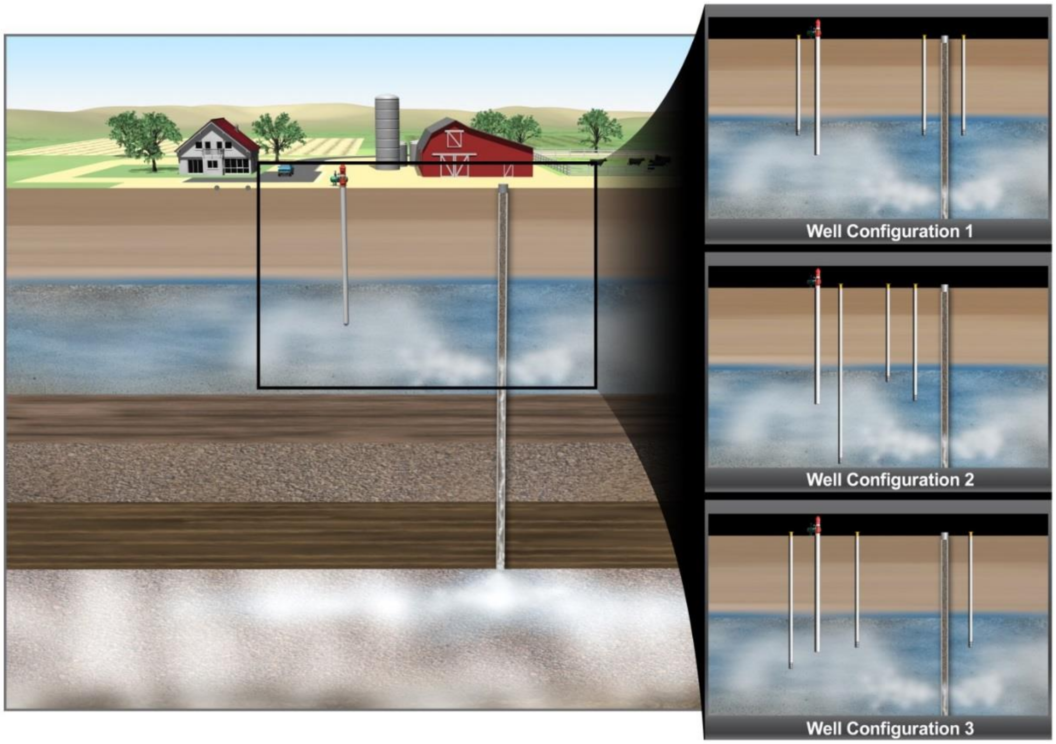

Designs for Risk Evaluation and Management (DREAM) Tool User's Manual, Version: 2020.01-2.0

January 31, 2020

Office of Fossil Energy

Disclaimer

Cover Illustration: A hypothetical visualization of a DREAM application to a leak from subsurface storage into an overlying aquifer through an abandoned wellbore. The inserts visualize three of many monitoring configurations that DREAM would generate and assess during the iterative procedure.

Suggested Citation: Yonkofski, C. M.; Whiting, J. M.; Huang, B. Z., Hanna, A. C. *Designs for Risk Evaluation and Management (DREAM) Tool User's Manual, Version: 2020.01-2.0;* NRAP-TRS-III-001-2020; NRAP Technical Report Series; U.S. Department of Energy, National Energy Technology Laboratory: Morgantown, WV, 2020; p 45.

An electronic version of this report can be found at:
https://edx.netl.doe.gov/organization/nrap-tools/folder/080f6c7e-7a40-43c2-9c44-551bcc16ed7d

Designs for Risk Evaluation and Management (DREAM) Tool User's Manual, Version: 2020.01-2.0

Catherine M. Yonkofski, Jonathan M. Whiting, Brian Z. Huang, Alexander C. Hanna

Pacific Northwest National Laboratory, 902 Battelle Boulevard, Richland, WA 99354

NRAP-TRS-III-001-2020

Level III Technical Report Series

January 31, 2020

This page intentionally left blank.

Table of Contents

List of Figures

List of Tables

Acronyms, Abbreviations, and Symbols

Term	Description
Acronyms/Abbreviations	
3D	Three-dimensional
ASCII	American Standard Code for Information Interchange
CO_2	Carbon dioxide
DOE	U.S. Department of Energy
DREAM	Designs for Risk Evaluation and Management
EDX	Energy Data Exchange
GUI	Graphical user interface
HDF5	Hierarchical data format
IAM	Integrated Assessment Model
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LLNL	Lawrence Livermore National Laboratory
NETL	National Energy Technology Laboratory
NRAP	National Risk Assessment Partnership
NUFT	Nonisothermal, Unsaturated Flow and Transport model
PC	Personal computer
PNNL	Pacific Northwest National Laboratory
RCSP	Regional Carbon Sequestration Partnership
STOMP	Subsurface Transport Over Multiple Phases model
TTD	Time to detection
USDW	Underground source of drinking water
VAD	Volume of aquifer degraded
Units/Symbols	
cm	centimeter
L	Liter
mg	Milligram
mg/L	Milligrams per liter
min	Minute
mol	Mole
Pa	Pascal
yr	Year

Acknowledgments

This work was completed as part of the National Risk Assessment Partnership (NRAP) project. Support for this project came from the U.S. Department of Energy's (DOE) Office of Fossil Energy's Crosscutting Research program. The authors wish to acknowledge Traci Rodosta (Carbon Storage Technology Manager), Kanwal Mahajan (Carbon Storage Division Director), M. Kylee Rice (Carbon Storage Division Project Manager), Mark Ackiewicz (Division of CCS Research Program Manager), Robert Romanosky (NETL Crosscutting Research, Office of Strategic Planning), and Regis Conrad (DOE Office of Fossil Energy) for programmatic guidance, direction, and support. The authors wish to thank Art Sadovsky, Jason Gastelum, Ellen Porter, Luke Rodriguez for their early development work on the DREAM tool.

ABSTRACT

This manual provides a brief guide for the use of the Designs for Risk Evaluation and Management (DREAM) tool Version 2.0, developed as part of the effort to quantify the risk of geologic storage of carbon dioxide (CO_2) under the U.S. Department of Energy's (DOE) National Risk Assessment Partnership (NRAP). DREAM is an optimization tool created to identify optimal monitoring schemes that minimize the time to first detection of CO_2 leakage from a subsurface storage formation. DREAM optimizes across user-provided output from subsurface leakage simulations or using outputs from reduced order models. While DREAM was developed for CO_2 leakage scenarios, it is applicable to any subsurface leakage simulation of the same output format.

The DREAM tool is comprised of four main components: (1) a Java wizard used to configure and execute the simulations, (2) a visualization tool to view the domain space and optimization results, and (3) plotting scripts used to analyze the results, and (4) a Java application to aid users in converting common American Standard Code for Information Interchange (ASCII) output data to the standard DREAM hierarchical data format (HDF5).

DREAM employs a simulated annealing approach that searches the solution space by iteratively mutating potential monitoring schemes built of various configurations of monitoring locations and leak detection parameters. This approach has proven to be orders of magnitude faster than an exhaustive search of the entire solution space. This user's manual illustrates the program graphical user interface (GUI), describes the tool inputs, and includes an example application.

This page intentionally left blank.

1. INTRODUCTION

The Designs for Risk Evaluation and Management (DREAM) tool was developed at Pacific Northwest National Laboratory (PNNL) as a tool to assist in determining optimal placement of monitoring devices in order to detect carbon dioxide (CO_2) leakage from storage formations. The National Risk Assessment Partnership (NRAP) identified the need for a user-friendly tool with the ability to design site-specific risk-based monitoring strategies. NRAP is a U.S. Department of Energy (DOE) project tasked with conducting risk and uncertainty analysis in the areas of reservoir performance, natural leakage pathways, wellbore integrity, groundwater protection, monitoring, and systems level modeling. Monitoring designs produced by DREAM may be used by stakeholders and regulators to assist in compliance with regulatory requirements developed to ensure the safety of U.S. underground sources of drinking water (USDW) and ultimately lead to safe, permanent geologic CO_2 storage. Further, site-specific designs generated by DREAM allow for potential generalizations to other sites, as well as comparisons between risk-based monitoring designs and monitoring designs for other purposes, if such designs should already exist (e.g., from a Regional Carbon Sequestration Partnership [RCSP] site).

DREAM optimizes across user-provided output from subsurface leakage simulations, with the objective of configuring monitoring schemes that minimize time to first detection of user-specified leakage indicators. DREAM employs a simulated annealing approach that searches the solution space by iteratively mutating potential monitoring schemes built of various configurations of monitoring locations and leak detection parameters. Leakage indicators may include pressure, temperature, gas saturation, dissolved component concentrations, pH, or any other quantity that can be modeled in a physics-based simulation of porous media fluid transport. These variables are constrained by location and budget, where placement must be in a user-defined suitable location and the budget includes both the number of monitoring devices and the number of wells. The simulated annealing approach has proven to be orders of magnitude faster than an exhaustive search of the entire solution space (Yonkofski et al., 2016). While DREAM was designed with applications to CO_2 leakage in mind, this flexibility allows DREAM to determine optimal monitoring locations for any contaminant transport scenario.

Successful use of this software requires both a proper implementation of the mathematics by the tool developers and a proper application of the tool by the user. It is strongly recommended that the user develops an understanding of the leakage system in terms of the relevant hydrogeologic behavior and chemical properties as well as the practical aspects of site-specific monitoring prior to use the DREAM tool. Successful application of the DREAM tool facilitates decision support through an enhanced understanding of the leakage system and associated solution monitoring configurations. Unsuccessful application may lead to a false understanding of the leakage system and suboptimal monitoring configurations.

Development of DREAM began in 2012 as part of the NRAP project, with the first code version being released in 2016. The current version of the code began development during the second phase of the NRAP program. Subsequent versions, when completed, are planned to add flexibility in the objective function, allow for a broader range of input formats, and improve existing capabilities (e.g. faster computational speeds, additional geophysical monitoring technologies).

This manual illustrates the program GUI and describes the tool inputs. For a synopsis of the theoretical basis of DREAM, see Yonkofski et al. (2016). For an example application using point source monitoring technologies from leakage simulations, see Yonkofski et al. (2017). For an example application using Open-IAM, see Bacon et al. (2019).

2. SOFTWARE INSTALLATION AND REQUIREMENTS

DREAM requires that you have the most recent release of the Java Platform, currently version 8. If you already have Java installed, search for "About Java" to find your version. It is also recommended that the user installs an HDF5 reader, such as HDFView, for reading converted hierarchical data format (HDF5). Finally, it is recommended that the user has Python 3 with "numpy", "h5py", "matplotlib", and "pandas" packages installed for some post-processing scripts to work. If you already have Python installed, you can check your version by typing "python --version" into a command prompt. Download locations for these files are shown in Table 1.

Table 1: Supplementary Software

Software	Website
Java SE 8	https://www.oracle.com/technetwork/java/javase/downloads/jre8-downloads-2133155.html Required
HDFView 3.1	https://portal.hdfgroup.org/display/support/Download+HDFView Optional for viewing and editing HDF5 files
Python 3	https://www.python.org/downloads/ Optional for post-processing scripts

DREAM version 2.0 has been released within the NRAP Tools Beta Test Release Collaborative Workspace on the NETL Energy Data Exchange (EDX). Sign into EDX with an account that belongs to the workspace and download the DREAM tool: https://edx.netl.doe.gov/organization/nrap-tools/folder/080f6c7e-7a40-43c2-9c44-551bcc16ed7d. There are separate distributions for the Windows and Mac versions. Two sample input datasets are provided with the DREAM distribution at the link above:

- DREAM_2.0.jar (14.8 MB) – A runnable JAR file, which packages all the necessary libraries, images, and documentation into an executable program.
- HDF5_Example.zip (160 MB) – HDF5 files for 5 scenarios from modeling associated with Sminchak et al. (2014).
- IAM_Example.zip (2.7 MB) – Results from 480 scenarios generated with Open-IAM associated with Bacon et al. (2019).

Instructions:

1. Download the files and unzip the example folders.
2. Double click the JAR file to start DREAM and select an unzipped example folder during the Input Directory page.

3. USER INTERACE DESCRIPTION WITH AN EXAMPLE APPLICATION

The DREAM tool is comprised of three main components: 1) a Java wizard used to configure and execute the optimization algorithm; 2) a file converter to translate leakage simulation output from American Standard Code for Information Interchange (ASCII) data to the standard DREAM HDF5; and 3) a results directory to plot best configurations and analyze the performance of the iterative procedure.

The example will guide the user through the DREAM Java Wizard GUI while demonstrating an application to 19 randomly selected leakage scenarios generated for an NRAP Second-Generation Reduced-Order Model study (Carroll et al., 2014b). For context, a brief summary of the model set up from Carroll et al. (2014b) is provided below.

The NUFT numerical model (Figure 1) was comprised of a 3D heterogeneous domain that represented an unconsolidated aquifer consisting of layers of permeable sand and impermeable shale layers based on the lithology of the High Plains Aquifer. The aquifer was underlain by a hypothetical CO_2 storage reservoir and both aquifer and reservoir were penetrated by leaking wells. The model domain encompassed 10 km × 5 km × 240 m with 1 to 5 leakage sources per scenario placed at a depth of 198 m based on 48 known well locations. The wells were a mix of domestic, feedlot, irrigation, public water supply, and oil field water supply wells. Leakage rates were varied based on uncertainties in hydrogeologic properties.

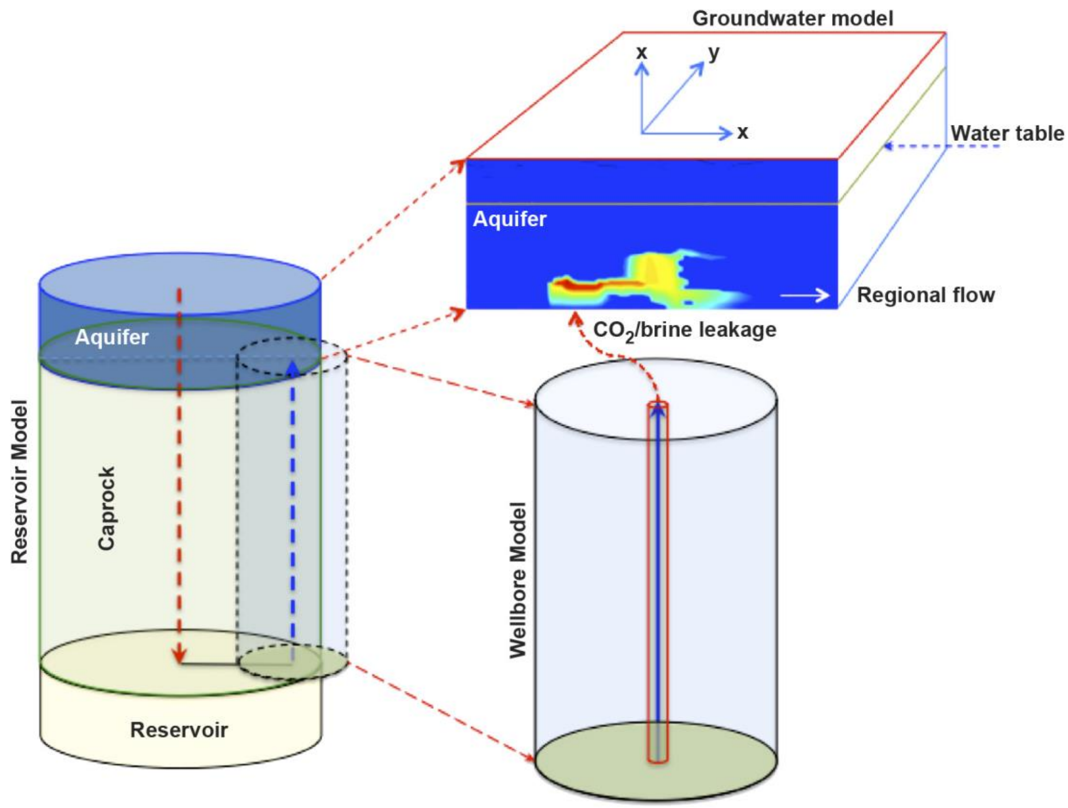

Figure 1: Beta Example Schematic. Figure from Carroll et al. (2014b) shows the links between reservoir, well leakage, and aquifer models using the alluvium case study. Links between reservoir, well leakage, and the carbonate case study are identical.

The included beta test files contain output data at specified times across all nodes representing hypothetical leakage scenarios from the CO_2 storage formation. DREAM will be used to optimize monitoring configurations that minimize the estimated time to first detection (TTD) of CO_2 leakage.

3.1 THE DREAM WIZARD

For best results, the DREAM GUI should be completed in the sequence with which windows progress (Figure 2).

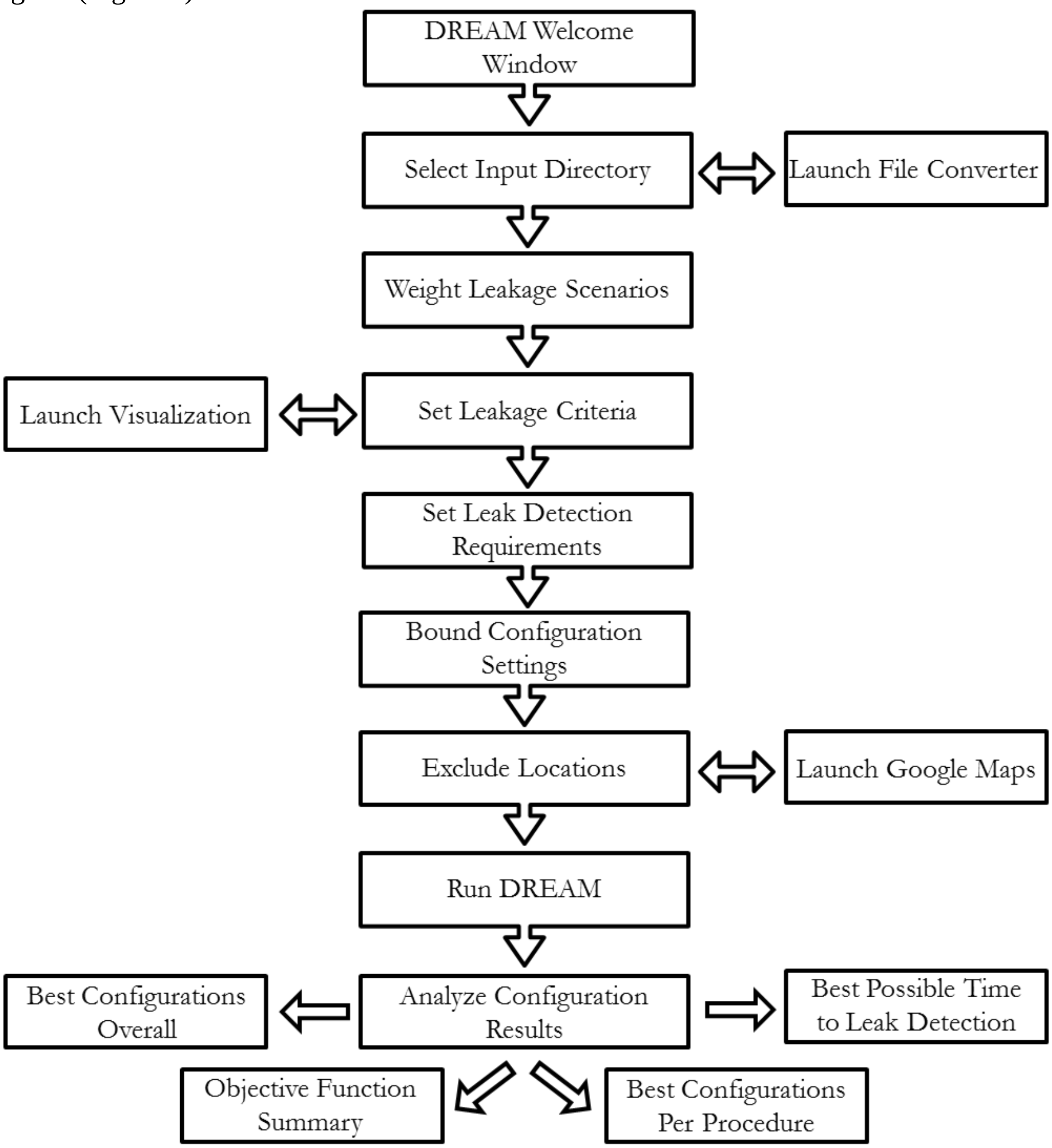

Figure 2: DREAM GUI Flow Chart.

3.1.1 DREAM Welcome Page

The DREAM *Welcome* page (Figure 3) provides links to the DREAM Tool User's Manual and literature detailing the technical development and theory behind the DREAM simulated annealing algorithm (Yonkofski et al., 2016). It is recommended the user reviews the cited paper to thoroughly understand the objective function, decision variables and constraints, as well as the process DREAM performs to approach the global minima.

A conceptual figure on the right side of the Welcome window shows a theoretical DREAM application, with a leak from subsurface storage entering an overlying aquifer through an abandoned wellbore. While the user must provide the leakage scenario, the inserts visualize three of many monitoring configurations that DREAM generates and assesses during the iterative procedure.

To continue to the example application, press *Next*.

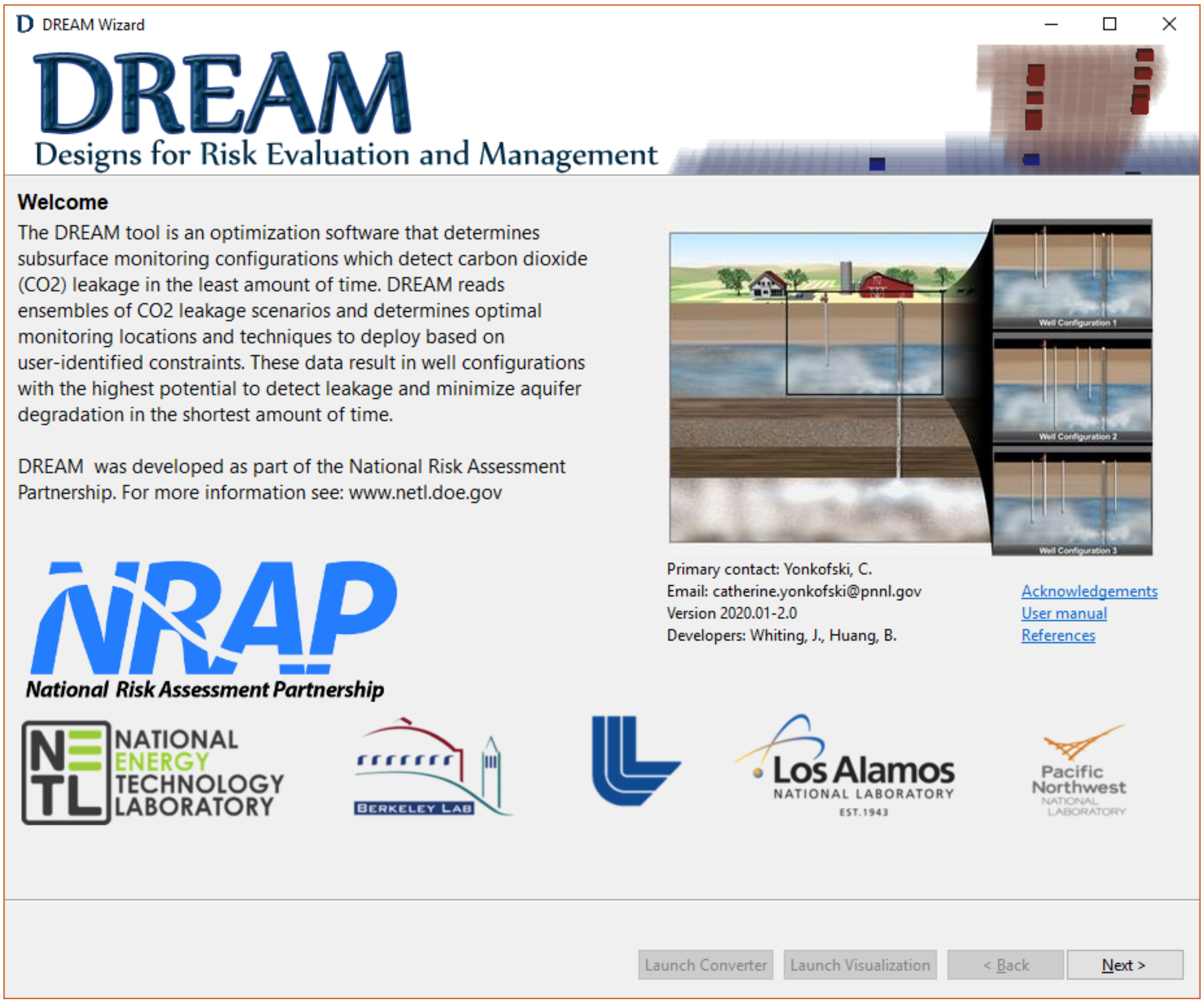

Figure 3: DREAM Welcome Page.

3.1.2 Input Directory Page

The *Input Directory* page (Figure 4) prompts the user to select the directory containing HDF5 or IAM files for all leakage scenarios to be analyzed. The HDF5 or IAM files must be directly available within the directory provided; they may not be in subdirectories. All scenarios within the directory should reference a single geographic location.

If the user has not converted ASCII simulation output data into DREAM readable HDF5 input files, the *Launch Converter* button will open a pop-up file converter tool. Read more about the DREAM HDF5 Converter tool in Section 3.2.

Note: The information icon in this and all subsequent windows provides brief instructions to those using DREAM without the manual.

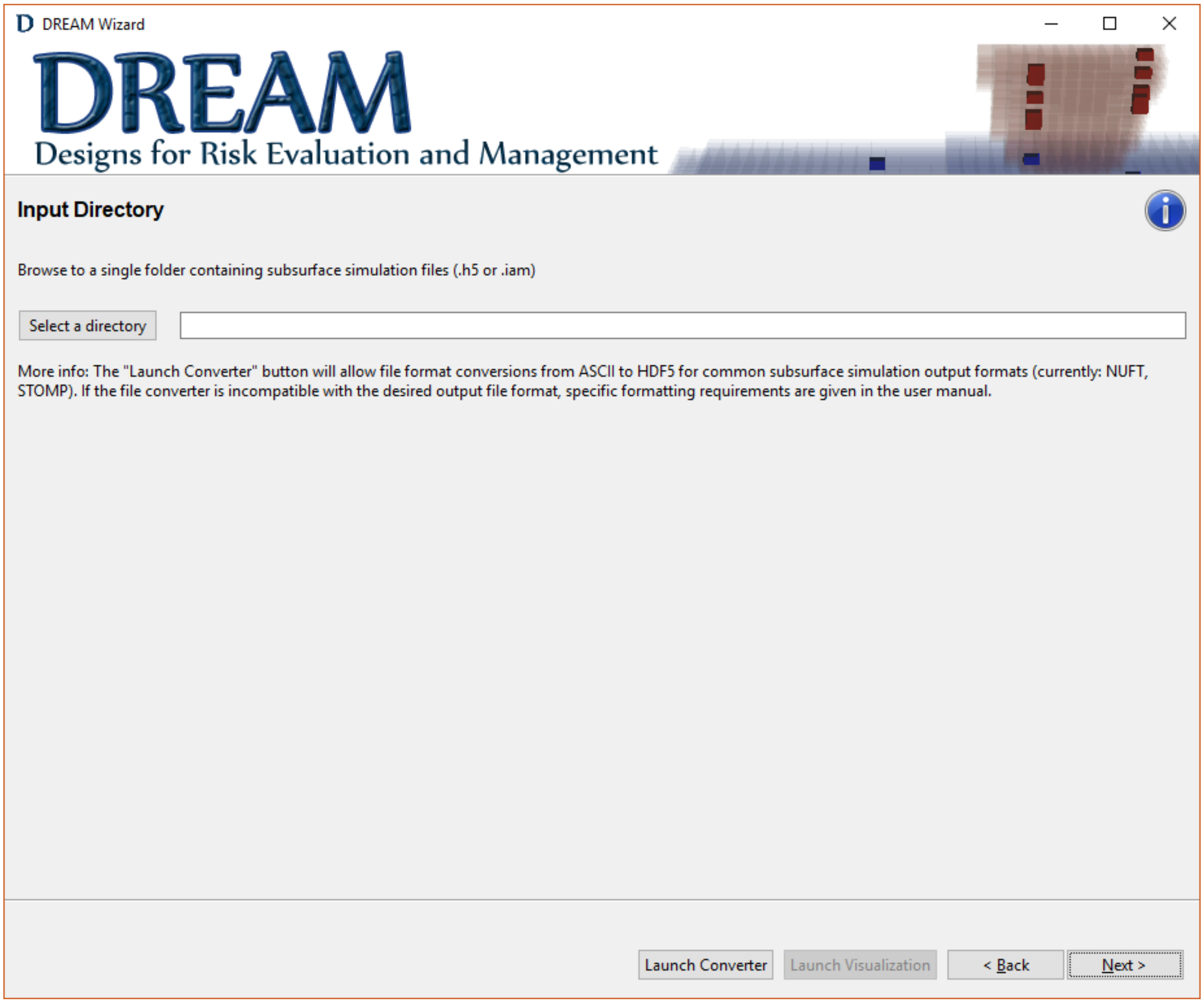

Figure 4: Input Directory Page.

For the purpose of this example, HDF5 files will be used as input files. From the *DREAM Input Directory* Window, navigate to the HDF5 files directory. Select *Next.*

A pop-up window (**Error! Reference source not found.**) may prompt the user to specify any information missing from the HDF5 files, including porosity, units, and elevation/depth (z-axis orientation). This information will be stored in HDF5 files as variables and attributes when available from the leakage simulation outputs, otherwise they will require this manual input. IAM files will usually require these additional inputs. The porosity property is not typically included in simulation output files but is useful in calculating the volume of aquifer degraded. A user may define homogeneous porosity for the entire model domain. Non-homogeneous porosity is possible only when porosity is included as a parameter during conversion to HDF5 files.

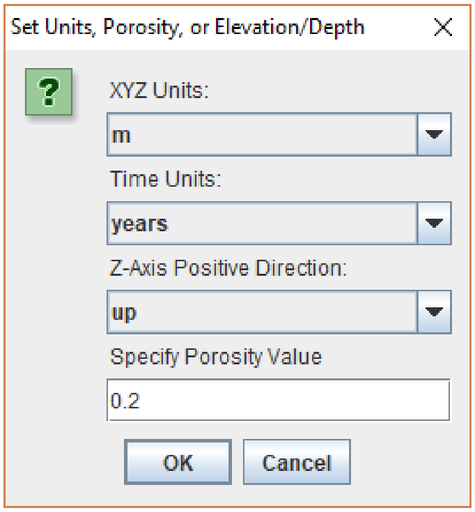

Figure 5: Pop-up to specify missing information

3.1.3 Scenario Weighting

The *Scenario Weighting* page (Figure 6) lists scenarios by the naming convention used in the leakage simulation input files. This allows the user to weight the leakage scenarios unequally if they have prior knowledge of leakage probabilities. By default, all scenarios are considered equally likely.

DREAM works to minimize the average time to leakage detection across all scenarios. Weighting scenarios non-uniformly has the effect of altering the average time to detection; therefore, monitoring configurations that solve for scenarios with higher weights will be given priority while DREAM iterates over monitoring configurations. Ultimately, results show both the unweighted and weighted times to detection to provide the user with an understanding of the impact scenario weighting has on each problem.

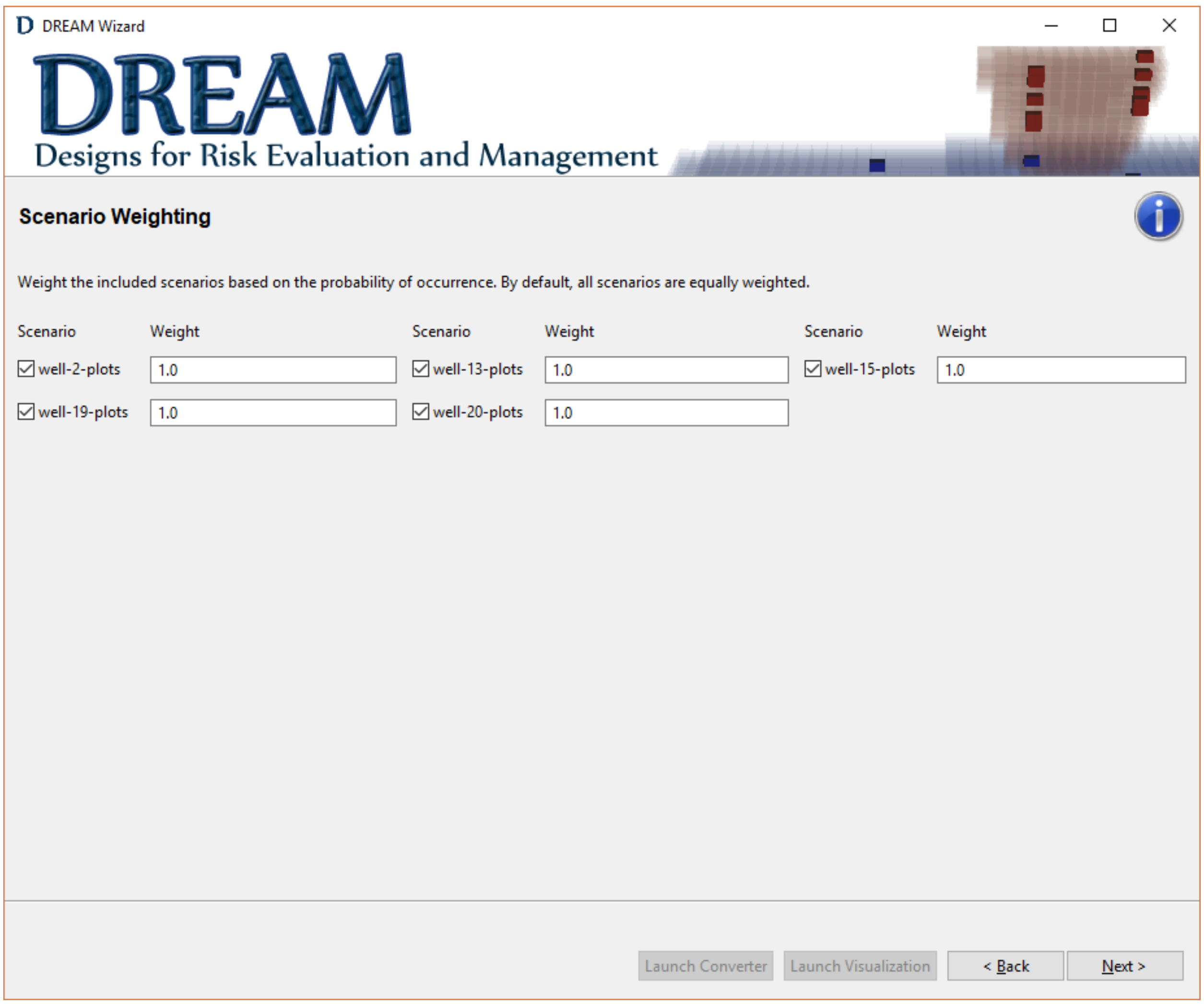

Figure 6: Scenario Weighting Page.

For the example problem, choose to leave all scenarios equally weighted, assuming they are all equally likely. Select *Next*.

3.1.4 Leakage Criteria

The *Leakage Criteria* page (Figure 7) allows the user to select monitoring technologies that are being optimized, providing a table of monitoring parameters from loaded scenarios.

The *plus box* allows technologies to be competed, creating a second monitoring parameter option that can have different cost, detection information, or zone limitations. The *check box* enables or disables a monitoring technology from the optimization. The *Alias for Monitoring Technology* input allows the user to assign a recognizable name to the technology. The *Cost* input allows the user to assign a value to each monitoring technology unit, which limits the optimization algorithm based on a later-assigned budget. The *Detection Criteria* and *Detection Value* define the technical capabilities of the monitoring technology and the magnitude of detection that will reliably identify a leak. "Absolute change" and "Relative change" define leaks as change across time and may be limited to positive or negative change by providing a +/- sign before the value. "Above threshold" and "Below threshold" define leaks as surpassing the given threshold. Hovering over the value input will display the global minimum, average, and maximum for the parameter across all timesteps and scenarios, helping the user make their selection. Lastly, the *Zone Bottom* and *Zone Top* inputs define depth limitations to where the monitoring technology can be placed. By default, these values are set to the global minimum and maximum. When loading IAM files, most user inputs are not available, as inputs are fixed during the process to generate IAM files.

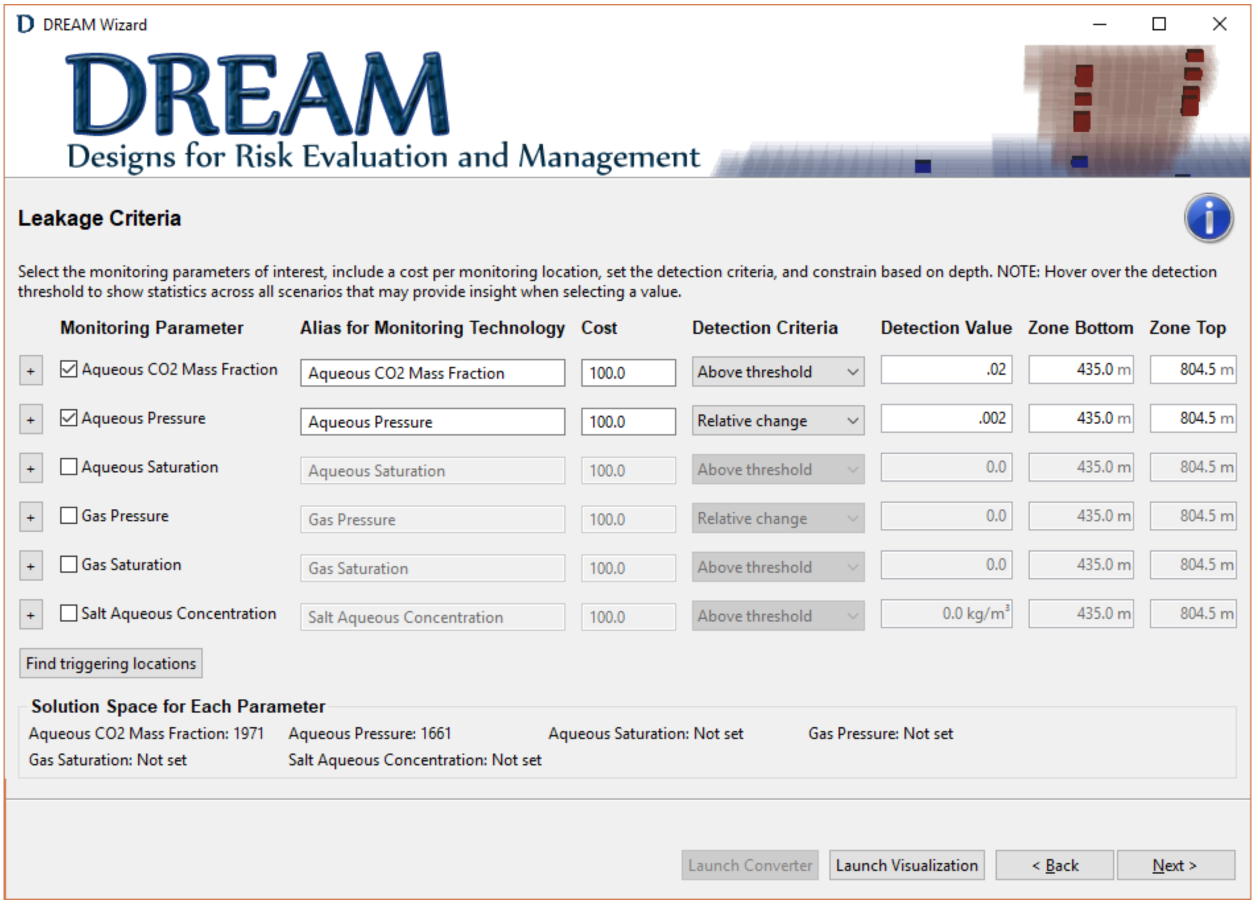

Figure 7: Leakage Criteria Page.

Select *Find triggering locations*. DREAM will calculate which nodes trigger for at least one scenario in the ensemble. Triggering means the node exceeds the entered threshold or experiences greater change than specified, implying that a leak has occurred. The following values should appear next to each selected parameter type at the bottom of the page (Table 2).

Note: While the process is working, a red box appears to the right of the progress bar. Pressing this box cancels the process before completion. Returning to a previously calculated value will not require additional processing.

Table 2: Triggering Locations

Monitoring Parameter	Solution Space
CO2 Mass Fraction	1971
Aqueous Pressure	1661

To visualize both the leakage solution space, press *Launch Visualization*.

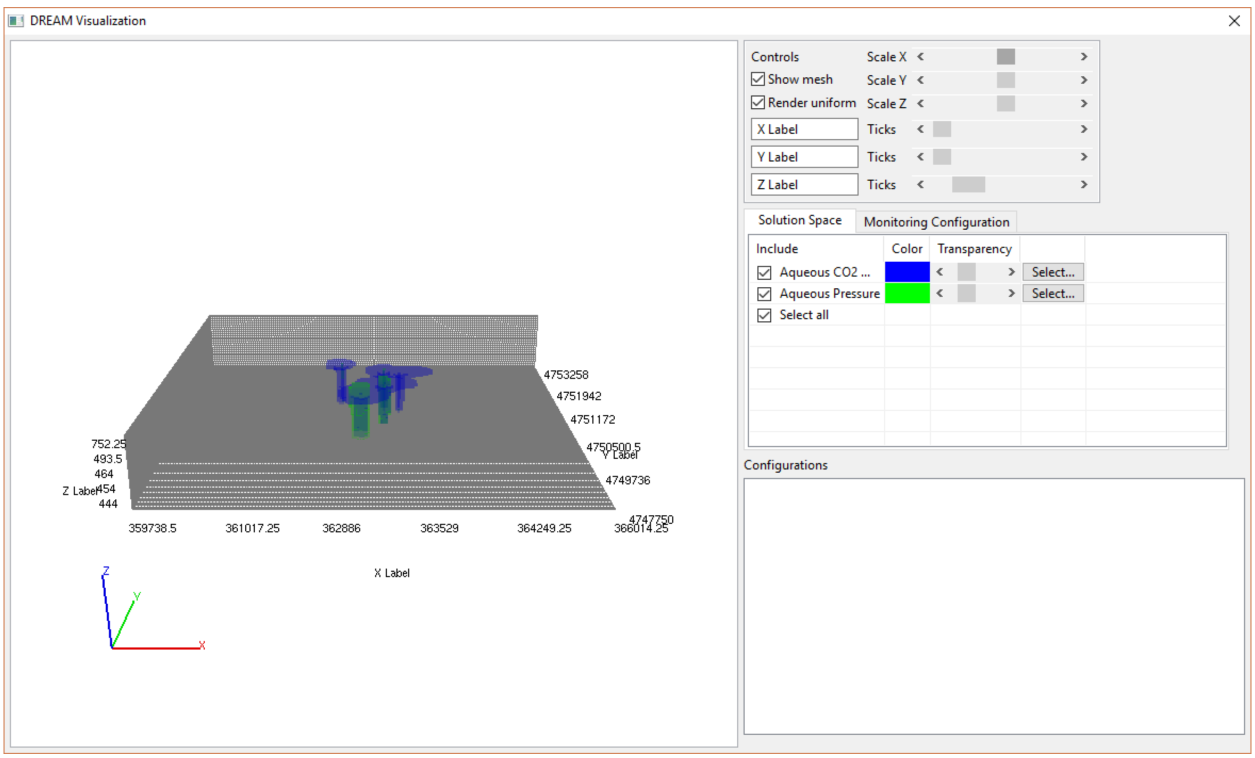

Figure 8: DREAM Visualization Tool.

The DREAM Visualization Tool (Figure 8) displays the full solution space (every leakage location). The user may toggle between views and change which parameters to display and what the color and transparency of the parameter should be. The user may zoom in and out with the mouse or scale the grid with the "Scale X/Y/Z" sliders. The monitoring configuration tab will become useful once the DREAM tool has run. Close out the Visualization Tool and select *Next* on the Leakage Criteria Window.

3.1.5 Detection Criteria

The *Detection Criteria* page (Figure 9) prompts the user to specify how many monitoring devices must be triggered to signify a leak has occurred. Multiple criteria can be created by selecting the *Add a new test* button. Within a given test, the user may select any combination of specific technologies will signify a leak.

Select Aqueous Pressure from the menu and click plus. This implies that two monitoring devices are required to signify a leak and that one device must be monitoring Aqueous Pressure. Select *Next*.

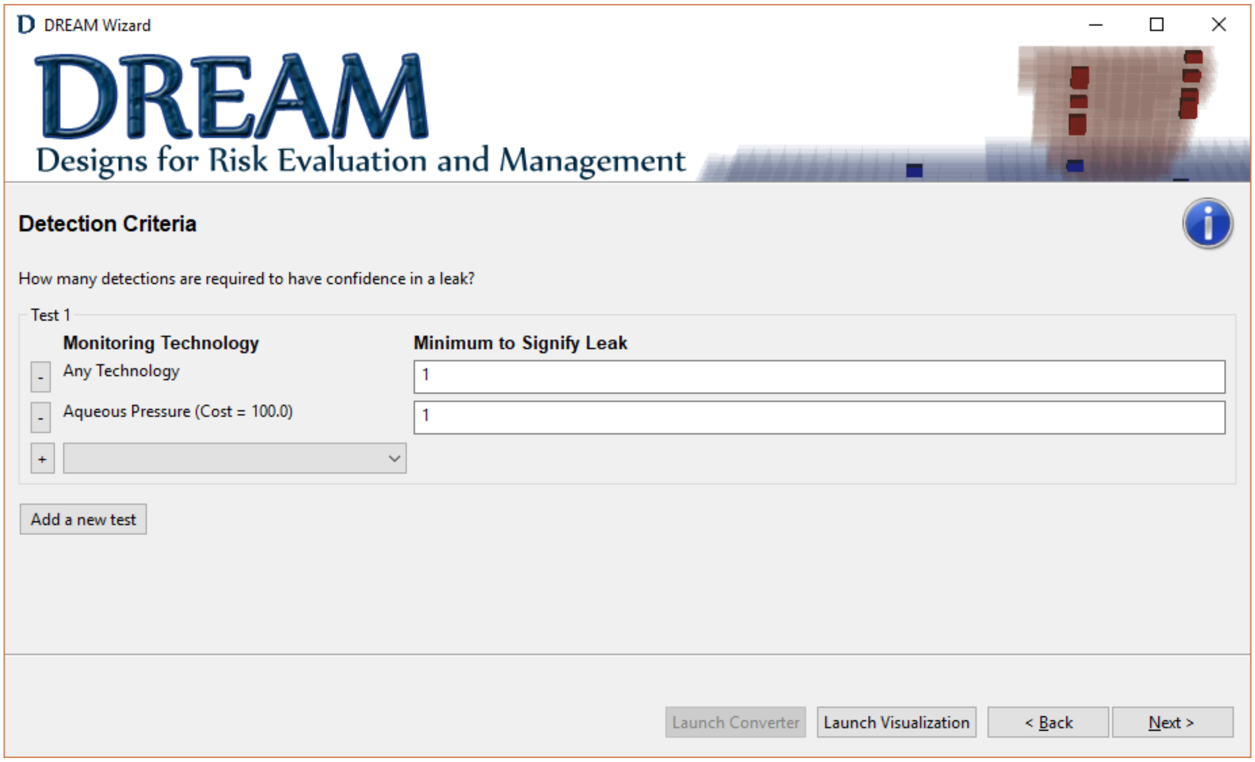

Figure 9: Detection Criteria Page.

3.1.6 Configuration Settings

The *Configuration Settings* page (Figure 10) allows the user to specify hard constraints for the optimization algorithm. The *Total Monitoring Budget* input specifies how much budget is available for monitoring technologies, acting as the primary limitation on the number of monitoring technologies can be added. The user is unable to select a budget less than the minimum constraints defined by the Detection Criteria page and associated costs. The *Maximum Number of Wells* and *Minimum Distance Between Wells* inputs can also constrain the optimization algorithm. The final three cost inputs do not affect the algorithm but are instead factored during post-processing to distinguish between the best configurations.

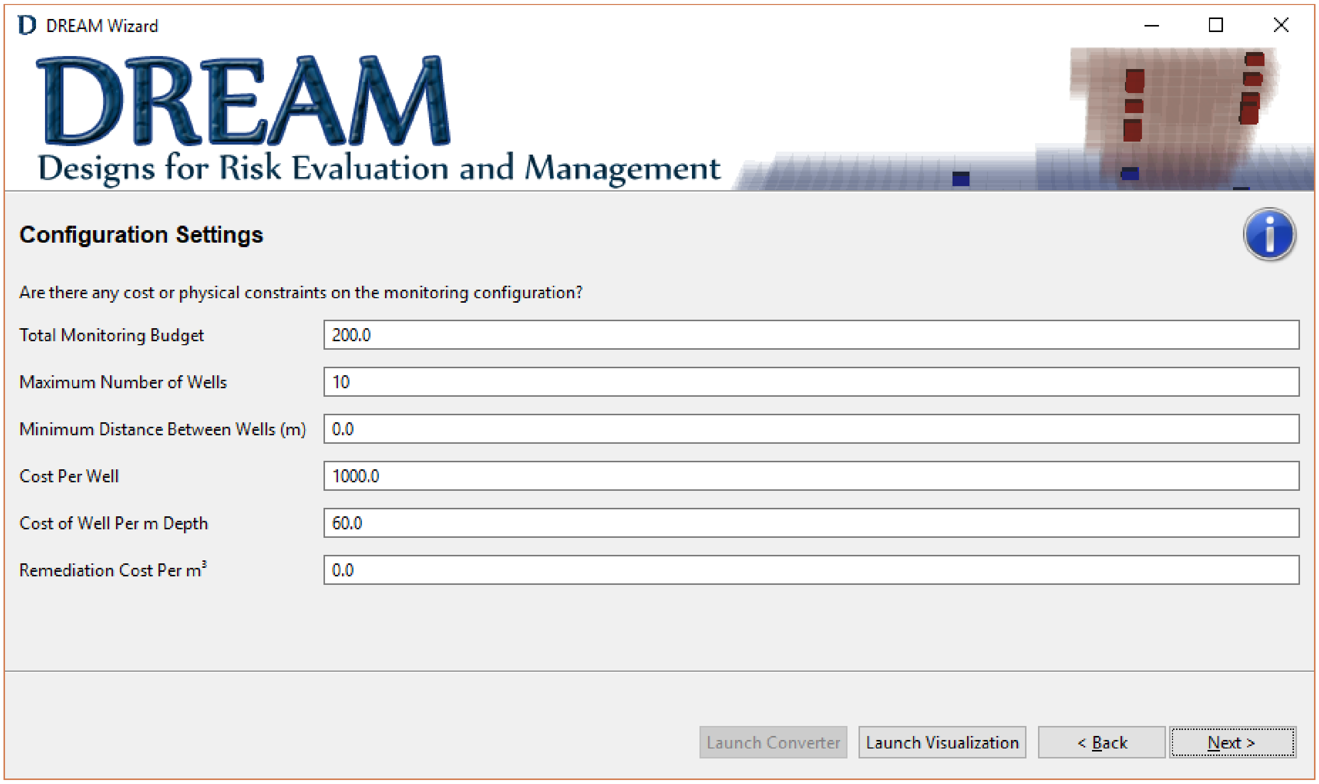

Figure 10: Configuration Settings Page.

Set the Total Monitoring Budget to 500, which will allow the algorithm to place up to 5 sensors based on the costs provided at the Leakage Criteria page. All other inputs can be left at default values. Select *Next*.

3.1.7 Exclude Locations

The Exclude Location page (Figure 11) allows the user to exclude (x, y) locations from the monitoring configuration that are infeasible or unapproved. This window allows the user to manually deselect nodes that should not be used in the optimization algorithm.

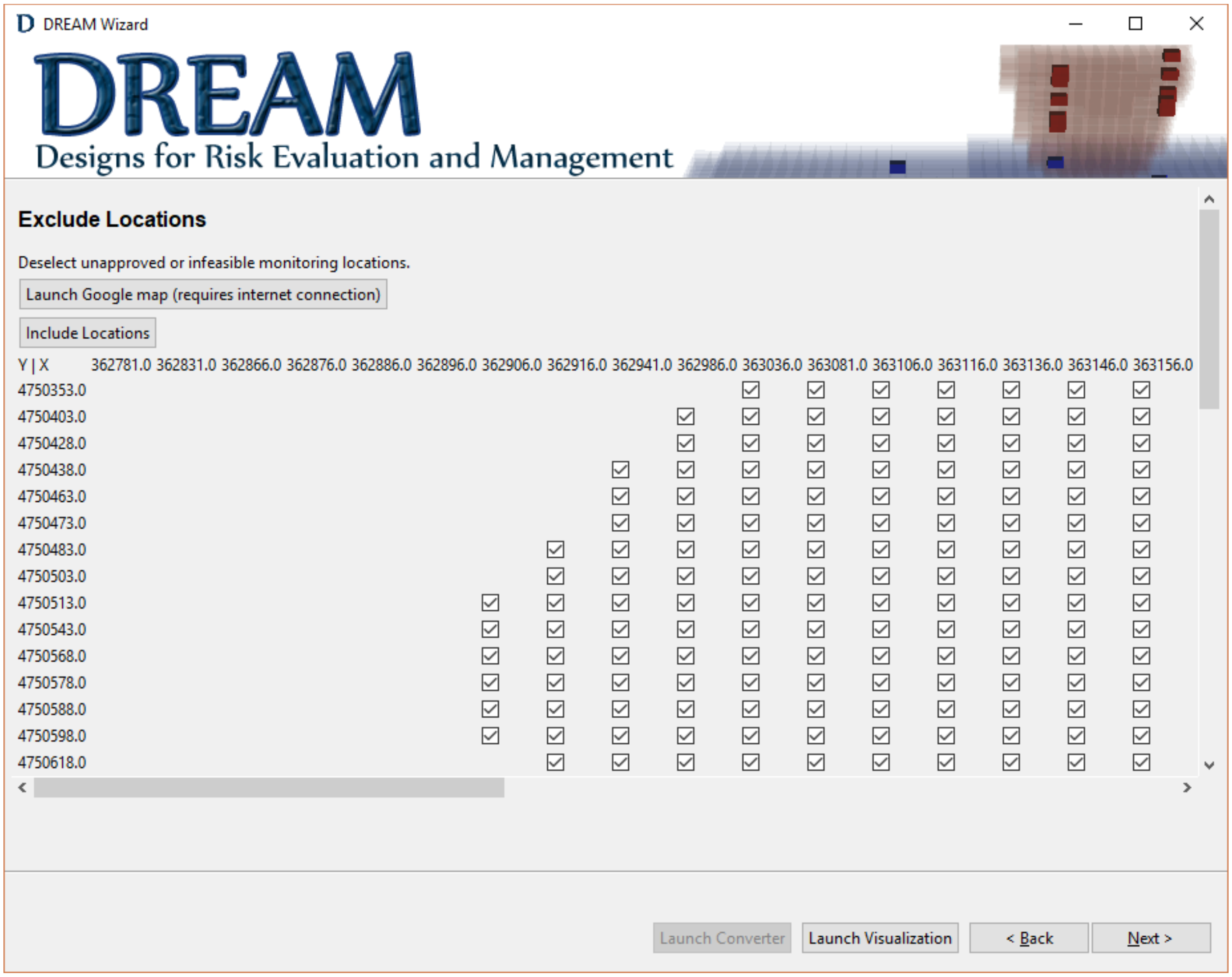

Figure 11: Exclude Locations Page.

If the user has an internet connection, the *Launch Google map* button will pop-up a map (Figure 12) which overlays the grid on a satellite map with zoom functionality enabled. The user will first be prompted to enter the UTM zone so the coordinates can be properly mapped – at this time, the overlay functionality only works with a UTM coordinate system. Enter "17N" to view the map. Nodes appear as greyed boxes that can be deselected to exclude from the optimization algorithm. The extents of the model grid are shown as a red box (not pictured below).

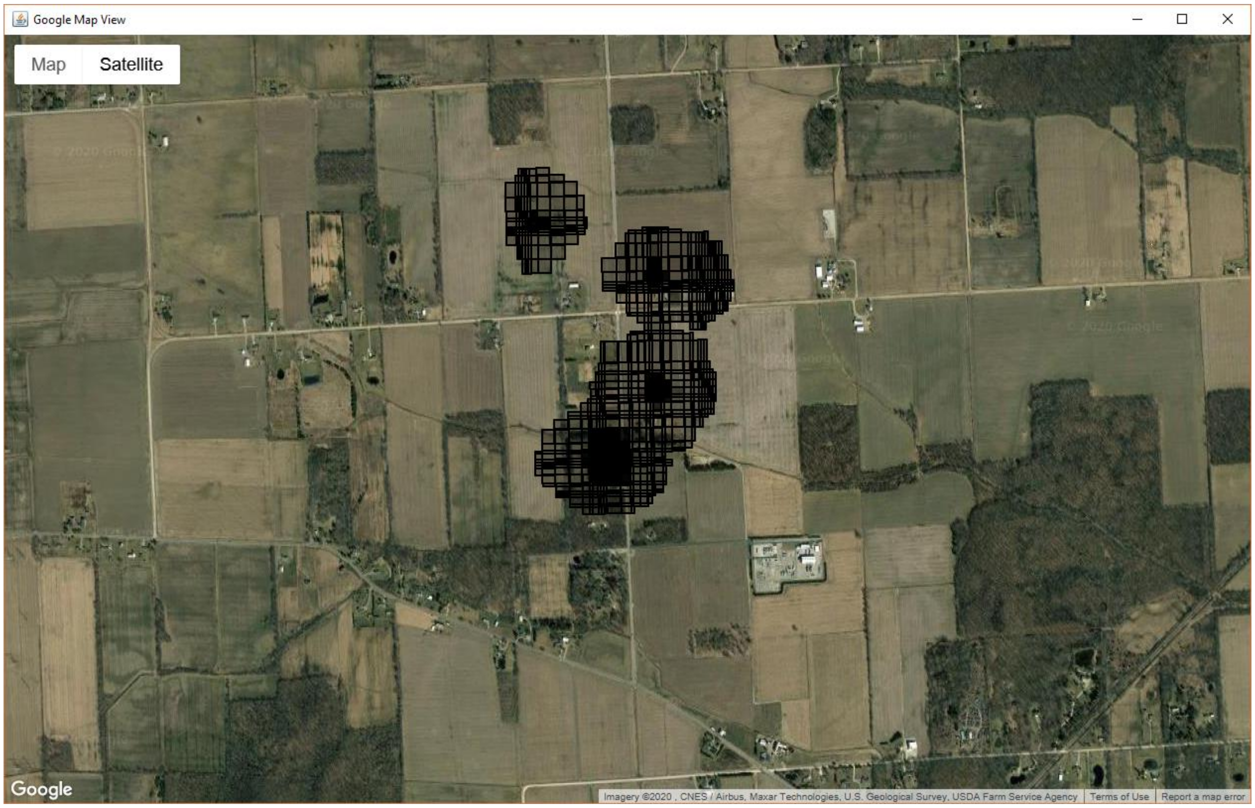

Figure 12: Google Map view to exclude locations.

DREAM also allows the user to enter locations of existing wells (Figure 13). Dream will then search the solution space for the entered well and output the time to detection of each parameter to a csv file. This is meant to be a diagnostic tool to identify the value of instrumenting existing wells, but inputs are not used in the optimization algorithm.

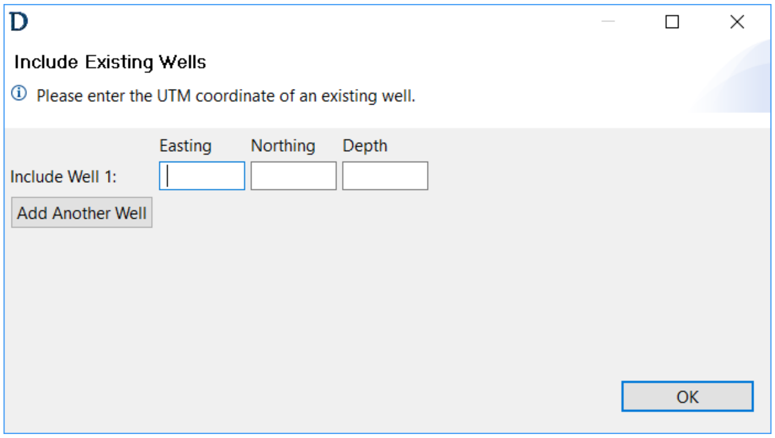

Figure 13. Diagnostic tool to explore the viability

Do not deselect any boxes, rather exit out of this window. Select *Next.*

3.1.8 Run DREAM

The *Run DREAM* page (Figure 14) provides a summary of the user inputs to the left. By default, a new "results" directory will be created to store output files. The *Run Iterative Procedure* button will run the simulated annealing optimization algorithm the number of times specified on the number of configurations specified. For more information on the Simulated Annealing algorithm, see Section 3.1.9 The *Show Plots* box determines whether results are actively plotted and displayed in the visualization window. The *Plot Results* box determines whether to generate additional output plots (Python3 is required).

A few additional outputs are available as diagnostic tools. The *Best TTD Possible per Technology* button quickly generates a table providing the shortest time to detection for each monitoring technology, if hypothetically every node in the solution space was monitored. This provides no indication of optimal monitoring configurations but allows the user to understand the problem before running the iterative procedure. The *Volume of Aquifer Degraded* button quickly generates a table showing the average, minimum, and maximum volume of aquifer degraded across all scenarios at each time step, providing insight into the magnitude of leaks across the provided scenarios.

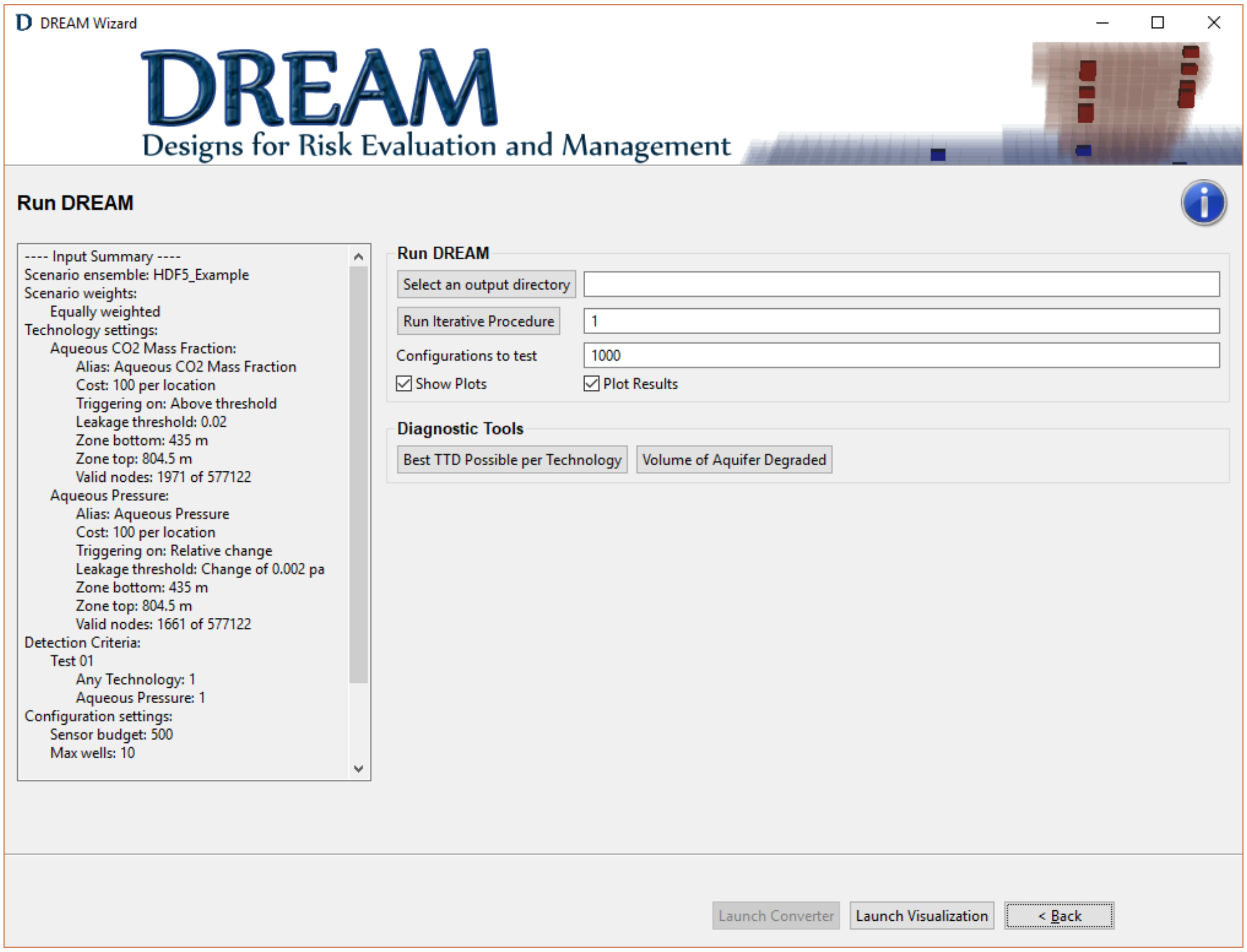

Figure 14: Run DREAM Page.

For the example problem, follow this progression:

1. Choose *Best TTD Possible per Technology* to view a summary of the lowest possible times to leakage detection. An excel file is created in the results directory specified ("best_ttd_table.csv").
2. Choose *Volume of Aquifer Degraded* to view a summary of the volume of aquifer degraded (VAD) per timestep ("VolumeOfAquiferDegraded.csv").
3. Next, choose to run the procedure five times for 500 configurations. Select *Run Iterative Procedure*.

While DREAM is running, two pop-up windows display the optimization performance. One is the DREAM Visualization Tool (Figure 15), which dynamically updates to show configurations being tested. Results for all unique configurations are stored in the Configurations tree, with the best results near the top.

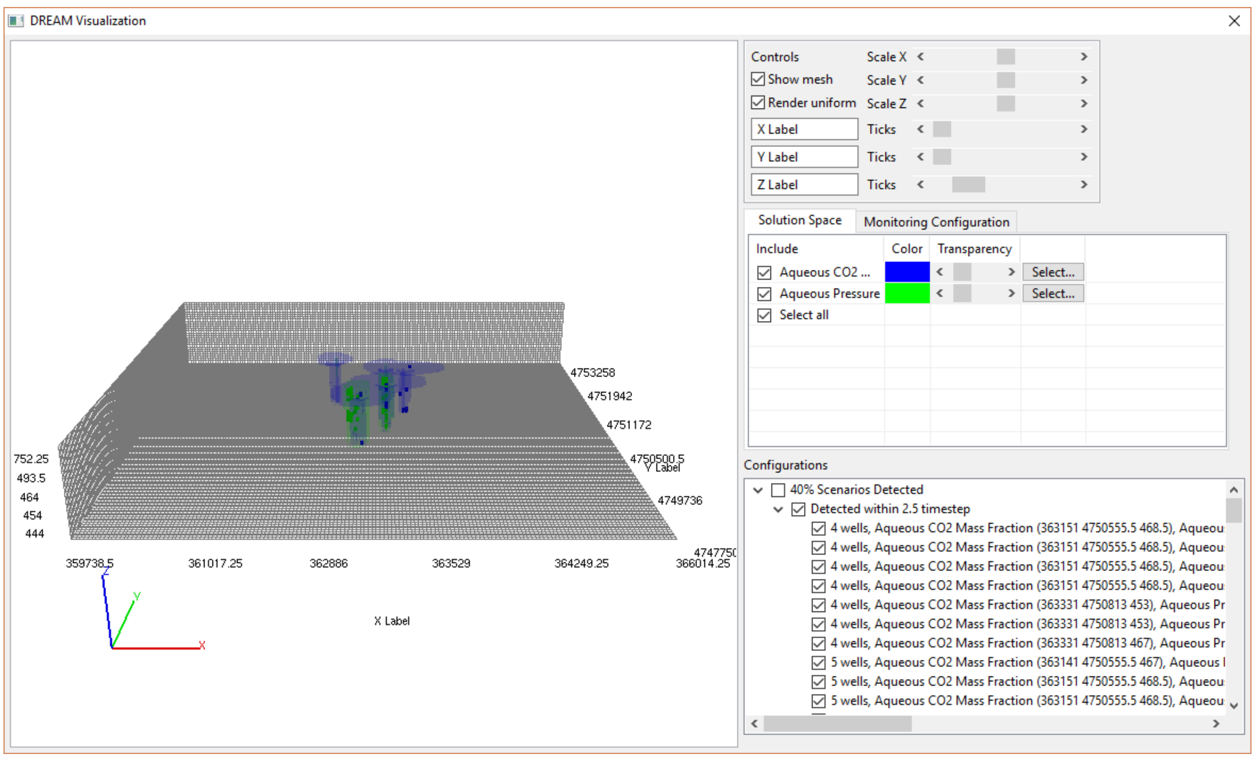

Figure 15: Tested configurations during optimization.

The second window shows the performance of the iteration procedure through two plots (Figure 16). The left plot shows the running TTD of the newest configuration, for each simulated annealing iteration, or new monitoring configuration. The right plot shows the percent of scenarios in which the leak was detected as new configurations are being tested.

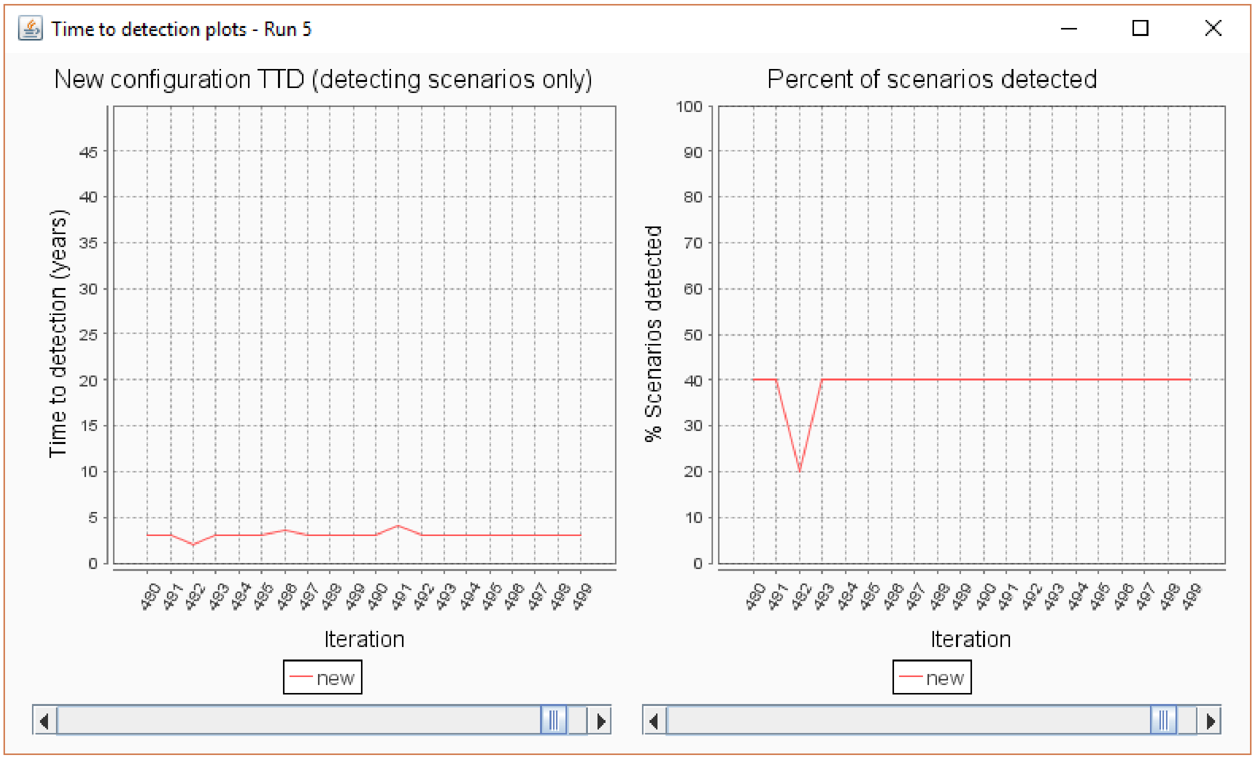

Figure 16: Algorithm performance plots.

Additionally, DREAM loads results files into the specified directory. The user can view output files summarizing the iteration procedure and results. These include:

- **best_configurations.csv**
  - One of the most useful output files is the best_configurations.csv, which provides the weighted and unweighted percent of scenarios where the leak was detected using the best configuration(s), weighted and unweighted average TTD across all successful scenarios, the range of TTD across all successful scenarios, the scenarios where the configuration(s) did not detect a leak, the number of wells, the cost of the well configuration factoring monitoring technology and well costs, the average volume of aquifer degraded at the time of detection, and the monitoring technologies locations of the best configuration(s).
- **objective_summary_best.csv, objective_summary_current.csv, objective_summary_new.csv**
  - These files provide summaries of each simulated annealing procedure performed. The iterations listed count the best, current, and new configurations tested. The respective weighted TTD and percent of scenarios detected are given so the user can visualize the algorithm performance.
- **run_0_best.csv, run_0_current.csv, run_0_new.csv**
  - These files provide summaries of the specific configurations tested during iterations. The first column is the iteration number, the second column is the TTD, and from the third column on, the node number and sensor type are given. Note: DREAM uses random seeding so results can be reproduced.
- Optional Python-Generated Plots:

- **Best configuration time to detection plots**
  - This script plots the time to detection spread per scenario for each configuration. The x-axis shows the time to detection and the y-axis shows the number of scenarios detected (Figure 17).

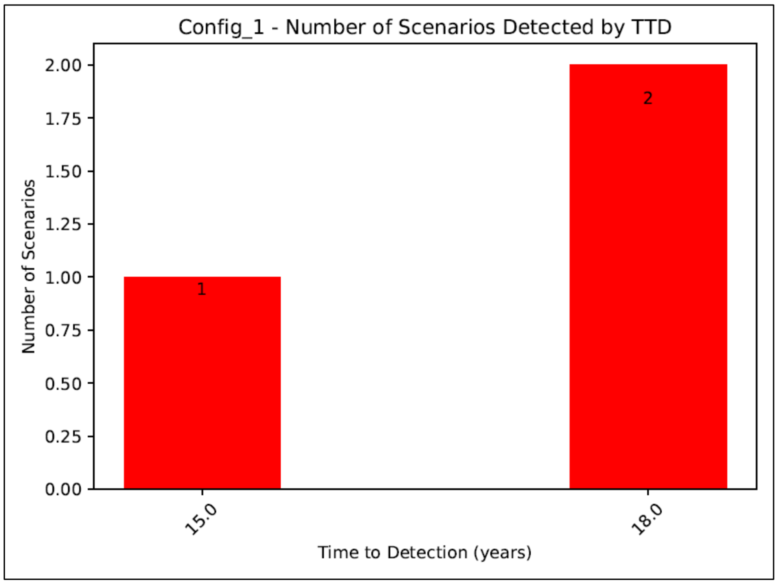

Figure 17. Best Configuration TTD Plot Example.

- **Best configuration volume of aquifer degraded plots**
  - This script plots the volume of aquifer degraded per scenario for each configuration. The x-axis shows the Volume of Aquifer degraded and the y-axis shows the number of scenarios (Figure 18).

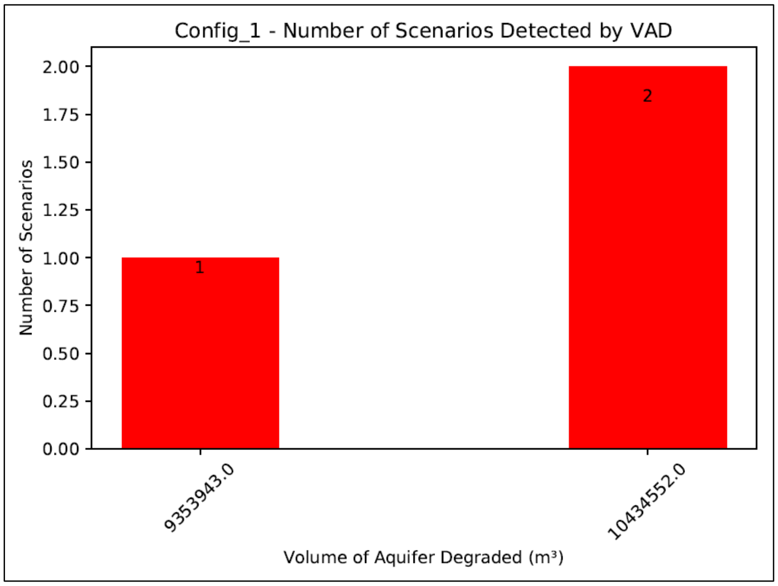

Figure 18. Best Configuration VAD Plot Example.

- **3-Panel plume plots**
  - This script plots DREAM's optimal sensor configurations on a 3-panel plume map for each configuration (Figure 19).

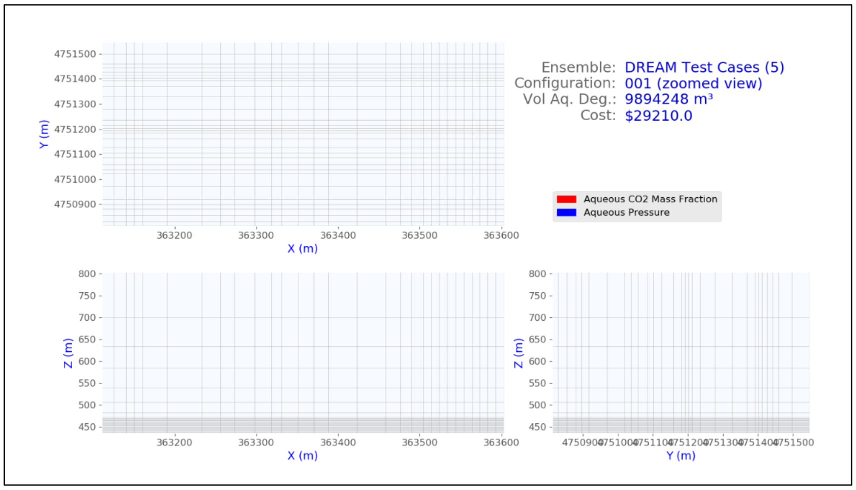

Figure 19. 3-Panel Plum Plot Example.

- Dreamout01.py
  - This script plots outputs from all iterations and runs tested, emulating the plots that appear in a window during the simulated annealing process (Figure 20).

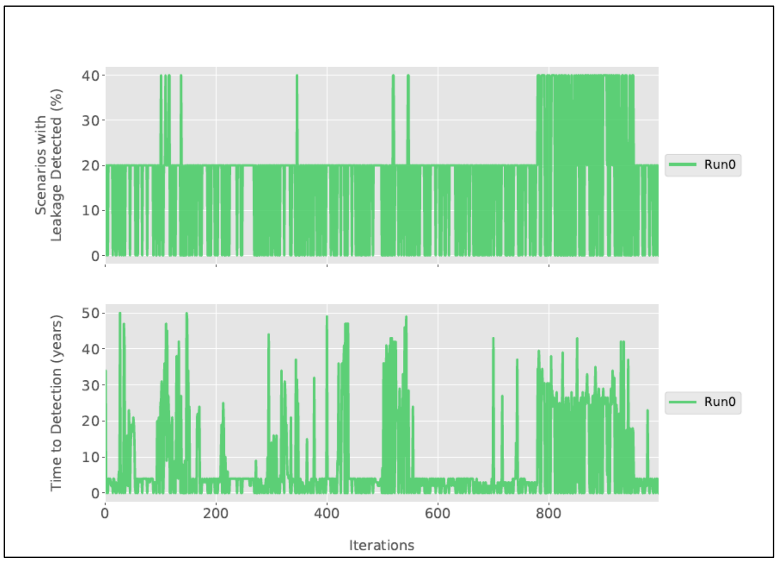

Figure 20. Iteration Output Plot Example.

3.2 SIMULATED ANNEALING ALGORITHM

DREAM is intentionally designed to run on a personal computer. Therefore, a complete enumeration of the solution space that tests all possible combinations and placements of monitoring technologies is not feasible. As an alternative, DREAM uses an optimization algorithm to approximate the optimal monitoring configurations. In the future, DREAM may provide multiple algorithm options.

Simulated annealing is the chosen algorithm for DREAM, found by Matott et al. (2011) to perform moderately well among evaluated algorithms for geoscience application and found by Bangerth et al. (2006) to be efficient at finding near-optimal solutions. Simulated annealing is an iterative search heuristic analogous to the physical process of annealing. At each iteration, the configuration is randomly mutated with one of the following actions:

- Add a random monitoring technology to a valid location
- Remove an existing monitoring location
- Swap an existing location with another valid monitoring technology
- Move an existing monitoring technology to another valid location
- Move an entire well to another valid location
- Shuffle all the monitoring locations with a single well

Each of the listed actions are limited by prior user inputs such as cost constraints, available locations, and the maximum number of wells. The first action (add a location) is weighted more heavily so that the iterations approach a maximized budget which is assumed to yield the best results, though randomization can result in configurations using less budget. All other actions are equally weighted. If one action is attempted and fails due to constraints (i.e. add a location when no budget is available), a new action is randomly selected until an action is successful.

Simulated annealing comes into play as the algorithm decides whether to keep the previous configuration or the mutated configuration at each iteration. Simply taking the better configuration every time is likely to trap the algorithm at a locally optimized result rather than the globally optimized result. Simulated annealing uses a temperature value that exponentially degrades from 1 to 0 through the iterations (Figure 21), used to determine the likelihood of keeping the worst of the two configurations. This allows the algorithm to act “risky” towards the start of the run and transition towards more “stable” changes as the solution converges on an optimized location at the end of the run. Best configurations are saved during the entire process.

An objective function is used to value each configuration for the above simulated annealing algorithm. Currently, DREAM optimizes exclusively on the shortest time to detection of leaks. Value is assigned based on the shortest time to detection for all scenarios, with a large penalty assessed if a leak is not detected.

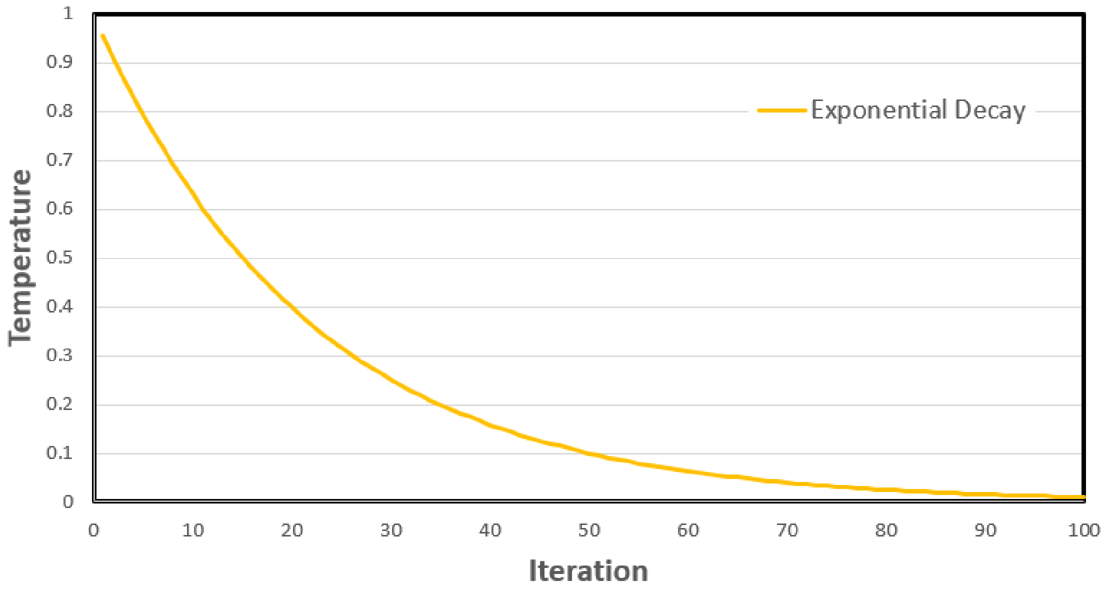

Figure 21: Exponential decay used for temperature function.

3.3 PRE-PROCESSING DATA

There are two different ways to use DREAM: (1) converting full leakage simulations into HDF5 files or (2) reading results from IAM, a reduced order model that uses a probabilistic framework.

To handle outputs from leakage simulations, DREAM provides the HDF5 Converter tool (Figure 22), which is pre-programmed to convert NUFT (Nonisothermal, Unsaturated Flow and Transport model; Nitao, 1998), STOMP (Subsurface Transport Over Multiple Phases model; White and Oostrom, 2000), and TECPLOT formatted output data to DREAM input files. The user must provide the directory containing the time plot files of all the scenarios, organized according to the selected folder structure. The converter quickly reads the basic structure and allows the user to select monitoring parameters of interest and deselect unwanted time steps or scenarios. Select *Run* to begin the conversion process.

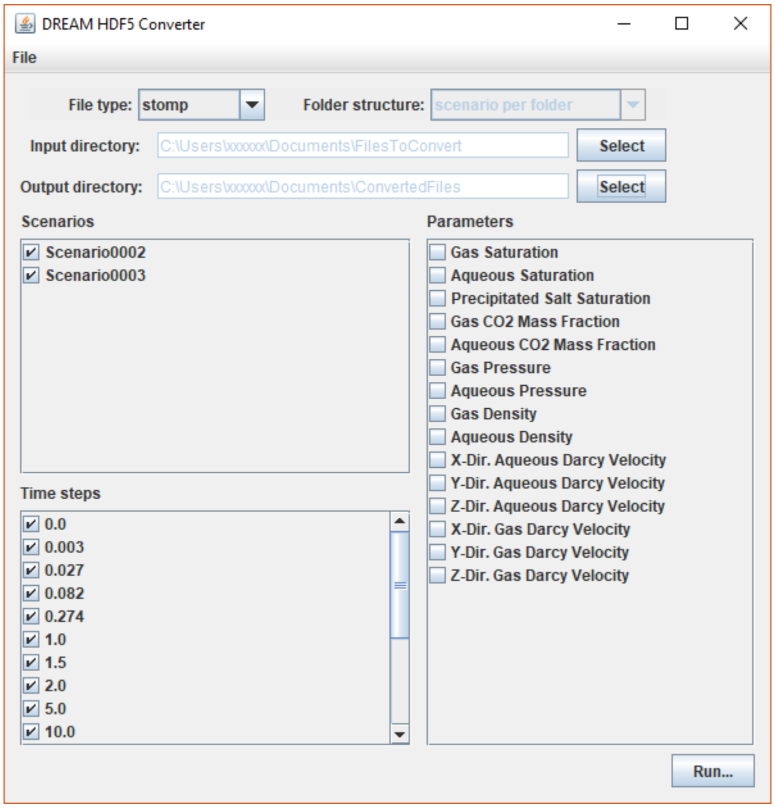

Figure 22: DREAM HDF5 Converter Tool.

3.3.1 STOMP Data

The DREAM file converter will accept most output types from STOMP. The required directory hierarchy is "ensemble folder\scenario folders\file per time step". Detailed information follows.

Folder Structure

For STOMP output, a folder with sub folders is expected. Each subfolder contains all the data for a given scenario. Within the scenario folder there should be one file for each time step that contains data for all the variables. Each scenario needs to have the same number of time steps and the same set of variables.

stomp_ensemble/scenario1/plot.1
stomp_ensemble/scenario1/plot.2
stomp_ensemble/scenario2/plot.1
stomp_ensemble/scenario2/plot.2

File Example: stomp_ensemble/scenario1/plot.1

This example file contains data for the first time step for the first scenario. XYZ data in STOMP is expected in x, then y, then z ordering. **Required** input are in bold, optional data is *italics*.

----------------------------- Beginning of File
Number of Time Steps = 2
Time = 1,yr
Number of X or R-Direction Nodes = 2
Number of Y or Theta-Direction Nodes = 2
Number of Z-Direction Nodes = 2
Number of Active Nodes = 8
Number of Vertices = 8
X-Direction Nodal Vertices, m
0 1 0 1 0 1 0 1
1 2 1 2 1 2 1 2
0 1 0 1 0 1 0 1
1 2 1 2 1 2 1 2
0 1 0 1 0 1 0 1
1 2 1 2 1 2 1 2
0 1 0 1 0 1 0 1
1 2 1 2 1 2 1 2
Y-Direction Nodal Vertices, m
0 0 1 1 0 0 1 1
0 0 1 1 0 0 1 1
1 1 2 2 1 1 2 2
1 1 2 2 1 1 2 2
0 0 1 1 0 0 1 1
0 0 1 1 0 0 1 1
1 1 2 2 1 1 2 2
1 1 2 2 1 1 2 2
Z-Direction Nodal Vertices, m
0 0 0 0 1 1 1 1
0 0 0 0 1 1 1 1
0 0 0 0 1 1 1 1
0 0 0 0 1 1 1 1

1 1 1 1 2 2 2 2
1 1 1 1 2 2 2 2
1 1 1 1 2 2 2 2
1 1 1 1 2 2 2 2
Data type 1, *units*
1.2 1.2 1.2 6.3 1.2 1.2 1.2 1.2
Data type 2, *units*
4.5 4.5 4.5 4.5 4.5 4.5 4.5 4.5

-------------------------------------- End of File

3.3.2 NUFT Data

The DREAM file converter will accept most output types from NUFT given in NTAB format. The required directory hierarchy is "ensemble folder\file per parameter and time step". Detailed information follows.

Folder Structure

For a NUFT output, a single folder is expected for the entire ensemble. Each file should represent a parameter for each scenario. All scenarios should have the same parameters. Each scenario needs to have the same number of time steps.

ntab_ensemble/parameter1_scenario1.ntab
ntab_ensemble/parameter1_scenario2.ntab
ntab_ensemble/parameter2_scenario1.ntab
ntab_ensemble/parameter2_scenario2.ntab

File Example: ntab_ensemble/parameter1_scenario1.ntab

This file contains data for all time steps of parameter 1. **Required** input are in bold, optional data is *italics*.

---------------------------- Beginning of File

index **i j k** *element_ref nuft_ind* **x y z dx dy dz volume 1.0y 2.0y**
1 1 1 1 52 1 0.5 0.5 0.5 1 1 1 1 1.2 1.2
2 2 1 1 52 2501 1.5 0.5 0.5 1 1 1 1 1.2 1.2
3 1 2 1 52 5001 0.5 1.5 0.5 1 1 1 1 1.2 6.3
4 2 2 1 52 7501 1.5 1.5 0.5 1 1 1 1 6.3 6.3
5 1 1 2 52 10001 0.5 0.5 1.5 1 1 1 1 1.2 1.2
6 2 1 2 52 12501 1.5 0.5 1.5 1 1 1 1 1.2 1.2
7 1 2 2 52 15001 0.5 1.5 1.5 1 1 1 1 1.2 1.2
8 2 2 2 52 17501 1.5 1.5 1.5 1 1 1 1 1.2 1.2

-------------------------------------- End of File

3.3.3 TECPLOT Data

If the user has plot files generated by another subsurface simulation code, it is recommended to reformat the plot file to fit an accepted ASCII format. TECPLOT formats are accepted due to their prevalent use in post-processing.

Folder Structure

For Tecplot output DREAM expects a single folder containing a TECPLOT file for each scenario. Each tecplot file is expected to contain all the time steps and all the data for that scenario. Each scenario needs to have the same number of time steps and the same set of variables.

tecplot_ensemble/scenario1.dat
tecplot_ensemble/scenario2.dat

File Example: tecplot_ensemble/scenario1.tecplot

This file contains data for all time steps and all data types. XYZ are expected to be nodal and should be in z then y then x ordering. All data is expected to be cell centered. **Required** keys are in bold, optional data is *italics*.

------------------------------ Beginning of File

TITLE = "Scenario 1"
VARIABLES = "X, m" "Y, m" "Z, m" "data type 1" "data type 2"
ZONE T = "1, y" , *STRANDID = 1*, **SOLUTIONTIME = 1**, **NODES = 64**, **ELEMENTS = 8**, *DATAPACKING = BLOCK, ZONETYPE = FEBRICK*
VARLOCATION = ([4,5] = CELLCENTERED)
0 1 0 1 0 1 0 1
0 1 0 1 0 1 0 1
0 1 0 1 0 1 0 1
0 1 0 1 0 1 0 1
1 2 1 2 1 2 1 2
1 2 1 2 1 2 1 2
1 2 1 2 1 2 1 2
1 2 1 2 1 2 1 2
0 0 1 1 0 0 1 1
0 0 1 1 0 0 1 1
1 1 2 2 1 1 2 2
1 1 2 2 1 1 2 2
0 0 1 1 0 0 1 1
0 0 1 1 0 0 1 1
1 1 2 2 1 1 2 2
1 1 2 2 1 1 2 2
0 0 0 0 1 1 1 1
1 1 1 1 2 2 2 2
0 0 0 0 1 1 1 1
1 1 1 1 2 2 2 2
0 0 0 0 1 1 1 1

1 1 1 1 2 2 2 2
0 0 0 0 1 1 1 1
1 1 1 1 2 2 2 2
1.2 1.2 1.2 6.3 1.2 1.2 1.2 1.2
4.5 4.5 4.5 4.5 4.5 4.5 4.5 4.5

ZONE T = "2, y" , *STRANDID = 1***, SOLUTIONTIME = 2**, **NODES = 64, ELEMENTS = 8**,
DATAPACKING = BLOCK, ZONETYPE = FEBRICK VARSHARELIST = ([1,2,3]=1),
CONNECTIVITYSHAREZONE = 1
VARLOCATION = ([4,5] = CELLCENTERED)
1.2 1.2 6.3 6.3 1.2 1.2 1.2 6.3
4.5 4.5 4.5 4.5 4.5 4.5 4.5 4.5

-------------------------------------- End of File

3.3.4 HDF5 Output

For each of the three examples, DREAM will create a directory with the same name as the parent directory with an "_hdf5" appended. Inside the directory will be an HDF5 file for each scenario that contains all the time steps for all the data types along with the grid information. All data will be cell centered.

File Example:

The hdf5 files can be viewed with HDFView (Figure 23).

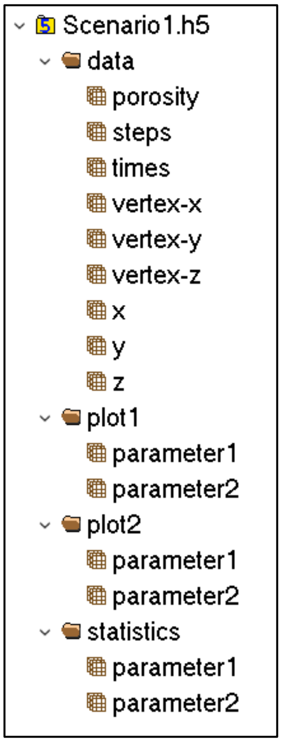

Figure 23: HDFView of DREAM input file structure.

Each scenario will contain a "data" group called that contains metadata about the scenario; porosity information, steps and their matching times, the grid XYZ vertices (edges), and the grid XYZ centers. There will also be a group for each time step containing 3D data for each parameter at that time step. Lastly, there is a "statistics" group that lists the global minimum, average, and maximum for each parameter to expedite future calculations.

3.3.5 IAM Output

IAM can quickly create many scenarios, all of which should be placed in a single directory. As part of the process of creating these files from IAM, the user must select detection criteria and threshold for each parameter. Therefore, the IAM files only contain detecting nodes for the inputted detection values, causing values to be greyed out on the Leakage Criteria page. To test different detection values, IAM must be rerun to generate a new set of IAM files.

File Example:

Each file has a header that lists IAM, scenario number, parameter, the detection criteria (relative change, absolute change, above, below), and the detection threshold. A negative or positive sign can be placed before the detection threshold to limit to a positive or negative change, otherwise the change threshold will work in both positive and native directions.

Following the header is a list of all detecting nodes for the given detection values. Each line represents a node and lists X, Y, Z, and time to first detection.

The same detection criteria and threshold should be used across all scenarios for a given parameter. All data is expected to be cell centered. **Required** keys are in bold, optional data is *italics*.

---------------------------- Beginning of File

IAM,1,Dissolved_CO2,relative,0.2,
776568.2414698162,14468825.459317585,-2343.3581219014286,25202.25
776568.2414698162,14468858.267716534,-2343.3581219014286,24837.0
776568.2414698162,14468891.076115485,-2343.3581219014286,25567.5
776601.0498687663,14468759.842519684,-2343.3581219014286,24106.5
776601.0498687663,14468792.650918635,-2343.3581219014286,21915.0

-------------------------------------- End of File

3.4 RANGE OF DREAM APPLICABILITY AND LIMITATIONS

DREAM version 2.0 is designed as a tool for additional analysis of subsurface CO_2 leakage simulations. However, it can be applied to any dataset of the formats described in Section 3.2. Users should take note of the following limitations:

- The only objective function solved is the time to first detection of leakage.
- The cost of monitoring devices is treated as a one-time fee, as opposed to incurring costs during operation.

- The constraint on the number of sensors is determined by the total monitoring budget compared to the cost of each technology. Costs for wells and remediation are not factored in the optimization but are post-processed for the best configurations.
- The monitoring configuration results produced by the simulated annealing algorithm are a function of the scenarios provided to DREAM as well as the number of iterative procedures and number of configurations tested. Users are encouraged to vary each of these parameters to determine the sensitivity of their results.
- DREAM was developed for use on PC and MAC and takes advantage of threading for some processes; therefore the speed of the tool is dependent on the capability of the specific PC or MAC to handle the size of the datasets.
- The interactive map feature (Section 3.1.7) cannot work without an internet connection.

4. REFERENCES

Bacon, D.H.; Yonkofski, C.M.; Brown, C.F.; Demirkanli, D.I.; Whiting, J.M. (2019). Risk-based post injection site care and monitoring for commercial-scale carbon storage: Reevaluation of the FutureGen 2.0 site using NRAP-Open-IAM and DREAM. *Intl. J. Greenhouse Gas Control*, 90, 102784.

Carroll, S. A.; Keating, E.; Mansoor, K.; Dai, Z.; Sun, Y.; Trainor-Guitton, W.; Brown, C.; Bacon, D. (2014a). Key factors for determining groundwater impacts due to leakage from geologic carbon sequestration reservoirs. *Intl. J. Greenhouse Gas Control*, 29, 153–168.

Carroll, S. A.; Mansoor, K.; Sun, Y. (2014b). *Second-Generation Reduced-Order Model for Calculating Groundwater Impacts as a Function of pH, Total Dissolved Solids, and Trace Metal Concentration*; NRAP-TRS-III-002-2014; NRAP Technical Report Series; U.S. Department of Energy, National Energy Technology Laboratory: Morgantown, WV, p 40.

Last, G. V.; Murray, C. J.; Brown, C. F.; Jordan, P. D.; Sharma, M. (2013). *No-Impact Threshold Values for NRAP's Reduced Order Models*; Pacific Northwest National Laboratory, Richland, Washington, p.72.

Nitao, J. J. (1998). *Reference manual for the NUFT flow and transport code, version 2.0*; Lawrence Livermore National Laboratory, Livermore, CA.

Sminchak, J. R.; Moody, M.; Theodos, A.; Larsen, G.; Gupta, N. (2014). Investigation of Wellbore Integrity Factors in Historical Oil and gas Wells for CO2 Geosequestration in the Midwestern US. *Energy Procedia*, 63, 5787-5797.

White, M. D.; Oostrom M. (2000). *STOMP, Subsurface transport over multiple phases, Version 2.0, Theory Guide*; Pacific Northwest National Laboratory, Richland, WA.

Yonkofski, C. M.; Gastelum, J. A.; Porter, E. A.; Rodriguez, L. R.; Bacon, D. H.; Brown, C. F. (2016). An optimization approach to design monitoring schemes for CO_2 leakage detection. *Intl. J. Greenhouse Gas Control*, 47, 233–239.

Yonkofski C.; Davidson, C.L.; Rodriguez, L.R.; Porter, E.A.; Bender, S.R.; Brown, C.F. (2017). Optimized, budget-constrained monitoring well placement using DREAM. *Energy Procedia*, 114, 3649-3655.

This page intentionally left blank.

NRAP is an initiative within DOE's Office of Fossil Energy and is led by the National Energy Technology Laboratory (NETL). It is a multi-national-lab effort that leverages broad technical capabilities across the DOE complex to develop an integrated science base that can be applied to risk assessment for long-term storage of carbon dioxide (CO_2). NRAP involves five DOE national laboratories: NETL, Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), and Pacific Northwest National Laboratory (PNNL).

Technical Leadership Team

Diana Bacon
Lead, Groundwater Protection Working Group
Pacific Northwest National Laboratory
Richmond, WA

Jens Birkholzer
LBNL Lab Lead
Lawrence Berkeley National Laboratory
Berkeley, CA

Grant Bromhal
Technical Director, NRAP
Research and Innovation Center
National Energy Technology Laboratory
Morgantown, WV

Chris Brown
PNNL Lab Lead
Pacific Northwest National Laboratory
Richmond, WA

Susan Carroll
LLNL Lab Lead
Lawrence Livermore National Laboratory
Livermore, CA

Abdullah Cihan
Lead, Reservoir Performance Working Group
Lawrence Berkeley National Laboratory
Berkeley, CA

Tom Daley
Lead, Strategic Monitoring Working Group
Lawrence Berkeley National Laboratory
Berkeley, CA

Robert Dilmore
NETL Lab Lead
Research and Innovation Center
National Energy Technology Laboratory
Pittsburgh, PA

Nik Huerta
Lead, Migration Pathways Working Group
Research and Innovation Center
National Energy Technology Laboratory
Albany, OR

Rajesh Pawar
LANL Lab Lead
Lead, Systems/Risk Modeling Working Group
Los Alamos National Laboratory
Los Alamos, NM

Tom Richard
Deputy Technical Director, NRAP
The Pennsylvania State University
State College, PA

Josh White
Lead, Induced Seismicity Working Group
Lawrence Livermore National Laboratory
Livermore, CA

Sean Plasynski
Executive Director
Technology Development and Integration Center
National Energy Technology Laboratory
U.S. Department of Energy

Heather Quedenfeld
Associate Director
Coal Development and Integration
National Energy Technology Laboratory
U.S. Department of Energy

Traci Rodosta
Technology Manager
Strategic Planning
Science and Technology Strategic Plans and Programs
National Energy Technology Laboratory
U.S. Department of Energy

Mark Ackiewicz
Director
Division of Carbon Capture and Storage
Office of Fossil Energy
U.S. Department of Energy

NRAP Executive Committee

Cynthia Powell
Executive Director
Research and Innovation Center
National Energy Technology Laboratory

Donald DePaolo
Associate Laboratory Director
Energy and Environmental Sciences
Lawrence Berkeley National Laboratory

Roger Aines
Chief Energy Technologist
Lawrence Livermore National Laboratory

Melissa Fox
Program Manager
Applied Energy Programs
Los Alamos National Laboratory

George Guthrie
Chair, NRAP Executive Committee
Earth and Environmental Sciences
Los Alamos National Laboratory

Alain Bonneville
Laboratory Fellow
Pacific Northwest National Laboratory

Grant Bromhal
Technical Director, NRAP
Senior Research Fellow
Research and Innovation Center
National Energy Technology Laboratory