
5	1	1	1	1	1	1	1	1	1	1
6	1	1	1	1	1	1	1	1	1	1
7	1	1	1	1	1	1	1	1	1	1
8	1	1	1	1	1	1	1	1	1	1
9	1	1	1	1	1	1	1	1	1	1
10	1	1	1	1	1	1	1	1	1	1
11	1	1	1	1	1	1	1	1	1	1
12	1	1	1	1	1	1	1	1	1	1

Grid Specific Efficiency

Choose grid specific efficiency factor ranges to account for formation heterogeneity
*Default setting uses values set in step 2

Grid #	Lithology and Depositional Environment	User Specified									
		E_1	E_2	E_3	E_4	E_5	E_6	E_7	E_8	E_9	E_{10}
1	Default	0	0	0	0	0	0	0	0	0	0
2	Default	0	0	0	0	0	0	0	0	0	0
3	Default	0	0	0	0	0	0	0	0	0	0
4	Default	0	0	0	0	0	0	0	0	0	0
5	Default	0	0	0	0	0	0	0	0	0	0
6	Default	0	0	0	0	0	0	0	0	0	0
7	Default	0	0	0	0	0	0	0	0	0	0
8	Default	0	0	0	0	0	0	0	0	0	0
9	Default	0	0	0	0	0	0	0	0	0	0
10	Default	0	0	0	0	0	0	0	0	0	0
11	Default	0	0	0	0	0	0	0	0	0	0
12	Default	0	0	0	0	0	0	0	0	0	0

Figure 1: CO₂-SCREEN Saline (Inputs) tab.

The General Information section (Figure 2) is not required to run CO₂-SCREEN, but it provides useful information that will be exported through to the Saline (Outputs) tab. It is recommended to fill this out for better organization and record keeping.

General Information

Researcher Name	Jane Smith
Formation Name	Example Formation
Date	1/1/2017
Run ID	123-Clastics

Figure 2: General Information section in the Saline (Inputs) tab of CO₂-SCREEN.

Storage efficiency factors (Figure 3) can be manually entered by the user or auto-populated based on a selected lithology and depositional environment. In CO₂-SCREEN, the efficiencies representing three lithologies and ten depositional environments are taken directly from the report compiled by IEA GHG (2009). Each efficiency factor can be set separately to provide greater constraints on the parameters for which more data are available for the formation of interest.

2	Storage Efficiency Factors								
	Auto-populate: Choose lithology and depositional environment								
	User Specified: Directly enter P ₁₀ and P ₉₀ values								
	Lithology and Depositional Environment	Clastics: Unspecified							
		Auto-populated		User Specified					
		P ₁₀	P ₉₀	P ₁₀	P ₉₀	X ₁₀	X ₉₀	μ _x	σ _x
	Net-to-Total Area	0.20	0.80	0	0	-1.39	1.39	0.00	1.08
	Net-to-Gross Thickness	0.21	0.76	0	0	-1.32	1.15	-0.09	0.97
	Effective-to-Total Porosity	0.64	0.77	0	0	0.58	1.21	0.89	0.25
	Volumetric Displacement	0.16	0.39	0	0	-1.66	-0.45	-1.05	0.47
	Microscopic Displacement	0.35	0.76	0	0	-0.62	1.15	0.27	0.69

Figure 3: Storage Efficiency Factors section in the Saline (Inputs) tab of CO₂-SCREEN.

The physical parameters (Figure 4) include area, thickness, porosity, pressure, and temperature. Mean and standard deviation values for each parameter (except area) are required as inputs. If data are limited and only average values are known, then the standard deviation can be set to zero. If formation data are expressed in a grid, separate storage parameter values can be entered for each grid cell. If grid cells are not used, all unused cells must contain a 1 for GoldSim to function (see rows 6–12 in Figure 4 as an example of grids not being used).

3	Physical Parameters									
	Mean and standard deviation values for each grid									
	Grid #	Area* (km²)	Gross Thickness* (m)		Total Porosity* (%)		Pressure[†] (MPa)		Temperature[†] (°C)	
		Mean	Mean	Std Dev	Mean	Std Dev	Mean	Std Dev	Mean	Std Dev
	1	100	50	0	5	0	25	0	100	0
	2	100	50	0	5	0	25	0	100	0
	3	100	50	0	5	0	25	0	100	0
	4	100	50	0	5	0	25	0	100	0
	5	100	50	0	5	0	25	0	100	0
	6	1	1	1	1	1	1	1	1	1
	7	1	1	1	1	1	1	1	1	1
	8	1	1	1	1	1	1	1	1	1
	9	1	1	1	1	1	1	1	1	1
	10	1	1	1	1	1	1	1	1	1
	11	1	1	1	1	1	1	1	1	1
	12	1	1	1	1	1	1	1	1	1

Figure 4: Physical Parameters section in the Saline (Inputs) tab of CO₂-SCREEN.

The Grid Specific Efficiency (Figure 5) section allows a user to set grid specific storage efficiency values. A user can use a “default” setting which automatically populates the storage efficiency factors set in Figure 3 or choose a different lithology and depositional environment on a grid by grid basis. Values are populated in the “Calculations” tab to be accessed by GoldSim. After choosing the lithology and depositional environment for a grid, individual storage efficiency factors can be altered to further refine the storage efficiency. Any cell containing a “0” value will use the value based on the selected lithology and depositional environment.

Grid Specific Efficiency Choose grid specific efficiency factor ranges to account for formation heterogeneity *Default setting uses values set in step 2											
4											
Grid #	Lithology and Depositional Environment	User Specified									
		E _A		E _h		E _φ		E _d		E _v	
		P ₁₀	P ₉₀	P ₁₀	P ₉₀	P ₁₀	P ₉₀	P ₁₀	P ₉₀	P ₁₀	P ₉₀
1	Default	0	0	0	0	0	0	0	0	0	0
2	Default	0	0	0	0	0	0	0	0	0	0
3	Default	0	0	0	0	0	0	0	0	0	0
4	Default	0	0	0	0	0	0	0	0	0	0
5	Default	0	0	0	0	0	0	0	0	0	0
6	Default	0	0	0	0	0	0	0	0	0	0
7	Default	0	0	0	0	0	0	0	0	0	0
8	Default	0	0	0	0	0	0	0	0	0	0
9	Default	0	0	0	0	0	0	0	0	0	0
10	Default	0	0	0	0	0	0	0	0	0	0
11	Default	0	0	0	0	0	0	0	0	0	0
12	Default	0	0	0	0	0	0	0	0	0	0

Figure 5: Grid Specific Efficiency section in the Saline (Inputs) tab of CO₂-SCREEN.

3.2 OUTPUTS

The Saline Outputs tab (Figure 6) of the CO₂-SCREEN Excel file displays the results generated from the GoldSim Player. Results are displayed as P₁₀, P₅₀, and P₉₀ values for mass CO₂ in million metric tons (Mt) for each grid. The Excel tab is formatted (Figure 7) to permit printing a summary of results and pertinent information.

Prospective CO ₂ Storage Resource				Grid	P ₁₀ (Mt)	P ₅₀ (Mt)	P ₉₀ (Mt)	Lithology and Depositional Environment	Saline Efficiency (%)		
									P ₁₀	P ₅₀	P ₉₀
Information				1	0.613	2.209	5.795	Clastics: Unspecified	0.42	1.50	3.94
				2	1.134	3.197	6.936	User Specified	0.77	2.17	4.71
				3	2.731	8.315	14.792	User Specified	1.86	5.65	10.05
				4	0.395	1.426	3.734	User Specified	0.27	0.97	2.54
Researcher Name	Jane Smith			5	5.034	15.907	30.015	User Specified	2.50	7.90	14.92
Formation Name	Example Formation			6	0.000	0.000	0.000	Clastics: Unspecified	0.65	2.44	6.77
Date	1/1/2016			7	0.000	0.000	0.000	Clastics: Unspecified	0.42	1.50	3.94
Depositional Environment	Clastics: Unspecified			8	0.000	0.000	0.000	Clastics: Unspecified	0.42	1.50	3.94
Number of Grids	5			9	0.000	0.000	0.000	Clastics: Unspecified	0.48	1.80	4.88
Run ID	123-Clastics			10	0.000	0.000	0.000	Clastics: Unspecified	0.42	1.50	3.94
				11	0.000	0.000	0.000	Clastics: Unspecified	0.42	1.50	3.94
CO₂ Storage Statistics				12	0.000	0.000	0.000	Clastics: Unspecified	0.42	1.50	3.94
				13	0.000	0.000	0.000	Clastics: Unspecified	0.42	1.50	3.94
Summed CO ₂ Total	9.91	31.06	61.27	14	0.000	0.000	0.000	Clastics: Unspecified	0.42	1.50	3.94
Average CO ₂ per Grid	1.98	6.21	12.25	15	0.000	0.000	0.000	Clastics: Unspecified	0.42	1.50	3.94
				16	0.000	0.000	0.000	Clastics: Unspecified	0.42	1.50	3.94
Summed CO ₂ Total	0.010	0.031	0.061	17	0.000	0.000	0.000	Clastics: Unspecified	0.42	1.50	3.94
Average CO ₂ per Grid	0.002	0.006	0.012	18	0.000	0.000	0.000	Clastics: Unspecified	0.42	1.50	3.94
				19	0.000	0.000	0.000	Clastics: Unspecified	0.42	1.50	3.94
				20	0.000	0.000	0.000	Clastics: Unspecified	0.42	1.50	3.94

Figure 6: Saline (Outputs) tab in CO₂-SCREEN displaying CO₂ storage results.

Prospective CO₂ Storage Resource

Information

Researcher Name	Jane Smith
Formation Name	Example Formation
Date	1/1/2016
Depositional Environment	Clastics: Unspecified
Number of Grids	5
Run ID	123-Clastics

CO₂ Storage Statistics

	P ₁₀	P ₅₀	P ₉₀	
Summed CO ₂ Total	9.91	31.06	61.27	Mt
Average CO ₂ per Grid	1.98	6.21	12.25	Mt
Summed CO ₂ Total	0.010	0.031	0.061	Gt
Average CO ₂ per Grid	0.002	0.006	0.012	Gt

Figure 7: Print screen display of CO₂-SCREEN Saline (Outputs) tab.

4. GOLDSIM MODEL

4.1 INTRODUCTION

GoldSim is primarily a Monte Carlo simulation program that is capable of modeling complex systems within a visual interface. It is a visual-based model in which a user structures icons and arrows in lieu of text based code. GoldSim is a licensed program, but provides a free Player version that can run pre-constructed GoldSim models such as CO₂-SCREEN. The free Player can be downloaded at <http://www.goldsim.com/forms/playerdownload.aspx>. GoldSim can only be run on a Windows Operating system and is supported on Windows 7, 8, and 10.

4.2 MODEL STRUCTURE

CO₂-SCREEN's GoldSim structure is divided into a main model and a submodel. The main model (Figure 8) contains the P₁₀, P₅₀, and P₉₀ probability estimates generated from the submodel and an output function linked to Excel.

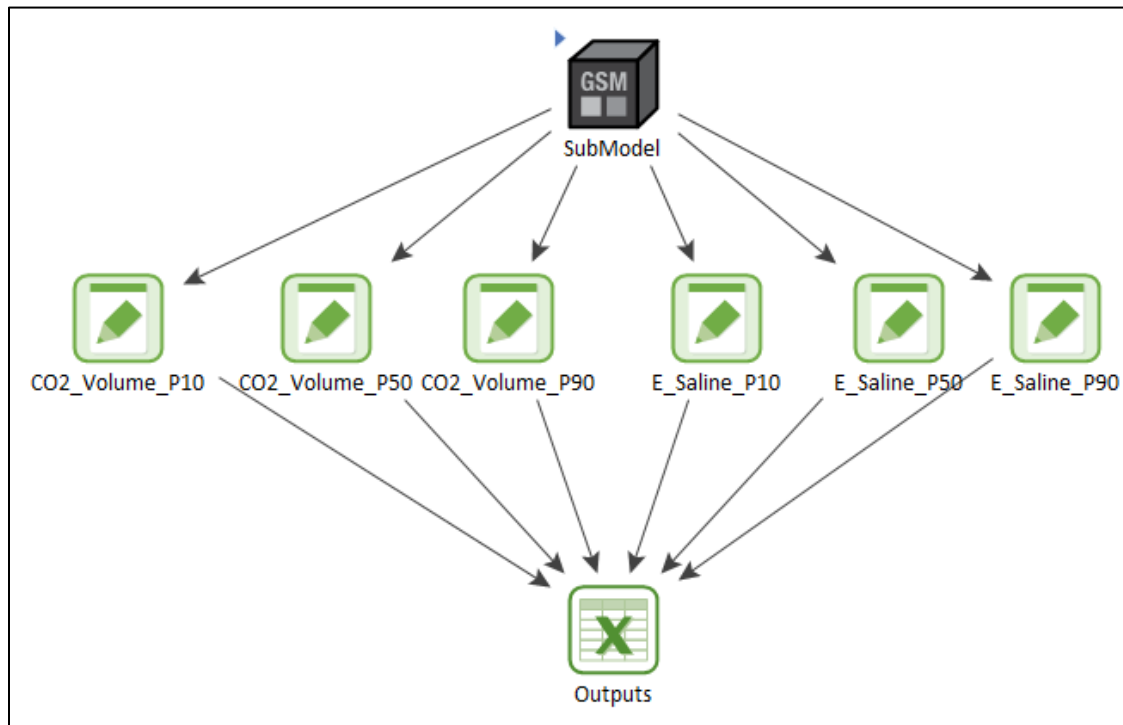


Figure 8: GoldSim main model structure of CO₂-SCREEN.

The submodel (Figure 9) is composed of an Excel input function, data distributions for the input parameters, a lookup table (LUT) to calculate CO₂ density, embedded equations to calculate prospective CO₂ storage resource, and generated results that are relayed to the main model to be exported to the corresponding Excel file.

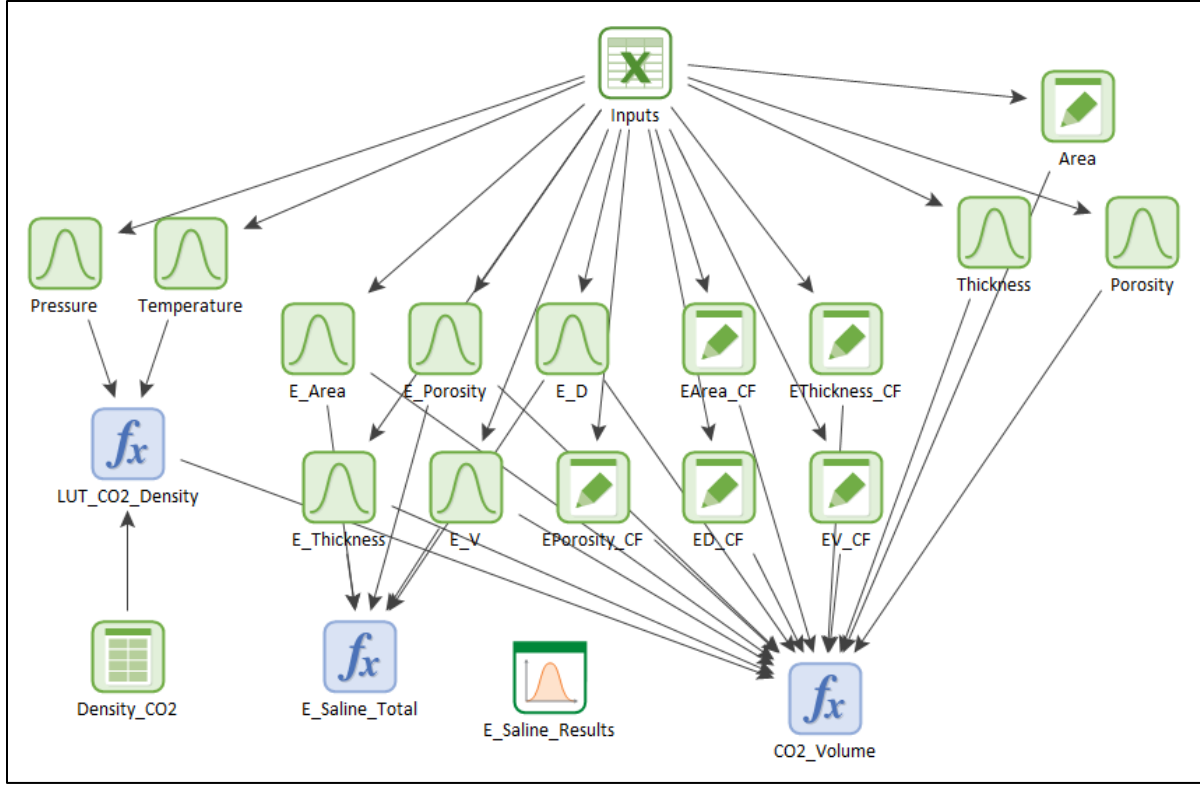


Figure 9: GoldSim submodel structure of CO₂-SCREEN.

The Excel input and output functions are the link between the CO₂-SCREEN Excel file and GoldSim Player file. This data link will only work if the Excel file name “NETL-CO₂-SCREEN.xlsx” remains unchanged and this file must be closed when running the GoldSim Player.

The distribution functions, displayed as icons with a red bell curve with blue axes, are generated by GoldSim for each input except the area term. Each of the five efficiency values are treated with a Log-Odds transformation. The pressure and temperature values are treated with normal distributions. A lookup table based on Duan and Sun (2003) is used to calculate CO₂ density from the pressure and temperature inputs which can range between 0.1–60 MPa and 1–180°C respectively. Log-normal distributions are generated for the thickness and porosity physical parameters, while a mean value is used for the area parameter.

GoldSim then performs Monte Carlo sampling from these distributions using the following equation:

$$G = A h \phi \rho \frac{1}{(1+e^{(-XA)})} * \frac{1}{(1+e^{(-Xh)})} * \frac{1}{(1+e^{(-X\phi)})} * \frac{1}{(1+e^{(-XV)})} * \frac{1}{(1+e^{(-XD)})} , \quad (1)$$

where G is the mass estimate of the saline formation for prospective CO₂ storage resource, A is the area (km²) (map view) that defines the formation being assessed for CO₂ storage, h is the thickness (m) of the formation being assessed as defined by A , ϕ is the porosity (represented as a percentage) or volume of void space per volume of rock, ρ is density (kg/m³) of CO₂ evaluated

at the pressure (MPa) and temperature (°C) that represents storage conditions defined by A and h , and 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 CO₂ mass storage resource are calculated and automatically exported to the Saline (Outputs) tab in the Excel file.

5. **INSTRUCTIONS FOR USE**

Using CO₂-SCREEN is designed to be straightforward and user-friendly. Only two files are necessary: the Excel file titled NETL-CO₂-SCREEN.xlsx and the GoldSim Player file titled NETL-CO₂-SCREEN.gsp. The three basic steps required to use CO₂-SCREEN are: 1) data input into the Excel file, 2) running the GoldSim Player file, and 3) data output into the Excel file.

5.1 **INPUTS**

Before entering inputs, download and save the NETL-CO₂-SCREEN.xlsx Excel file onto any computer directory without changing the file extension name. Then open this file and go to the Read Me tab. This tab contains general instructions and a link to download the free GoldSim Player. Be sure to place the Excel file and GoldSim Player file in the same directory. Follow the series of steps below to run CO₂-SCREEN.

1. **General information section (light blue)**

Enter in the researcher's name, the formation name, the date and the run ID. This information will be carried through to the Saline (Outputs) tab but is not necessary for CO₂-SCREEN to run properly.

2. **Storage efficiency factor ranges (purple)**

There are two options available for entering storage efficiency factors. Option one is to choose a lithology and depositional environment from the drop-down list in cell I17 (yellow). Choosing one of these fifteen options will auto-populate P₁₀ and P₉₀ values for all five efficiency factors (see Appendix A for details regarding these values). Option two allows the user to manually enter their own P₁₀ and P₉₀ efficiency values into cells K21:K25 and L21:L25 respectively. The values entered should range between 0 and 1 and represent the efficiency fraction for each specific storage parameter. For example, if a user enters a P₁₀ of 0.4 and a P₉₀ of 0.7, the efficiency range of that parameter ranges between 40% and 70%. The user also has the option of putting in the same value for P₁₀ and P₉₀ to use a single efficiency factor instead of a range of values. User specified values will receive preference over auto-populated values and thus a user does not need to delete auto-populated values when running the model. Users are encouraged to modify the efficiency factor ranges for Net-to-Total Area, Net-to-Gross Thickness, and Effective-to-Total Porosity in cells K21:K23 and L21:L23 based on geologic properties of the formation being assessed. For the efficiency factor ranges for Volumetric Displacement and Microscopic Displacement in cells K24:K25 and L24:L25, these terms are evaluated at a well scale and are not modified at the formation scale. Users are cautioned to only modify Volumetric Displacement and Microscopic Displacement efficiency factors with detailed reservoir simulation results for the formation being assessed.

3. **Physical parameters section (pale orange)**

Enter geologic data for the saline formation of interest here. If the formation has been divided into grids, enter each grid's data separately (up to 300 grids). If the formation has not been gridded then only use the first grid (row 35). Any grid that is not being used must have 1's in each of the 9 input cells for GoldSim to run correctly. This section is where the user provides data for area (km²), thickness (m), porosity (%), pressure (MPa), and temperature (°C). Area only requires an average value, while the rest of the

parameters require an average value and also have the option of a standard deviation value. If data are limited the standard deviation value can be set to zero.

The area, thickness, and porosity parameters should be gross values if using storage efficiency factors. If a user wants to use net values for any of these parameters, they must set the corresponding efficiency factor's P₁₀ and P₉₀ terms to 1 to avoid double reductions. For example, if a formation has a total area of 100 km² but only 60 km² meet CO₂ storage requirements, the user has three options on how to enter this data into CO₂-SCREEN.

The first option is to enter in 100 km² into the area cell of the Physical Parameters section. The user must then enter 0.6 into the net-to-total area P₁₀ and P₉₀ cells (K21 and L21) of the Storage Efficiency Factor section.

The second option is to enter 60 km² into the area cell of the Physical Parameters section and enter a 1 into the net-to-total area P₁₀ and P₉₀ cells of the Storage Efficiency Factor section.

The third option is a combination of the first two. A user can enter 60 km² into the area cell of the Physical Parameters Section, but instead of entering a 1 into the net-to-total area P₁₀ and P₉₀ cells of the Storage Efficiency Factor section, the user can enter a probability range to reflect uncertainty in net values.

All of these options will correctly only account for areal efficiency once.

4. Grid Specific Efficiency (blue)

Enter grid specific storage efficiency factor ranges here. First, choose the lithology and depositional environment for each grid. Choosing "default" will auto-populate values chosen/set in step two. After choosing the lithology and depositional environment for each grid, the user can further refine storage efficiency by setting ranges for each specific storage efficiency parameter. To use the auto-populated values based on lithology and depositional environment, leave a "0" in the cell.

Once all storage efficiency factors and geologic data are set, save the Excel file and close it. If the Excel file is not closed, GoldSim will not be able to run correctly.

5.2 SIMULATION

Open the GoldSim Player file titled NETL-CO₂-SCREEN.gsp (Figure 10). Simply click the green triangular "play" button (shown by red arrow) to run the simulation or press F5.

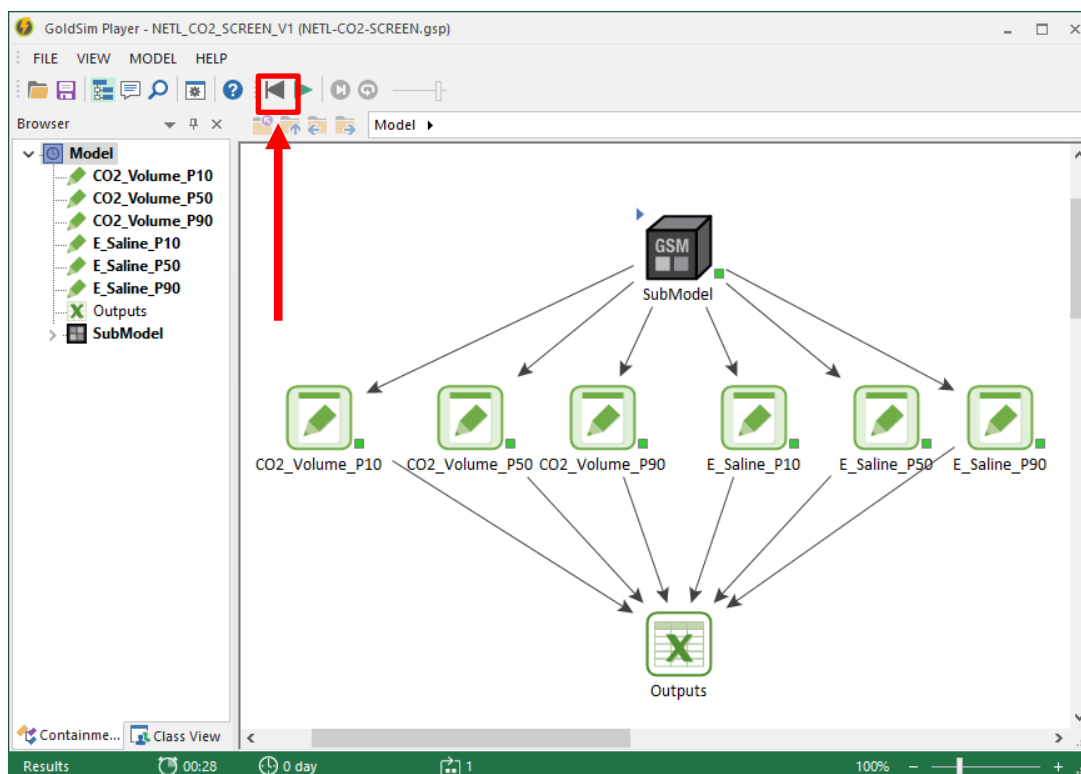


Figure 10: GoldSim Player interface.

Depending upon the amount of data and grids used, the simulation can take between 5 and 60 seconds. Once it is finished a dialog box titled GoldSim will pop up stating “Simulation Complete!” (Figure 11).

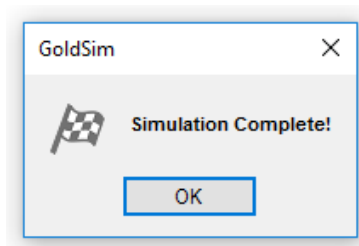


Figure 11: Pop-up dialog box indicating successful completion of GoldSim simulation.

5.3 OUTPUTS

After the GoldSim simulation is completed, open the CO₂-SCREEN Excel file. Navigate to the Saline (Outputs) tab (Figure 6) if necessary. The results will have auto-populated and a summary sheet can be printed without requiring any additional formatting. Results for CO₂ storage resources are presented as P₁₀, P₅₀, and P₉₀ probabilities. When running multiple simulations, the user must rename the file in order to avoid overwriting the data results in Excel. To preserve data outputs the user should copy and paste results to a new spreadsheet or save the current file under a new name so it will not be overwritten.

6. REFERENCES

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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 (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 10th and 90th percent probability based on a Gaussian function (Figure A1).

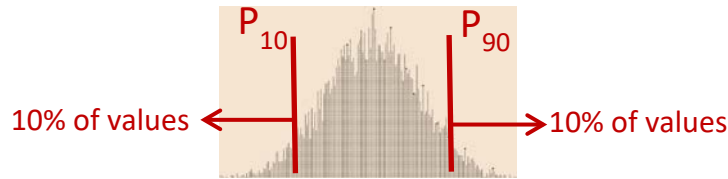


Figure A1: Gaussian function showing P_{10} and P_{90} range.

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

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

X_{10} and X_{90} values are calculated in Excel 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:

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

and

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

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.

A user can enter a specified range for P_{10} and P_{90} values or enter the same value for P_{10} and P_{90} to act as a single efficiency value. When the same value is entered for the P_{10} and P_{90} values, Excel calculates a mean (μ_X) and standard deviation (σ_X) using equations A2 and A3, but adds 0.0000001 to the P_{90} value. This has no significant effect on the calculations, but is necessary for GoldSim to function properly.

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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 CO₂ 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 CO₂-SCREEN (Figure B1) shows how Monte Carlo convergence occurs (Ballio and Guadagnini, 2004). Probabilistic CO₂ storage resource results are normalized to one million realizations and indicate a reasonable convergence by 10,000 realizations.

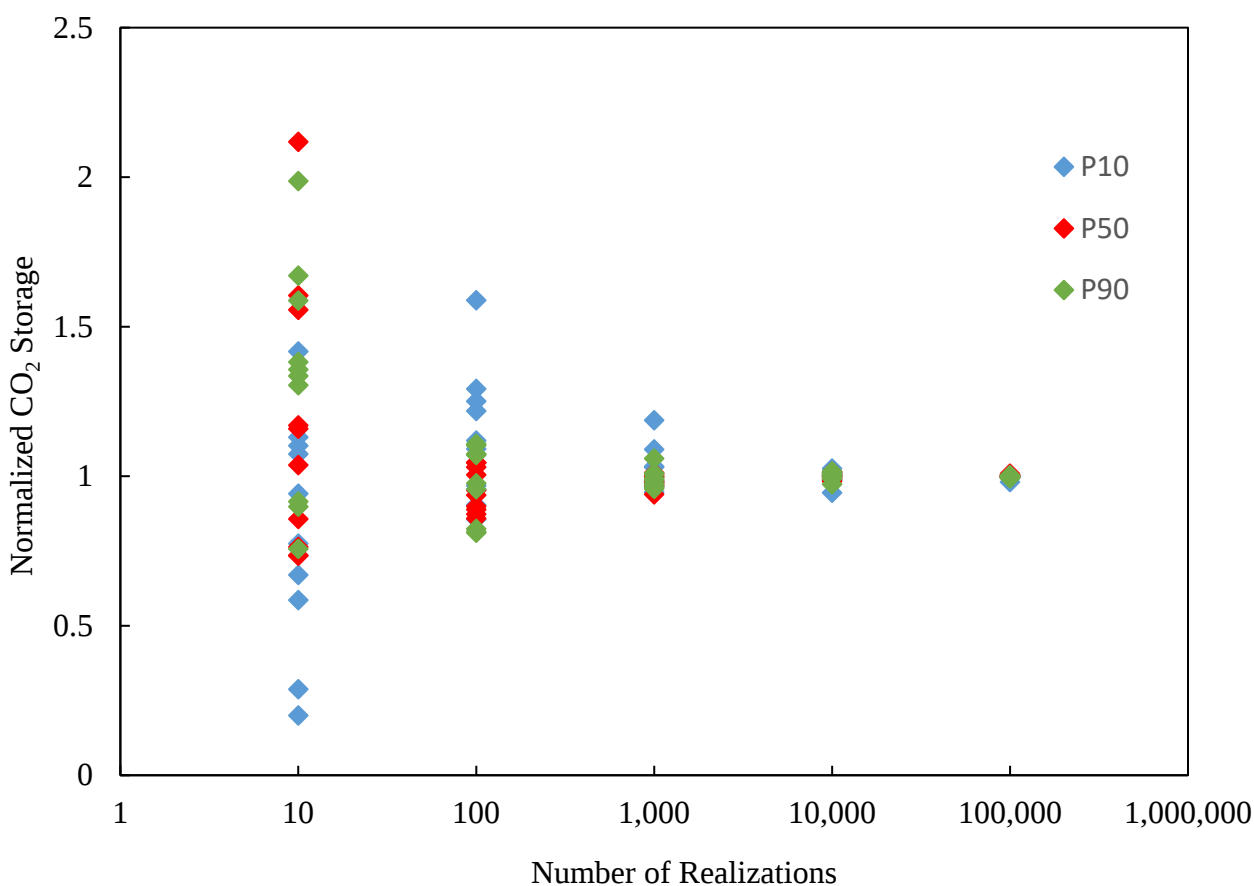


Figure B1: Sensitivity analysis showing probabilistic CO₂ storage resource values normalized to one million realizations plotted against the number of realizations for that simulation.

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