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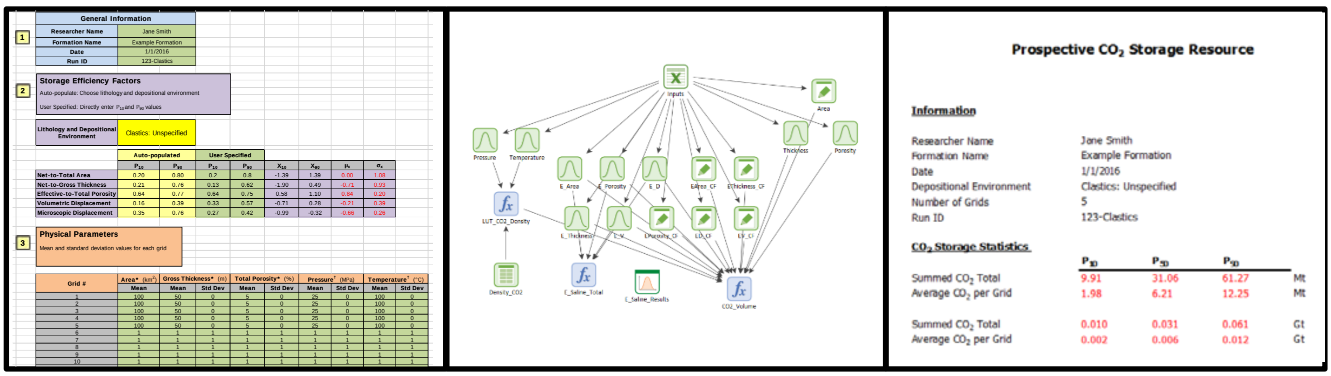

NETL CO_2 Storage prospeCtive Resource Estimation Excel aNalysis (CO_2-SCREEN) User's Manual

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Cover Illustration: Inputs, GoldSim Model Structure, and Outputs of CO_2-SCREEN.

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NETL CO_2 Storage prospeCtive Resource Estimation Excel aNalysis (CO_2-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		℃	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

Acknowledgments

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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 saline formations for prospective CO_2 storage resources. CO_2-SCREEN applies U.S. Department of Energy (DOE) methods and equations for estimating prospective CO_2 storage resources for saline formations. CO_2-SCREEN was developed to be substantive and user-friendly. It also provides a consistent method for calculating prospective CO_2 storage resources that allows for consistent comparison of results between different research efforts, such as the Regional Carbon Sequestration Partnerships (RCSP). CO_2-SCREEN consists of an Excel spreadsheet containing geologic inputs and outputs, linked to a GoldSim Player model that calculates prospective CO_2 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 (CO_2) 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 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 CO_2 Storage prospeCtive Resource Estimation Excel aNalysis (CO_2-SCREEN) tool: a tool which was developed by the DOE-NETL to screen saline formations for prospective CO_2 storage resources.

CO_2-SCREEN is available on the Energy Data eXchange (EDX). This manual describes CO_2-SCREEN, explains the organization and structure of the software files, and provides instructions for use.

2. TOOL DESCRIPTION

The NETL CO_2-SCREEN tool was developed to provide a substantive, user-friendly, and consistent mechanism to calculate CO_2 storage resources. CO_2-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 CO_2 storage resources using Monte Carlo methods, and outputs these values back into the Excel file in a separate tab.

CO_2-SCREEN includes the input of five storage efficiency factors (Table 1) which represent the fraction of formation volume accessible for CO_2 storage. These efficiency factors are entered as P_{10} and P_{90} 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 CO_2-SCREEN, efficiency factor ranges can be manually entered by the user based upon geologic properties. In the absence of detailed geologic information, CO_2-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. CO_2-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 CO_2-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 CO_2-SCREEN to function properly. Inputs and outputs are designated by two separate tabs in Excel.

Table 3: CO_2-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.

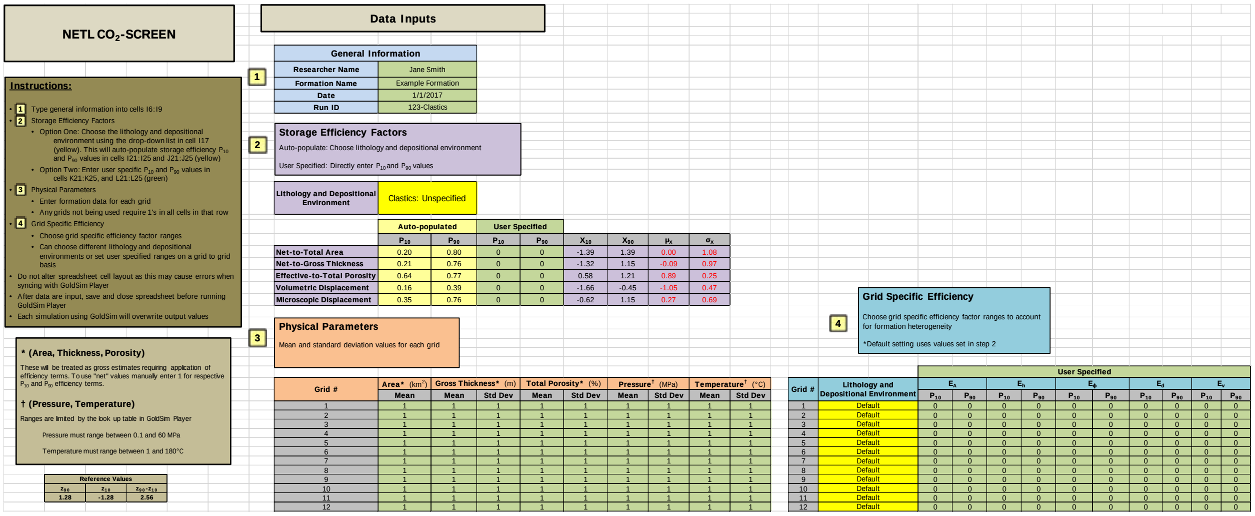

Figure 1: CO_2-SCREEN Saline (Inputs) tab.

The General Information section (Figure 2) is not required to run CO_2-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	
1	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 CO_2-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 CO_2-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 CO_2-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* (km^2)	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 CO_2-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

4

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_A P_{10}	E_A P_{90}	E_h P_{10}	E_h P_{90}	E_ϕ P_{10}	E_ϕ P_{90}	E_d P_{10}	E_d P_{90}	E_v P_{10}	E_v 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 CO_2-SCREEN.

3.2 OUTPUTS

The Saline Outputs tab (Figure 6) of the CO_2-SCREEN Excel file displays the results generated from the GoldSim Player. Results are displayed as P_{10}, P_{50}, and P_{90} values for mass CO_2 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

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

CO_2 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

Grid	P_{10} (Mt)	P_{50} (Mt)	P_{90} (Mt)	Lithology and Depositional Environment	Saline Efficiency (%) P_{10}	P_{50}	P_{90}
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
5	5.034	15.907	30.015	User Specified	2.50	7.90	14.92
6	0.000	0.000	0.000	Clastics: Unspecified	0.65	2.44	6.77
7	0.000	0.000	0.000	Clastics: Unspecified	0.42	1.50	3.94
8	0.000	0.000	0.000	Clastics: Unspecified	0.42	1.50	3.94
9	0.000	0.000	0.000	Clastics: Unspecified	0.48	1.80	4.88
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
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
14	0.000	0.000	0.000	Clastics: Unspecified	0.42	1.50	3.94
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
17	0.000	0.000	0.000	Clastics: Unspecified	0.42	1.50	3.94
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 CO_2-SCREEN displaying CO_2 storage results.

Prospective CO_2 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

CO_2 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 CO_2-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 CO_2-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

CO_2-SCREEN's GoldSim structure is divided into a main model and a submodel. The main model (Figure 8) contains the P_{10}, P_{50}, and P_{90} probability estimates generated from the submodel and an output function linked to Excel.

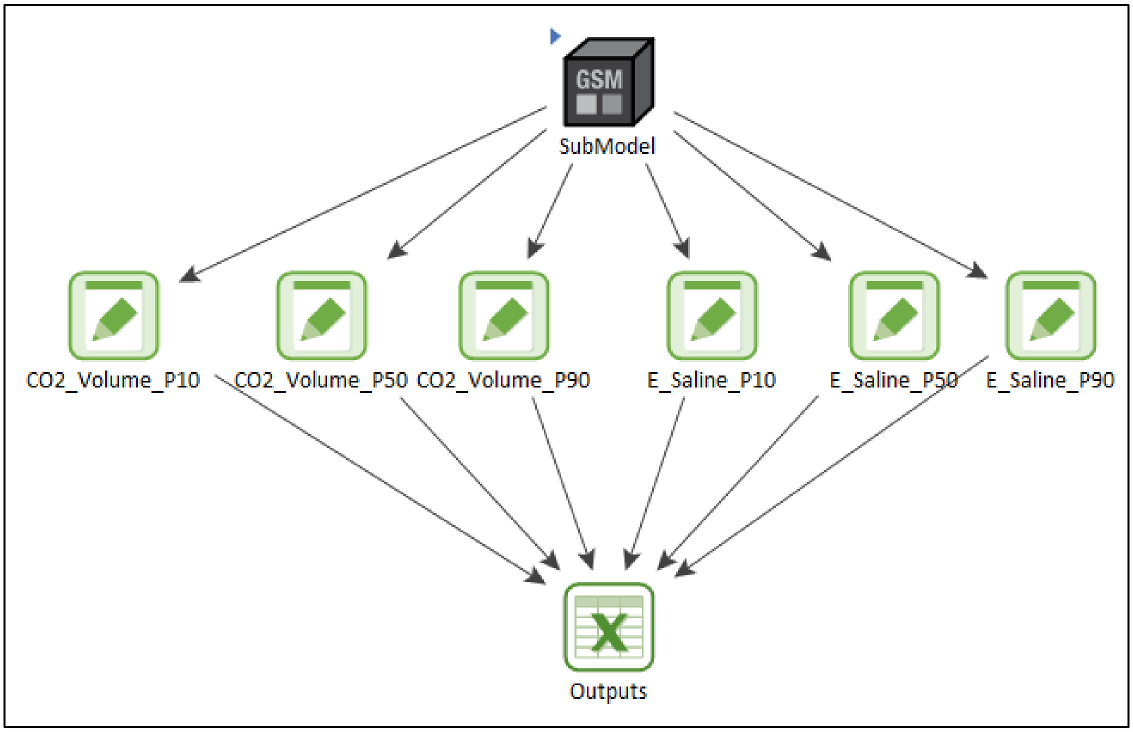

Figure 8: GoldSim main model structure of CO_2-SCREEN.

The submodel (Figure 9) is composed of an Excel input function, data distributions for the input parameters, a lookup table (LUT) to calculate CO_2 density, embedded equations to calculate prospective CO_2 storage resource, and generated results that are relayed to the main model to be exported to the corresponding Excel file.

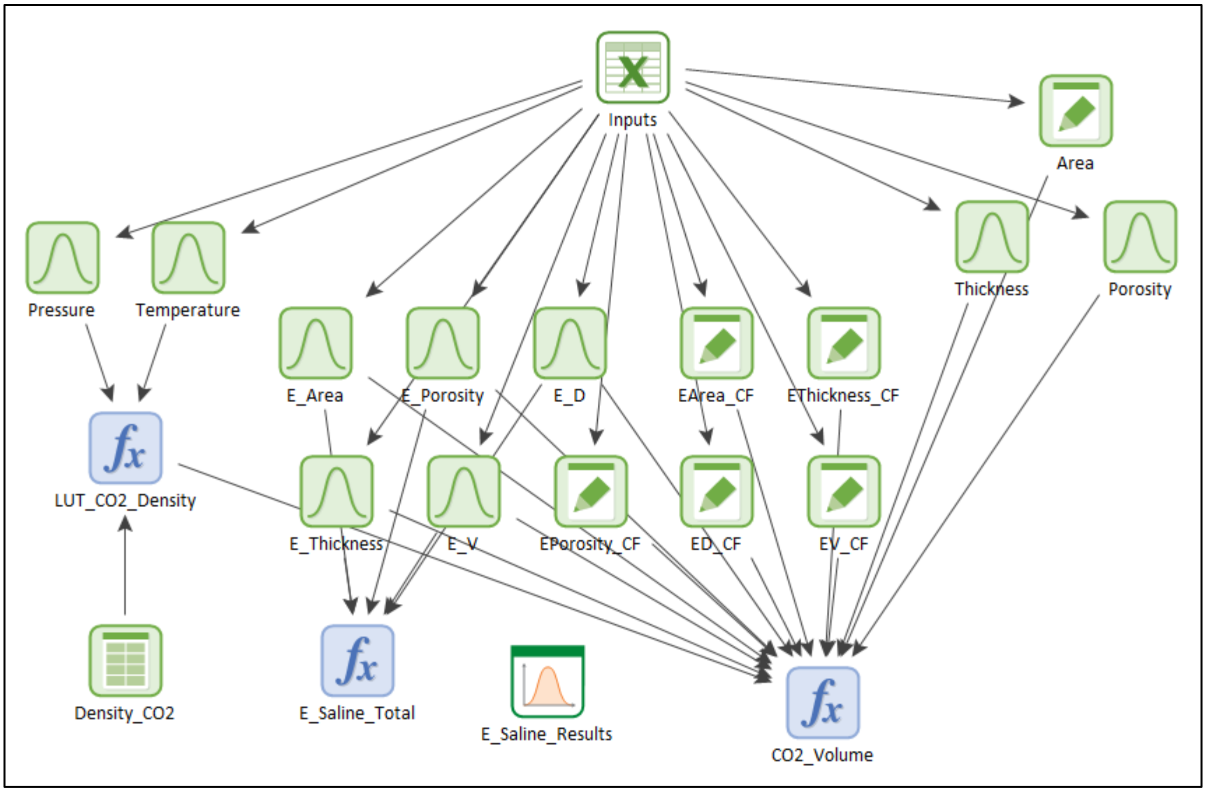

Figure 9: GoldSim submodel structure of CO_2-SCREEN.

The Excel input and output functions are the link between the CO_2-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 CO_2 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:

$$G = A\, h\, \phi\, \rho \frac{1}{\left(1+e^{(-X_A)}\right)} * \frac{1}{\left(1+e^{(-X_h)}\right)} * \frac{1}{\left(1+e^{(-X_\phi)}\right)} * \frac{1}{\left(1+e^{(-X_V)}\right)} * \frac{1}{\left(1+e^{(-X_D)}\right)}\ , \qquad (1)$$

where G is the mass estimate of the saline formation for prospective CO_2 storage resource, A is the area (km^2) (map view) that defines the formation being assessed for CO_2 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/m^3) of CO_2 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 CO_2 mass storage resource are calculated and automatically exported to the Saline (Outputs) tab in the Excel file.

5. INSTRUCTIONS FOR USE

Using CO_2-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 CO_2-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 CO_2-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 CO_2-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-drown list in cell I17 (yellow). Choosing one of these fifteen options will auto-populate P_{10} and P_{90} values for all five efficiency factors (see Appendix A for details regarding these values). Option two allows the user to manually enter their own P_{10} and P_{90} 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 P_{10} of 0.4 and a P_{90} 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 P_{10} and P_{90} 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 (km^2), 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 P_{10} and P_{90} terms to 1 to avoid double reductions. For example, if a formation has a total area of 100 km^2 but only 60 km^2 meet CO_2 storage requirements, the user has three options on how to enter this data into CO_2-SCREEN.

The first option is to enter in 100 km^2 into the area cell of the Physical Parameters section. The user must then enter 0.6 into the net-to-total area P_{10} and P_{90} cells (K21 and L21) of the Storage Efficiency Factor section.

The second option is to enter 60 km^2 into the area cell of the Physical Parameters section and enter a 1 into the net-to-total area P_{10} and P_{90} cells of the Storage Efficiency Factor section.

The third option is a combination of the first two. A user can enter 60 km^2 into the area cell of the Physical Parameters Section, but instead of entering a 1 into the net-to-total area P_{10} and P_{90} 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.

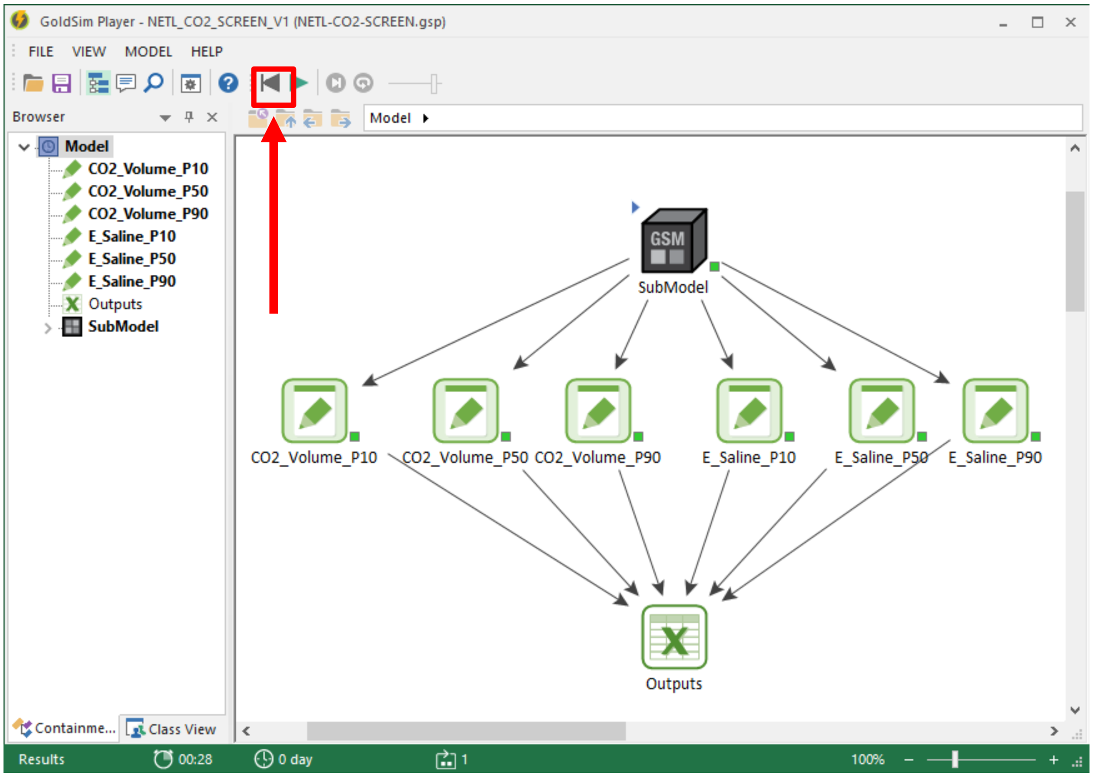

Figure 10: GoldSim Player interface.

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).

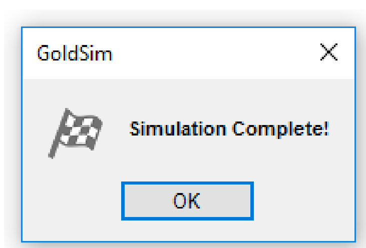

Figure 11: Pop-up dialog box indicating successful completion of GoldSim simulation.

5.3 OUTPUTS

After the GoldSim simulation is completed, open the CO_2-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 CO_2 storage resources are presented as P_{10}, P_{50}, and P_{90} 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.

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

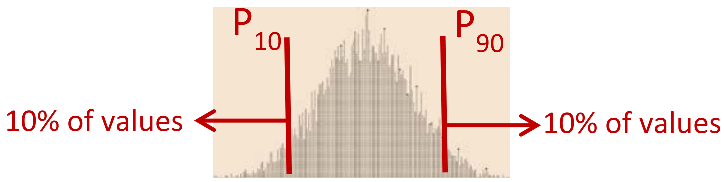

Figure A1: Gaussian function showing P_{10} and P_{90} range.

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

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

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:

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

and

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

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 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.

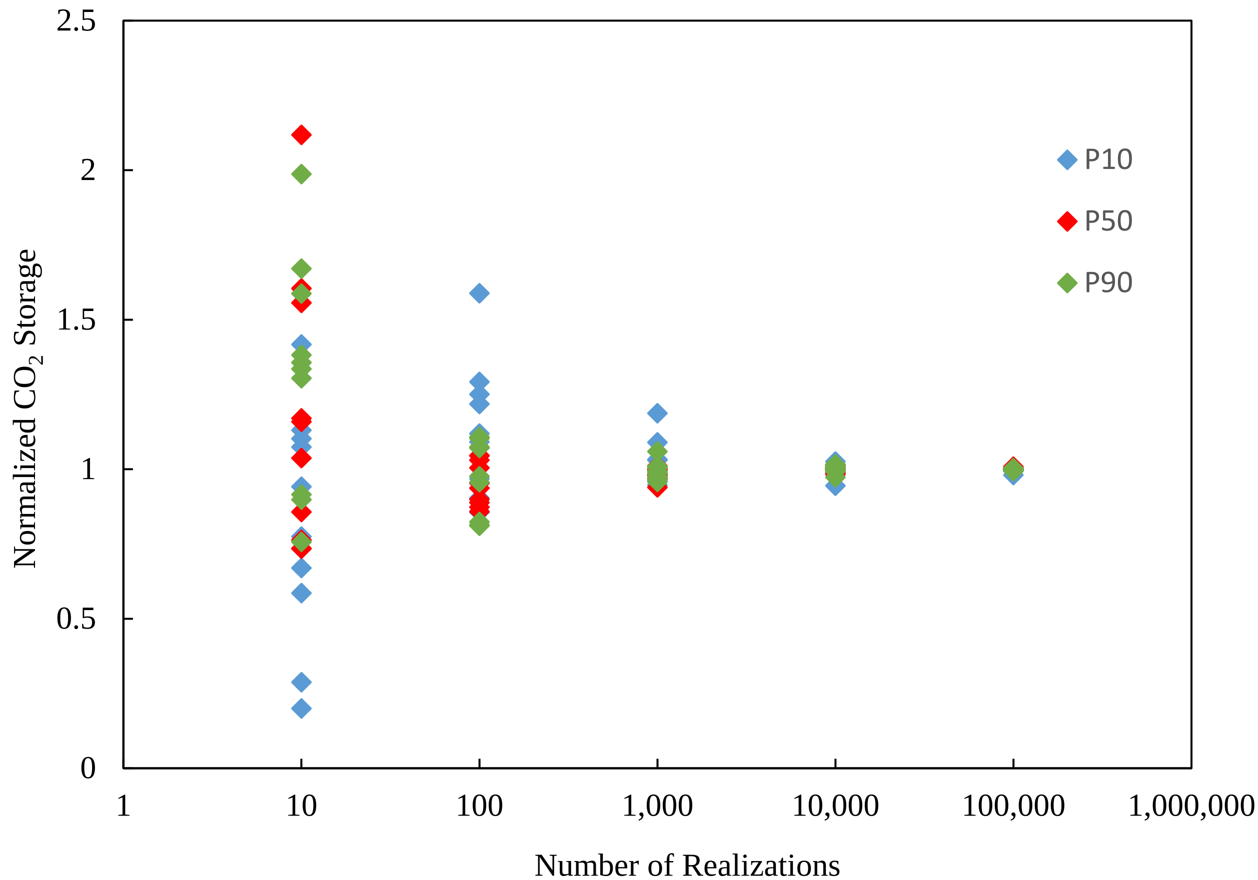

Figure B1: Sensitivity analysis showing probabilistic CO_2 storage resource values normalized to one million realizations plotted against the number of realizations for that simulation.

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