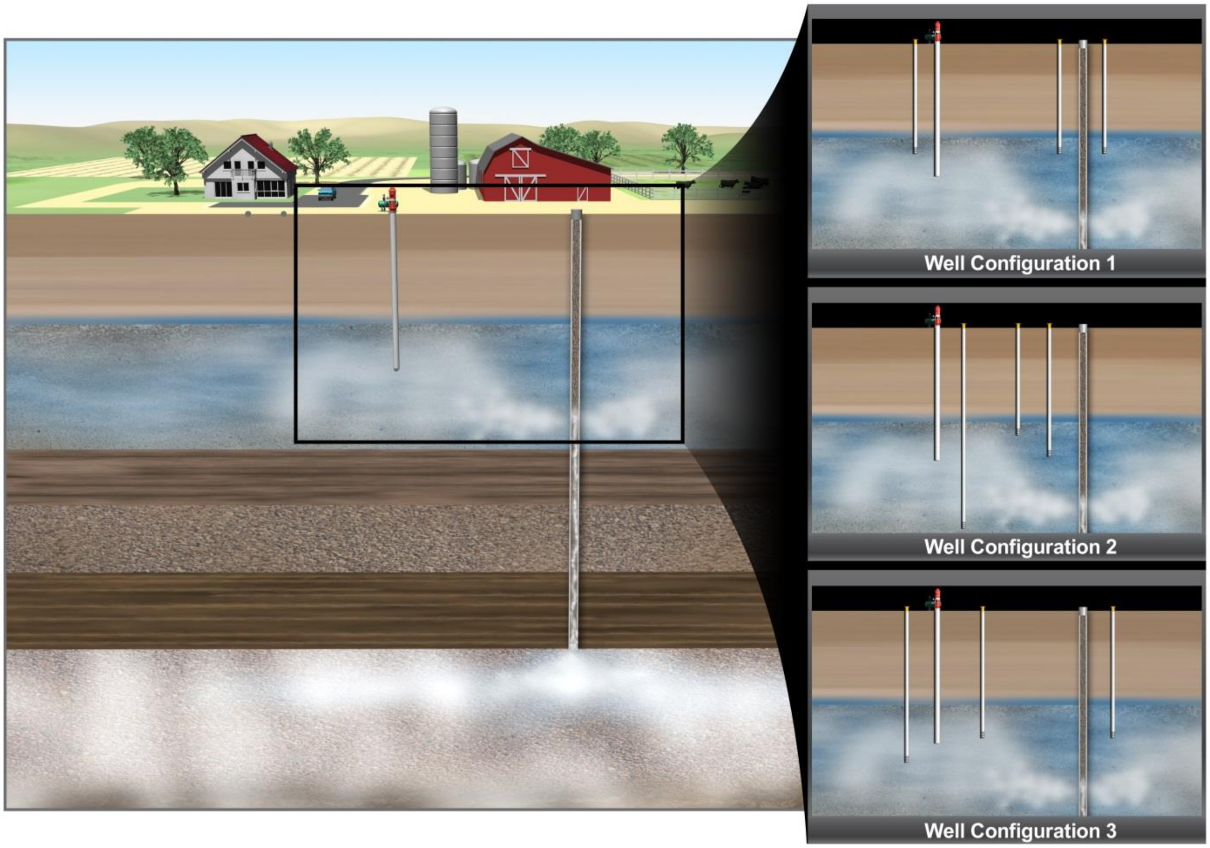
National Risk Assessment Partnership



Designs for Risk Evaluation and Management (DREAM) Tool User's Manual

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Cover Illustration: A hypothetical visualization of three CO_2 leakage with DREAM produced monitoring configurations.

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Designs for Risk Evaluation and Management (DREAM) Tool User's Manual

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Acronyms, Abbreviations, and Symbols

Term	Description
Acronyms/Abbreviations	
3-D	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
ETFD	Estimated time to first detection
GUI	Graphical user interface
HDF5	Hierarchical data format
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
Units/Symbols	
cm	centimeter
L	Liter
mg	Milligram
mg/L	Milligrams per liter
min	Minute
mol	Mole
Pa	Pascal
s	Second
wk	Week
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 technical effort described in this report was performed in support of the DOE National Energy Technology Laboratory’s (NETL) ongoing research. The author wishes to acknowledge Robert Romanosky and Traci Rodosta (NETL Strategic Center for Coal) and Regis Conrad and Mark Ackiewicz (DOE Office of Fossil Energy) for programmatic guidance, direction, and support.

In addition, special thanks to Jason Gastelum, Art Sadvosky, and Diana Bacon for their early contributions to DREAM development.

ABSTRACT

This manual provides a brief guide for the use of the Designs for Risk Evaluation and Management (DREAM) tool, 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 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 processes user-provided output from subsurface leakage simulations. 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 three 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) a plotting tool used to analyze the results. A secondary Java application is provided 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.

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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 need for a user-friendly tool with the ability to design site-specific risk-based monitoring strategies was identified by the National Risk Assessment Partnership (NRAP). 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 (USDWs) 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 reads user-provided output from subsurface leakage simulations, optimizing monitoring schemes based on the minimum 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. This approach has proven to be orders of magnitude faster than an exhaustive search of the entire solution space (Gastelum et al., 2015). 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. While DREAM was designed with applications to CO_2 leakage in mind, this flexibility allows DREAM to be used to determine optimal monitoring locations for any contaminant transport scenario.

Development of DREAM began in 2012 as part of work of the NRAP project. This code version began development in 2013 during the third-generation of the NRAP project. Subsequent versions, when completed, will add flexibility in the choice of the objective function (e.g. cost instead of time to detection), allow for a broader range of input formats, and improve existing capabilities (e.g. computational speed).

This manual illustrates the program graphical user interface (GUI), describes the tool inputs, and includes an example application. For a synopsis of the theoretical basis of DREAM, see Yonkofski et al. (2016).

2. SOFTWARE INSTALLATION AND REQUIREMENTS

Before DREAM installation, the most recent release of the Java Platform, Standard Edition Development Kit must be installed (jdk-8u71-windows-x64.exe is the most recent as of January 2016).

It is also recommend that the user install the most recent version of HDFView for reading converted hierarchical data format (HDF5). Download locations for these files are shown in Table 1.

The DREAM tool has been released within the NRAP August 2015 Tools Collaborative Workspace on the NETL Energy Data Exchange (EDX).

1. Sign into EDX with an account that belongs to the workspace and download the DREAM tool at: https://edx.netl.doe.gov/organization/nrap-tools-beta-testing-developer-uploads/folder/96ca4fa9-68c9-4795-a22d-164291336e45
2. Select the "DREAM V.1 - PC" link and download the zip file to your computer's hard drive
3. Also download all compressed files under "DREAM V.1 - PC Beta Test". These include BetaTest1_hdf5.zip, BetaTest2_hdf5.zip, and BetaTest_Results.zip.
4. Extract the all compressed folders to the same parent directory.
5. Run the "DREAM_v1.jar" file found within the extracted DREAM_v1 folder. This will launch the DREAM tool application.

Note: This software has been created for use on the Microsoft Windows operating system and requires a 64 bit system for operation.

Table 1: Supplementary Software

Software	Website
Java SE 7	http://www.oracle.com/technetwork/java/javase/downloads/jre7-downloads-1880261.html
HDFView 2.11	https://www.hdfgroup.org/products/java/release/download.html#download

3. USER INTERFACE 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. 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 User Interface (UI) while demonstrating an application to 19 randomly selected leakage realizations generated for an NRAP Second Generation Reduced-Order Model study (Carroll et al., 2013). For context, a brief summary of the model set up from Carroll et al. (2013) is provided:

The NUFT numerical model (Fig. 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. 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 realization 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.

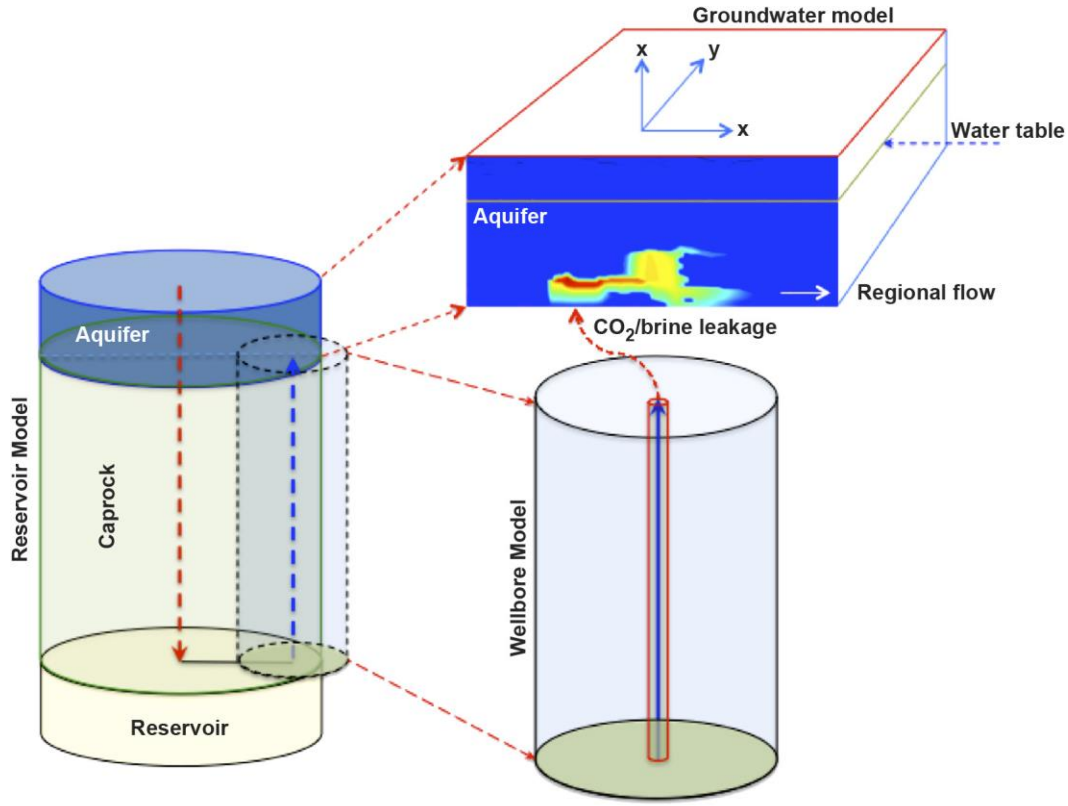


Figure 1: Beta Example Schematic. Figure from Carroll et al. (2013) shows the links between reservoir, well leakage, and aquifer models using the alluvium case study. Links between reservoir, well leakage, and the carbonate case study are identical.

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 UI should be completed in the sequence with which windows progress (Fig. 2).

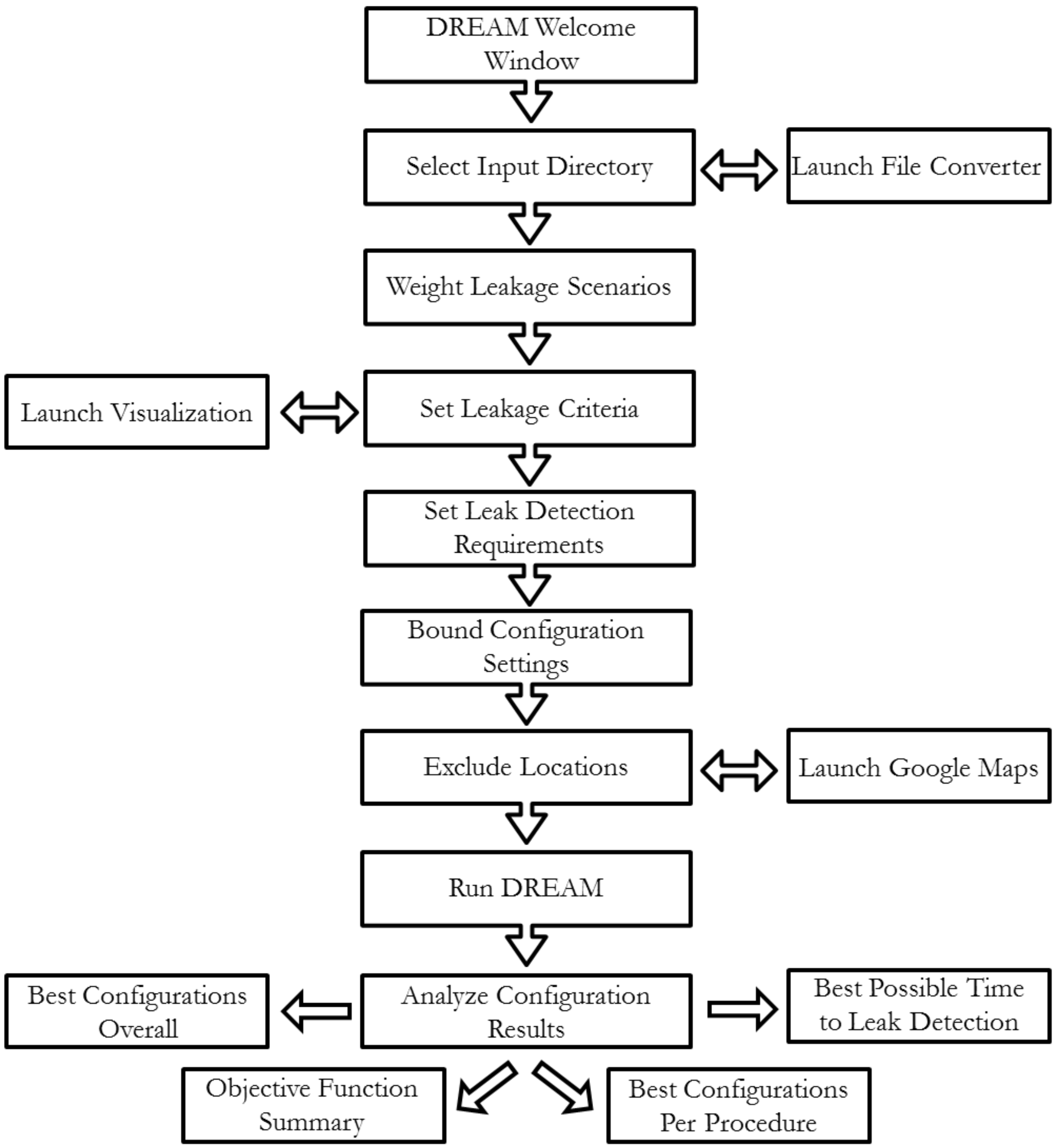


Figure 2: DREAM UI Flow Chart

3.1.1 DREAM Welcome Window

The DREAM Welcome page (Fig. 3Figure 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 review 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 shows a theoretical DREAM application, with a leak from subsurface storage entering an overlying aquifer through an abandoned well bore. 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*.

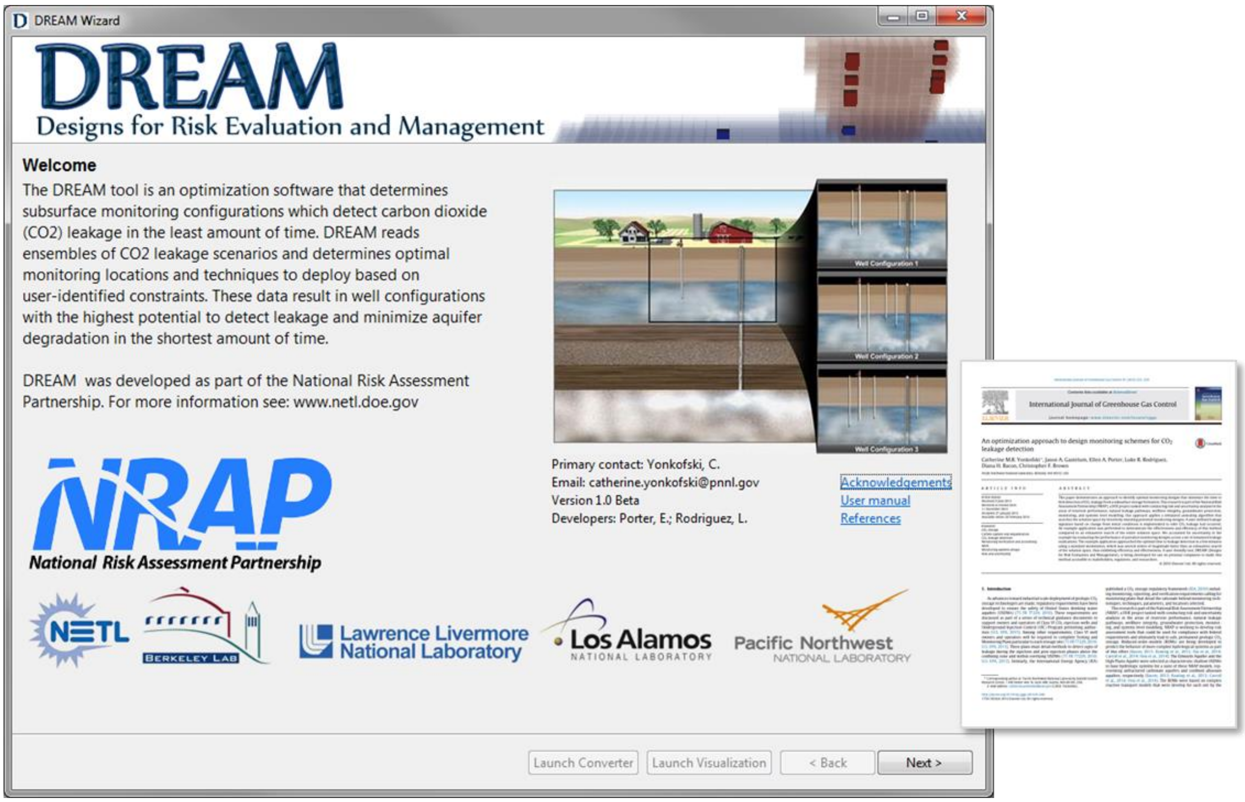


Figure 3: DREAM Welcome Window

3.1.2 Input Directory Selection

The "Input Directory" window (Fig. 4Figure 4) prompts the user to select the directory containing HDF5 files for all leakage simulations to be included. The current version of DREAM supports the "Sensor placement optimization tool: CCS9.1" and the model option, "Individual Sensors 2.1." The dropdown boxes provided were built with future versions of DREAM in mind, where the objective function parameters will be more flexible. The HDF5 files must be directly available within the directory provided; they may not be in subdirectories within the root directory.

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.

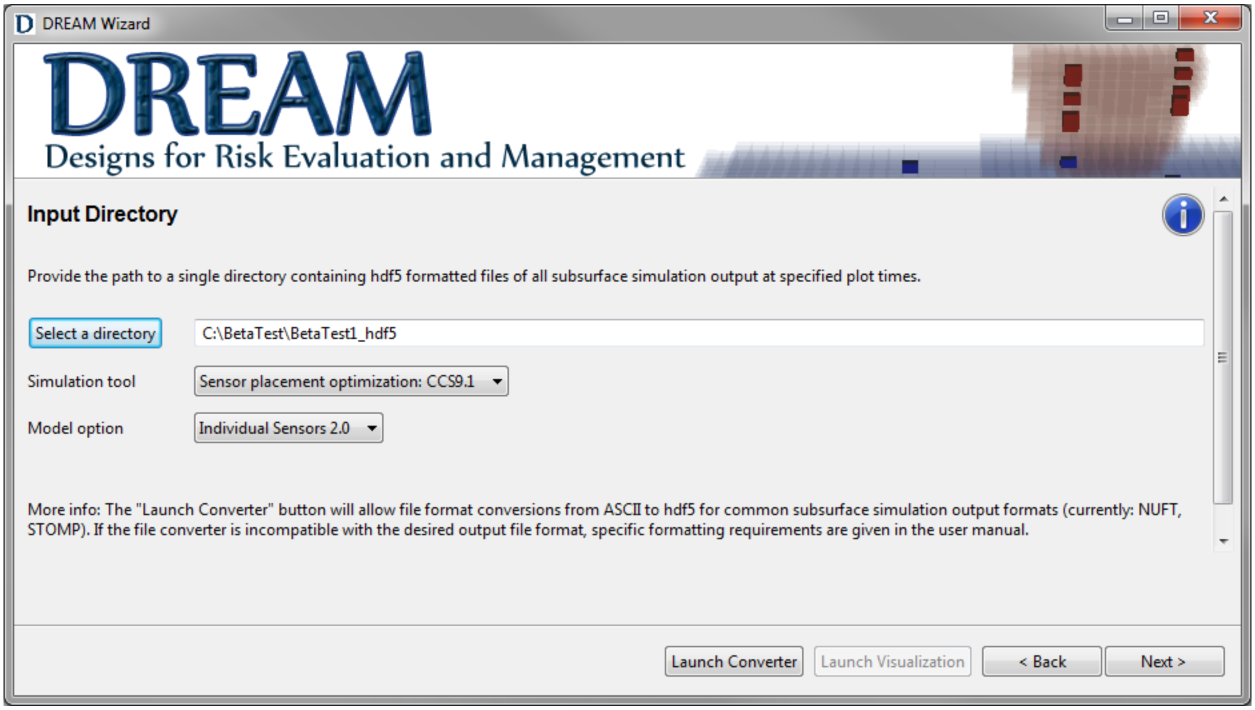


Figure 4: Input Directory Selection

To begin the example application, consolidate the BetaTest1_hdf5 and BetaTest2_hdf5 directories to BetaTest_hdf5. These directories were split for efficiency in uploading and downloading. From the DREAM Input Directory Window, navigate to the "BetaTest_hdf5" directory. Select *Next.*

3.1.3 Scenario Weighting

The Scenario Weighting window (Fig. 5) lists realizations by the naming convention used in the leakage simulation input files. If the user has prior knowledge of leakage probabilities or would like to choose to weight leakage scenarios unequally, they may do so in the Scenario Weighting window. 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 particular problem.

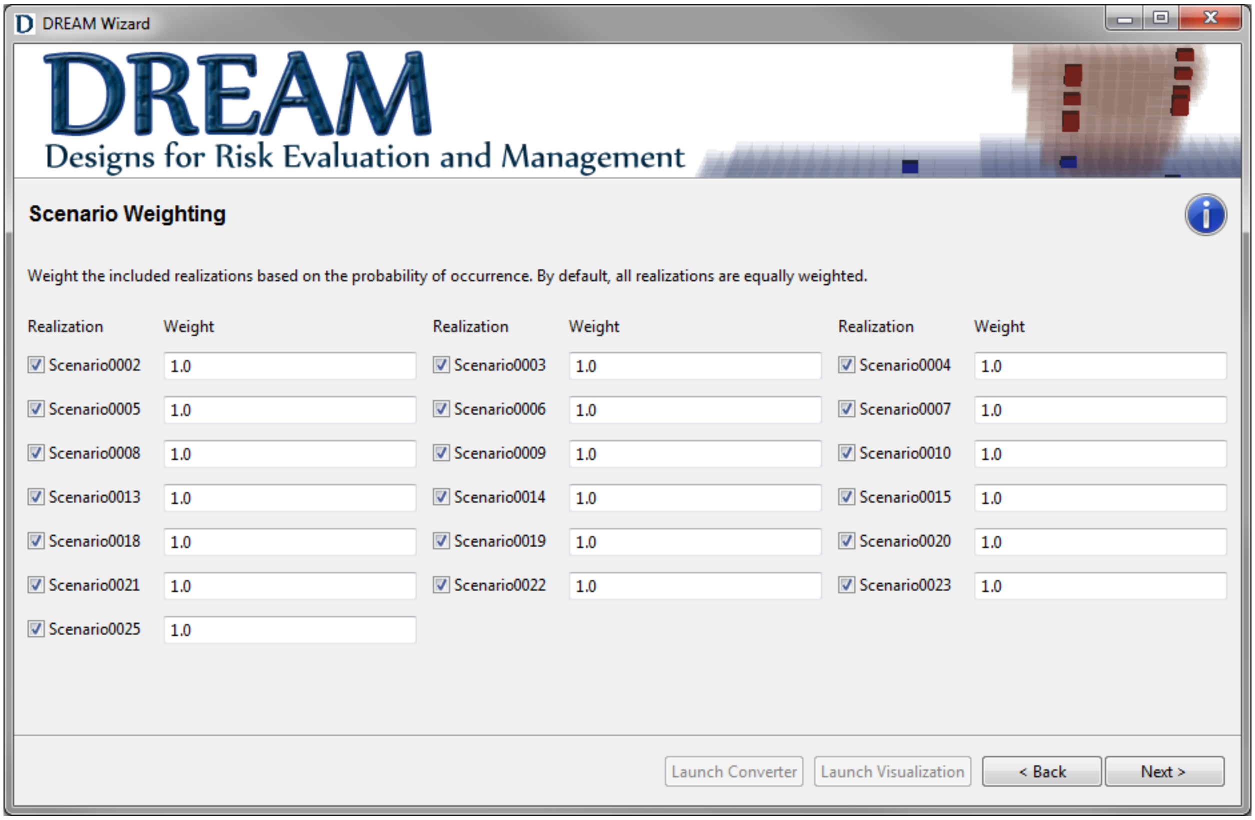


Figure 5: Scenario Weighting Window

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

3.1.4 Leakage Criteria for Monitoring Parameters

After reading through the directory of realization outputs, DREAM will generate a table of monitoring parameters that the user can select (Fig. 6). These parameters are specific to the included realizations. The selected monitoring parameters will be used in the optimization algorithm. The user may label what technology they will use to monitor each selected parameter in the “Alias for Monitoring Technology” box and then provide a realistic cost per monitoring technology if it is known; if not, the costs should be set equal. The detection criteria may be specified based on the relative change from initial conditions, absolute change from initial conditions, or a maximum or minimum threshold. If relative delta, absolute delta, or maximum threshold is selected, the given value and all values above are treated as detecting a leak. If minimum threshold is selected, that value and all values below are treated as detecting a leak.

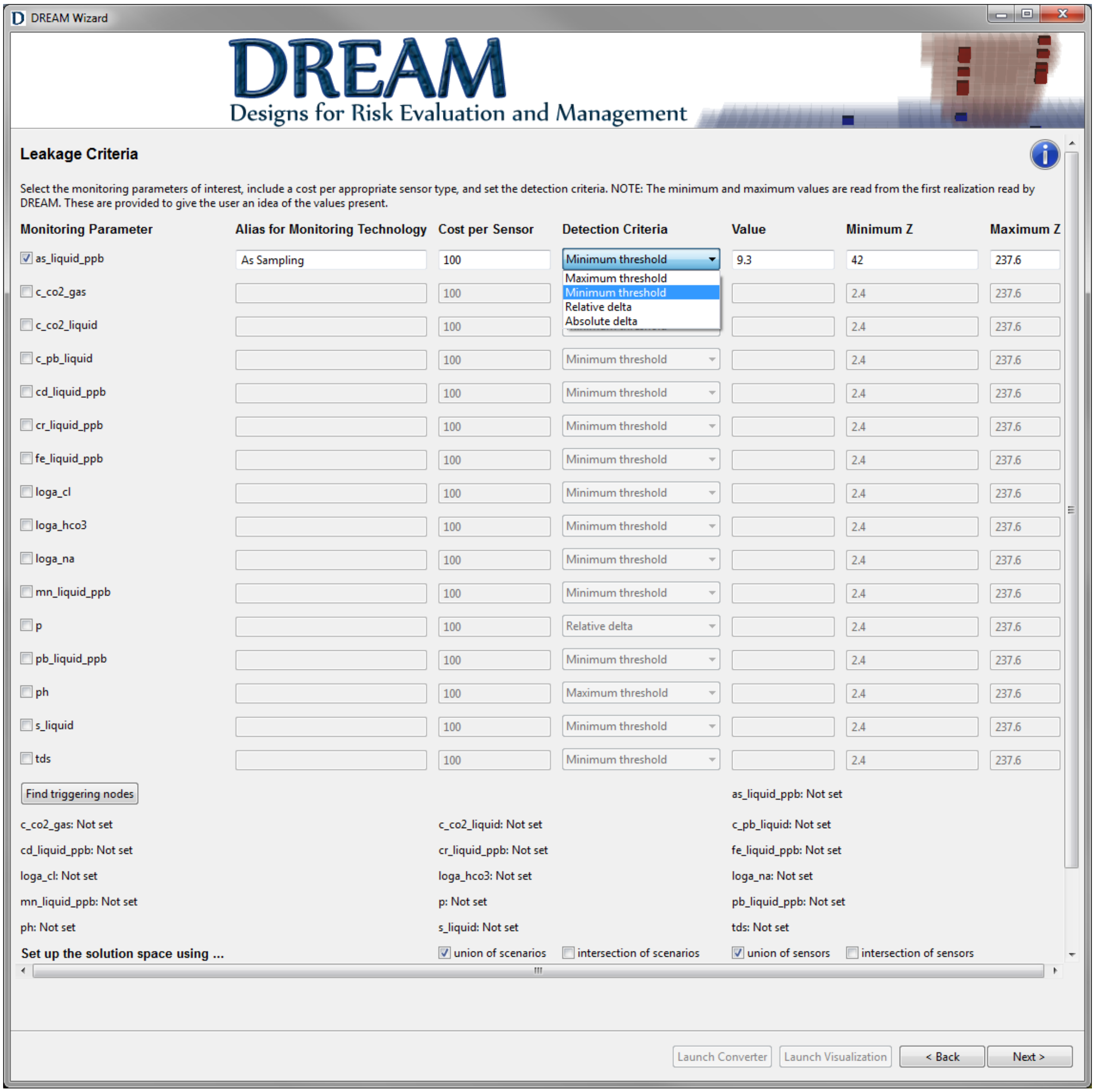


Figure 6: Leakage Criteria Window

For the example problem, select the listed monitoring parameters and enter in the following "no impact" criteria taken from Last et al. (2013) and Carroll et al. (2014) relating to arsenic, cadmium, chromium, lead, pH, and total dissolved solids in the High Plains Aquifer.

Table 2: Leakage Criteria Inputs

Monitoring Parameter	Cost per Sensor	Detection Criteria	Value	Minimum Z	Maximum Z
as_liquid_ppb	100	Minimum Threshold	9.3	42	237.6
cd_liquid_ppb	100	Minimum Threshold	0.25	42	237.6
cr_liquid_ppb	100	Minimum Threshold	3.9	42	237.6
pb_liquid_ppb	100	Minimum Threshold	0.63	42	237.6
pH	100	Maximum Threshold	6.5	42	237.6
tds	100	Minimum Threshold	1300	42	237.6

Leave the solution space settings to the union of scenarios and union of sensors. The *Find triggering node* button will read through all the realization files and select the nodes (or elements) that meet the detection criteria. Select *Find triggering nodes*. The following values should appear next to each selected parameter type at the bottom of the page.

Table 3: Triggering Nodes

Monitoring Parameter	Total Triggering Nodes
as_liquid_ppb	6
cd_liquid_ppb	28
cr_liquid_ppb	52
pb_liquid_ppb	35
pH	1307
tds	320

Note: While the *Find triggering nodes* button is working, a red box appears to the right of the progress bar. Pressing this box cancels the process before completion. This may be necessary if unphysical or incorrect values are entered for leakage criteria, sending DREAM into an excessively long process.

Select *Next*.

3.1.5 Minimum Triggered Monitoring Devices

The Detection Criteria window (Fig. 7) prompts the user to specify how many monitoring devices must be triggered to signify a leak has occurred. A leak may be defined in two ways. DREAM reads input provided as an "or"-statement, where it will determine a leak has occurred if (1) the specified value for any specific parameter has been met *or* (2) the overall number of locations exceeding the detection criteria is equal to or greater than the provided value. This allows for various combinations of monitoring device configurations to be tested.

Enter "1" for all minimum required number of sensors for all fields. Select *Next*.

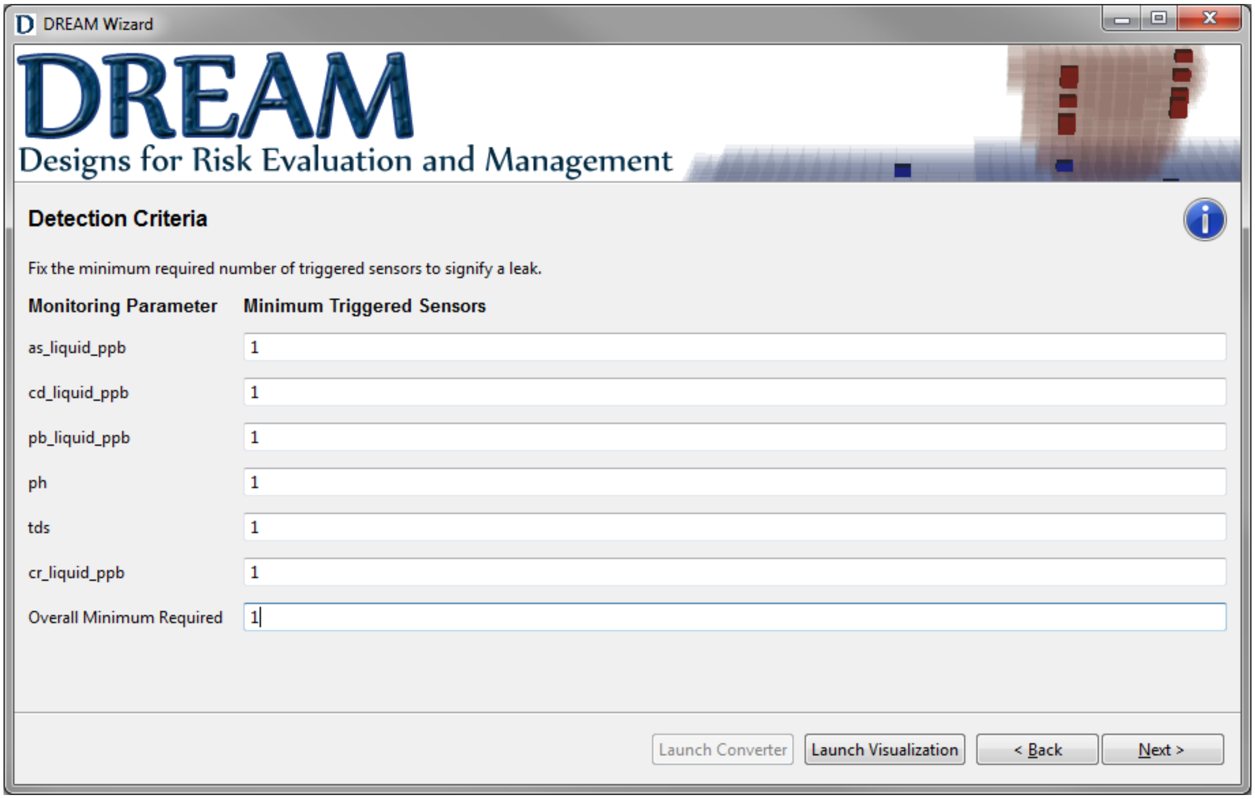


Figure 7: Detection Criteria Window

3.1.6 <u>Configuration Settings</u>

The configuration settings specify hard constraints for the optimization algorithm (Fig. 8). The solutions may not exceed the maximum cost or the maximum number of wells defined. The user must be careful to provide a high enough cost to meet the specified minimum requirements given in the previous window. The "Add starting point" field is the coordinate where the algorithm begins searching for new monitoring device placement. The *Use average time to detection* checkbox averages the time to first detection of leakage across all realizations using the same monitoring configuration.

Note: DREAM assumes that wells span the entire z-axis of simulation grids and multiple detection devices may be placed within a single well.

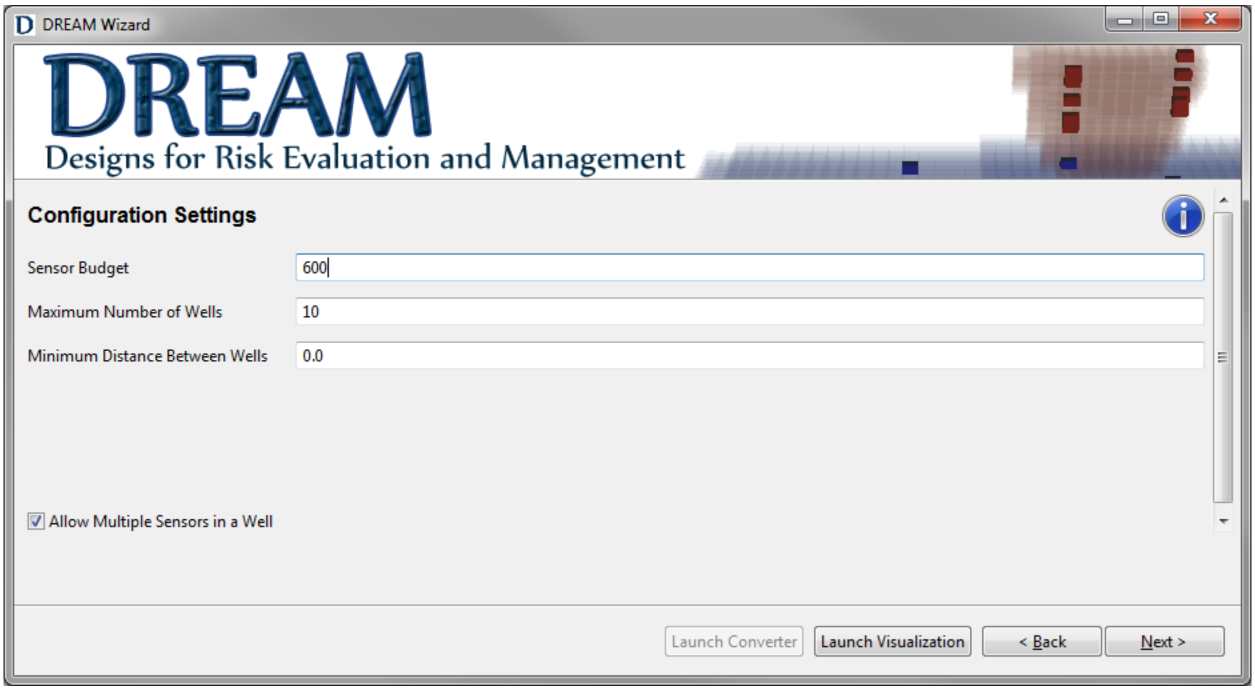


Figure 8: Configuration Settings

On the Configuration Settings page, enter "600" for the initial sensor budget. This strategy begins testing with the most conservative budget. Enter "6" for the maximum number of wells. Leave the "average time to detection" selected; this option optimizes based on the average minimum time to detection across all included realizations. Select *Next.*

3.1.7 <u>Exclude Locations</u>

The user may need 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 (Fig. 10Figure 9).

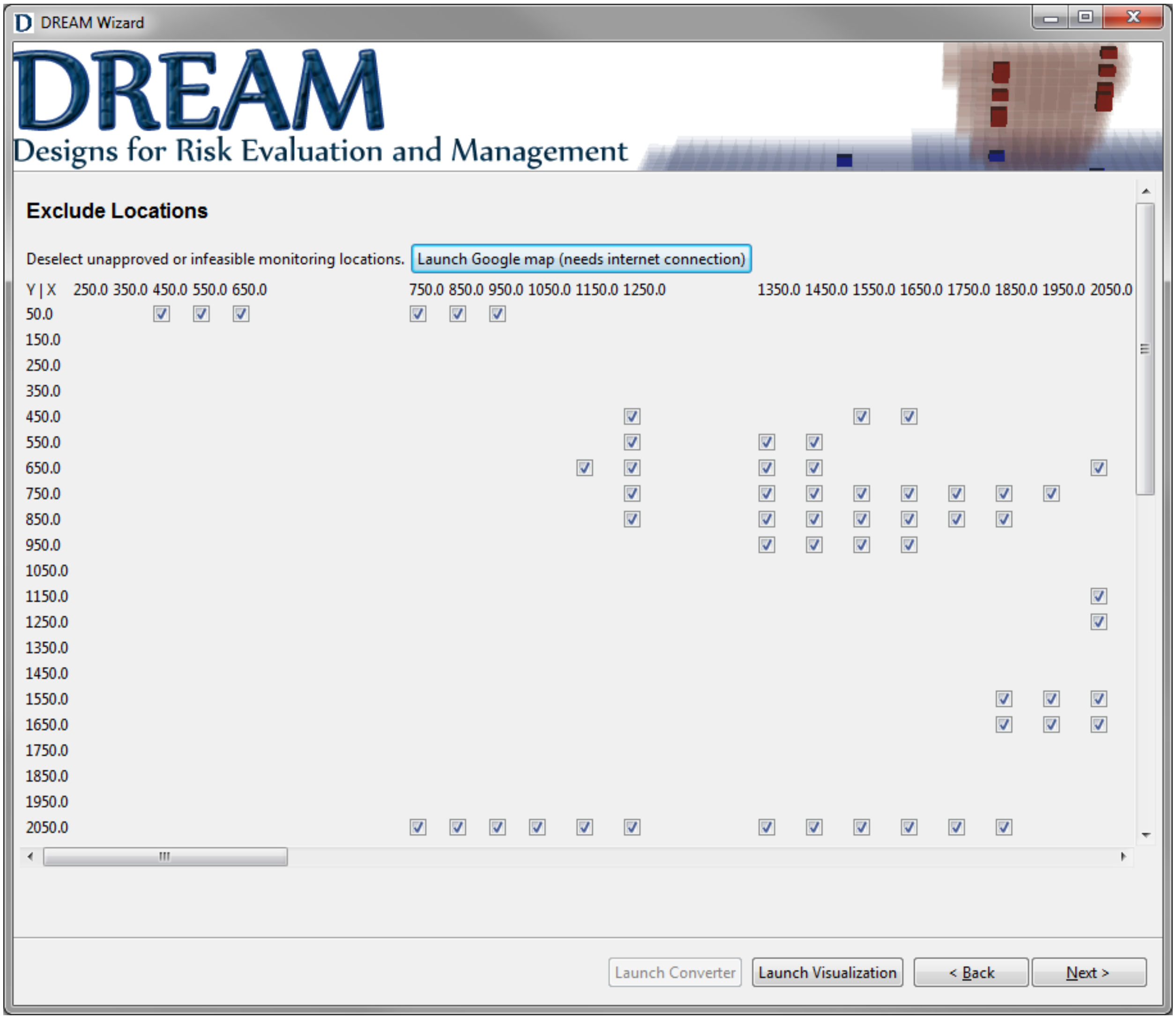


Figure 9: Exclude Locations by Node

If the user has an internet connection, the *Launch Google map* button will pop-up a map (Fig. 11) which the user can use to overlay the realization grid over the location of interest. The input coordinates should align with the upper left corner of the simulation grid (in plan view). The toolbar allows the user to zoom in or out and pivot the google map to achieve the appropriate view. Nodes that exceed one or more of the threshold criteria are shown in gray and may be de-selected by clicking on the (x, y) location.

Note: The image shown in Figure 10 is an arbitrary demonstration of this feature. It is *not* a location above a current CO_2 storage site.

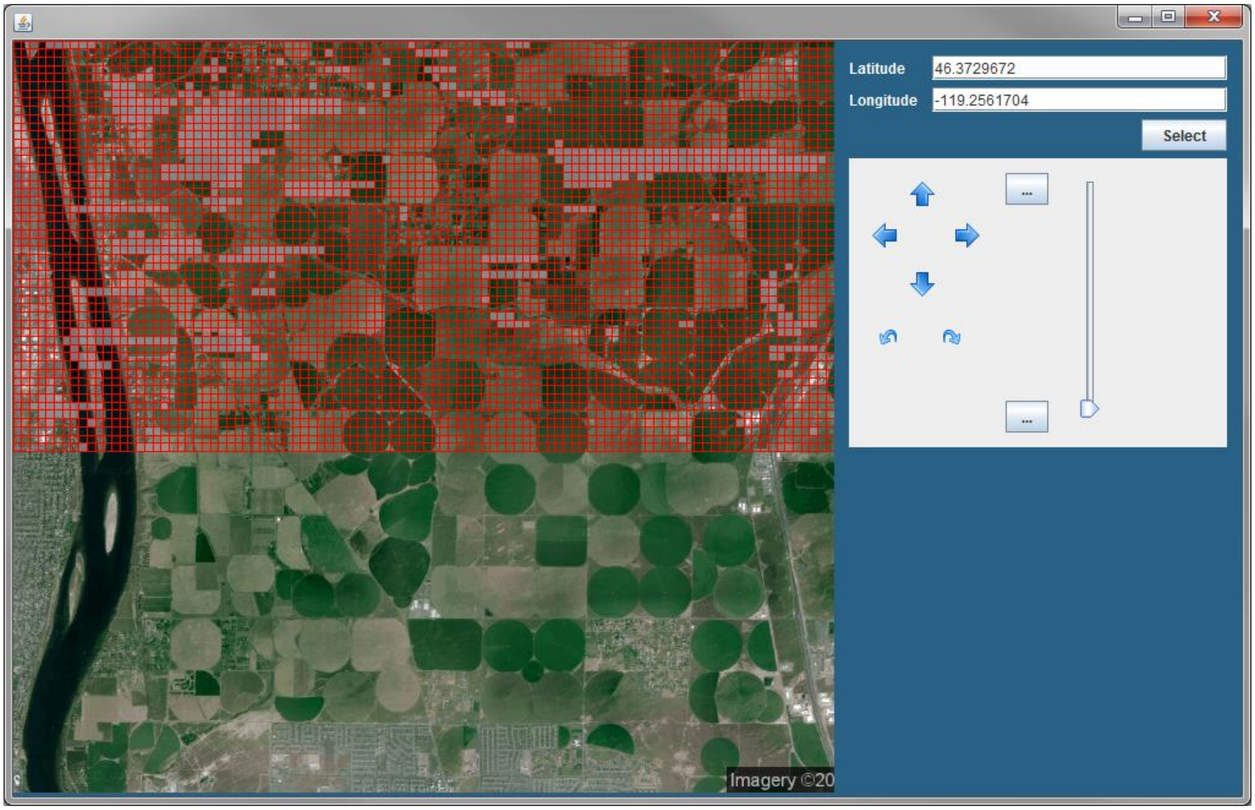


Figure 10: Google Map and Toolbar

Leave all the grayed out boxes included and exit out of this window. Select *Next*

3.1.8 Run DREAM

The "Run DREAM" window provides a summary of the scenario set and user-specified constraints. After reviewing run summary, the user must provide an output directory to store the resulting .csv files (Fig. 12Figure 11).

The *Best TTD Possible per Sensor-type* button allows the user to generate a summary of the average times to detection for all scenarios and all sensor-types individually and as a whole. The "Weighted percent of scenarios that are detectable" is also presented, giving the user an idea for how many of the leakage scenarios read into DREAM had leaks detected according to the leakage criteria specified. The algorithm behind this button assumes an unlimited budget and an unlimited number of wells to achieve this goal. In other words, a monitoring point is placed in every node in the solution space; therefore, the results give no indication of optimal monitoring configurations. The purpose of this button is to allow the user to have an understanding of the problem before running the iterative procedure. Results identify the best possible time to detection and highest percent of scenarios detecting a leak possible.

The *Run Iterative Procedure* button will run the simulated annealing optimization algorithm the number of times specified on the number of configurations specified.

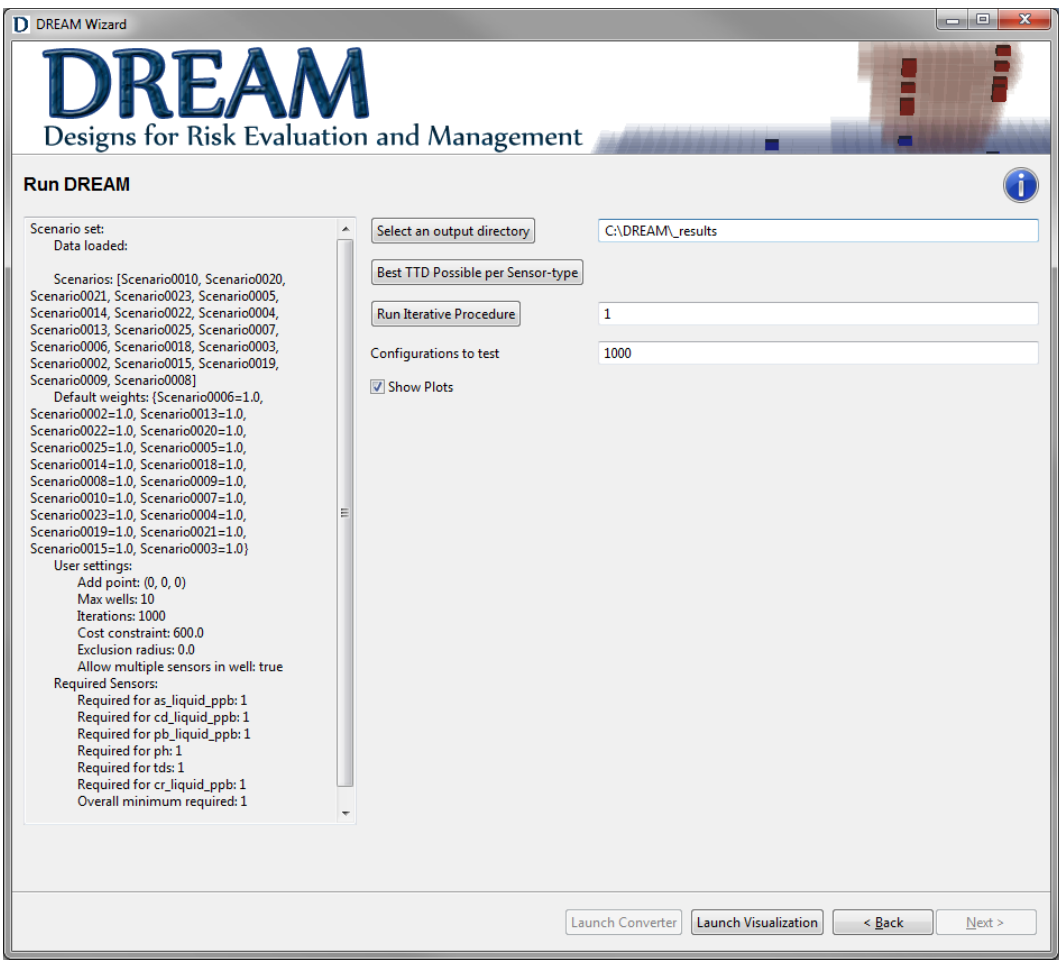


Figure 11: Run Optimization Window

For the example problem, enter an output directory for the example results files then follow this progression:

a. Choose *Best TTD Possible per Sensor-type* to view a summary of the lowest possible times to leakage detection. Compare your results to the copy found in BetaTest_Results_bak. Note the minimum time to leakage detection overall is 24.75 years and the weighted percent of scenarios that are detectable is 84.21%. These are the properties of the best possible configurations.

b. Next, choose to run the procedure one time for 1,000 configurations. Select *Run Iterative Procedure*.

   While DREAM is running, two pop-up windows display the optimization performance. The first is the 3-D Multi-Domain Viewer, which dynamically updates to show the current and best configurations being tested (Fig 13).

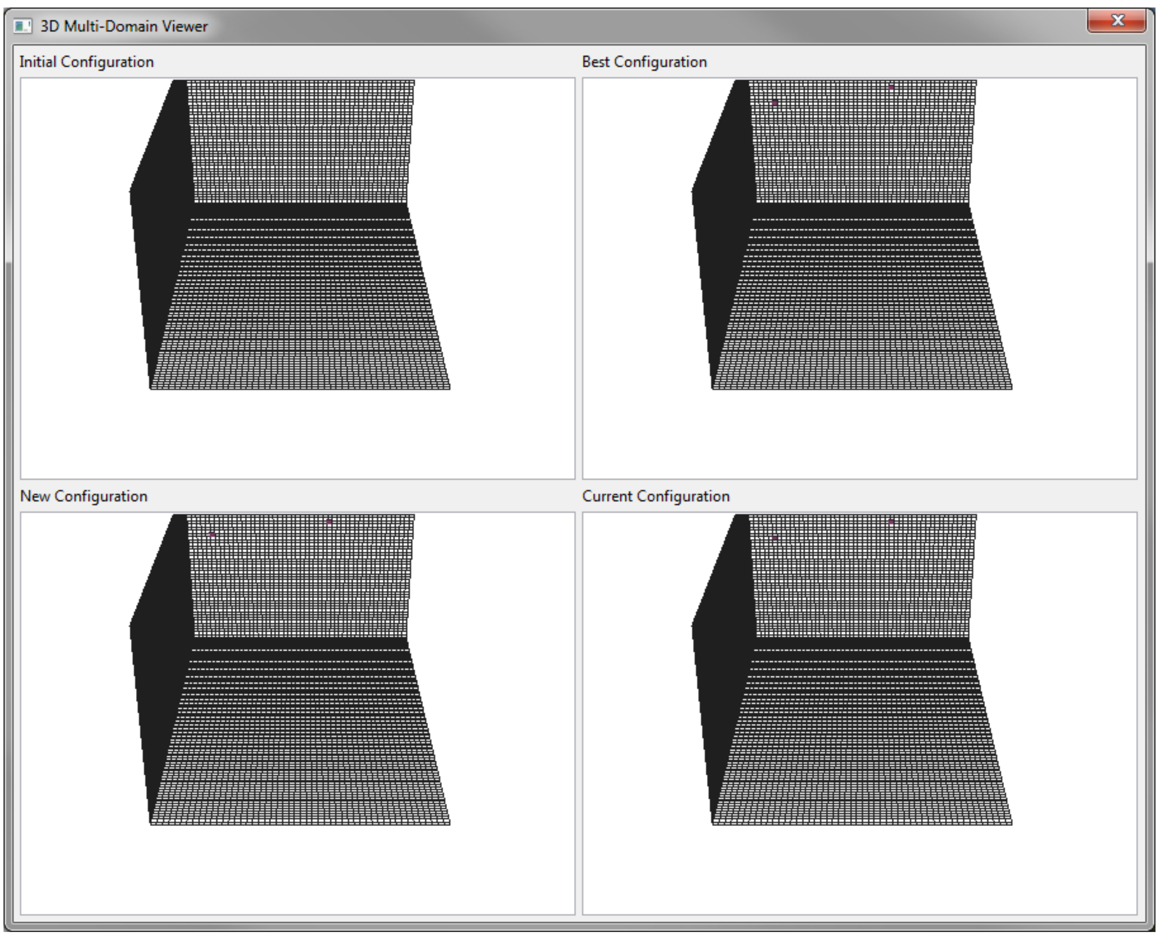


Figure 12: Tested configurations during optimization.

The second window to pop-up shows the performance of the iteration procedure through four plots (14). The upper-left plot shows the running first time to detection (TTD) of the newest configuration for each simulated annealing iteration, or new monitoring configuration. The upper-right plot shows the running TTD of the best configuration, or configuration with the lowest TTD. The bottom-left plot shows the TTD of each realization, or scenario, across all configurations. The bottom-right plot shows the percent of realizations, or scenarios, in which the leak was detected as new configurations are being tested.

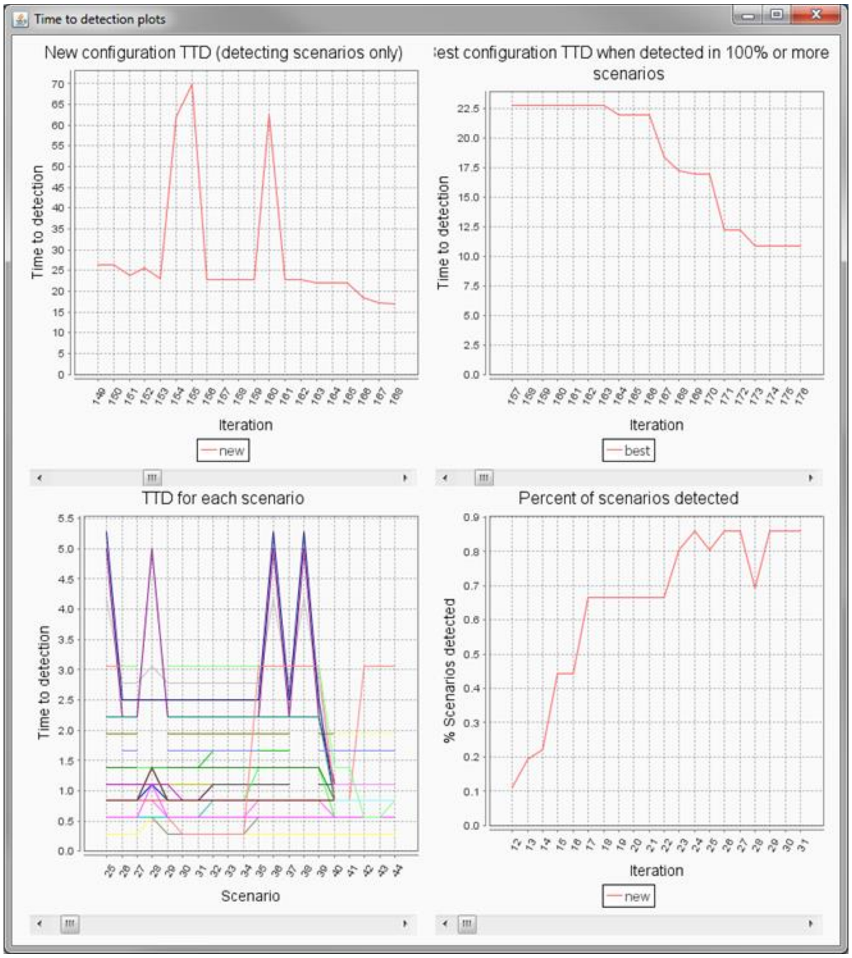


Figure 13: Algorithm performance plots.

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

best_configurations.csv

One of the most useful output files will be 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 time to detection (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 cost of the well configuration, the volume of aquifer degraded at the time of detection and the monitoring parameter and sensor locations of the best configuration(s).

Note: The cost of the well configuration and volume of aquifer degraded are under development. Current cost estimates are hardwired to assume $20 USD/ft well completion. The total length of each well spans from the surface to the deepest sensor location. These values are included to provide a ranking in circumstances where multiple configurations are identified with the same TTD.

Only detecting sensor locations are displayed. This is important to note in cases where the initial sensor budget is in excess of the number of sensors that actually detect.

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: There will likely be more than one configuration that provides the lowest TTD.

Open your results directory and compare your output files to those found in BetaTest_Results_6_1_1000_bak.

Note: DREAM_v1 is a special beta testing version where the random seeds usually included in the simulated annealing procedure have been removed in order to generate reproducible results.

c. The percent of scenarios where the leak was detected (found in best_configurations.csv) is much lower than the best possible (best_ttd_table.csv). Increase the iterative procedures to 10 to test a wider variety of configurations. Leave all else unchanged and close the current results files before re-running. Compare your new output files to those found in BetaTest_Results_6_10_1000_bak.

Use the objective_summary_best.csv to make plots of Iterations vs. TTDs for each scenario and Iterations vs. % Scenarios Detected.

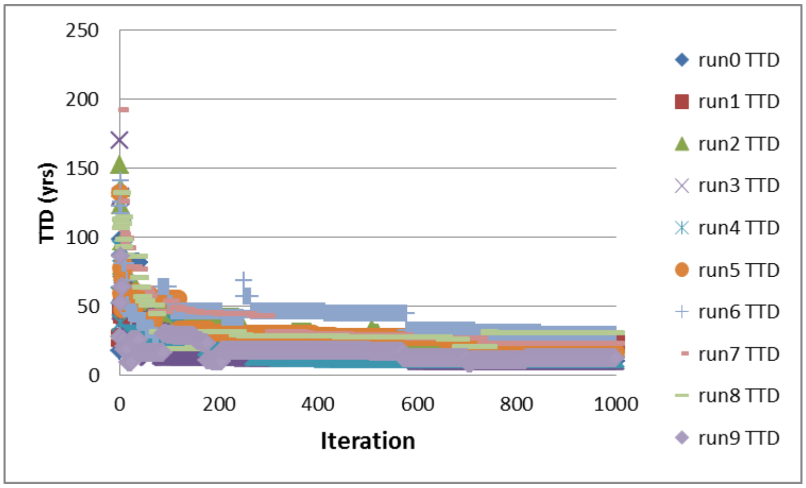


Figure 14: TTD performance for up to 6 sensors.

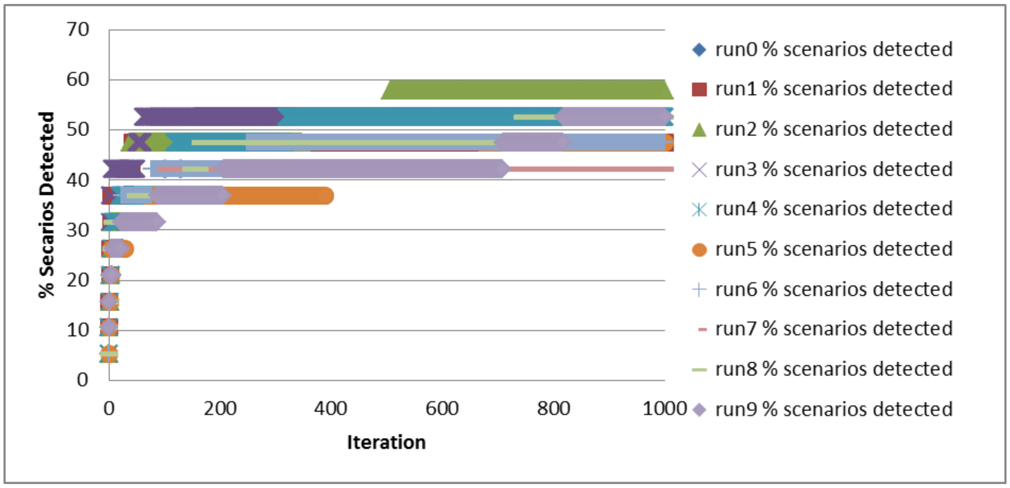


Figure 15: Detection performance for up to 6 sensors.

d. The percent of scenarios where the leak was detected is slightly higher but still much lower than the best, Select *Back* twice and increase the sensor budget to 1200 and the maximum number of wells to 12 for more coverage of the domain. Select *Next* twice.

   Update the output directory again. Choose to run the iterative procedure 10 times and test 1000 configurations. Close the current results files before re-running. Compare your new output files to those found in BetaTest_Results_12_10_1000_bak.

   Use the objective_summary_best.csv to make new plots of Iterations vs. TTDs for each scenario and Iterations vs. % Scenarios Detected.

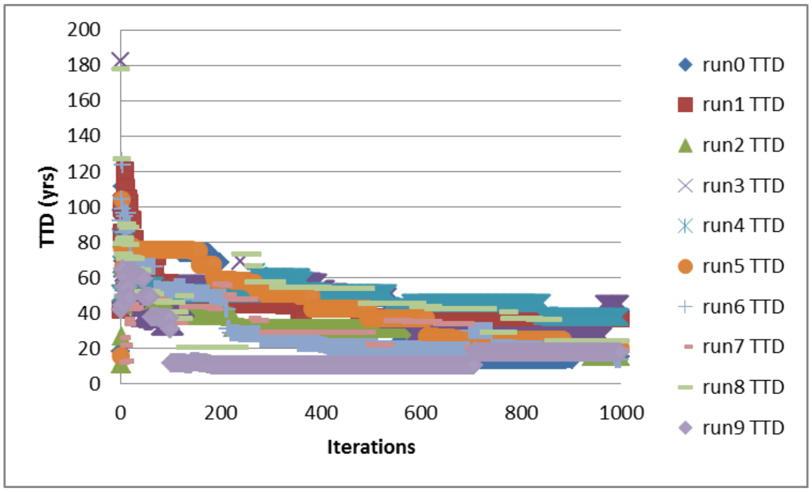


Figure 16: TTD performance for up to 12 sensors and 1,000 configurations.

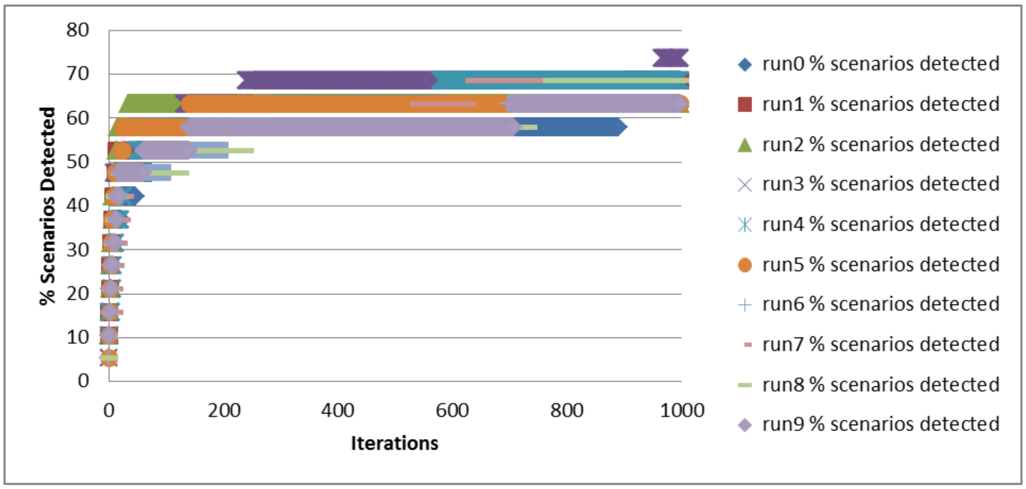


Figure 17: TTD performance for up to 12 sensors and 1,000 configurations.

e. The percent of scenarios where the leak was detected is significantly higher but the performance plots (Figures 20 and 21) show that a higher number of iterations are necessary for convergence. Increase the number of configurations tested to 10,000. Leave the number of iterative procedures at 10. Close the current results files before re-running.

   Note: This step will likely take several minutes.

   Compare your new output files to those found in BetaTest_Results_12_10_10000_bak.

   Use the objective_summary_best.csv to make new plots of Iterations vs. TTDs for each scenario and Iterations vs. % Scenarios Detected.

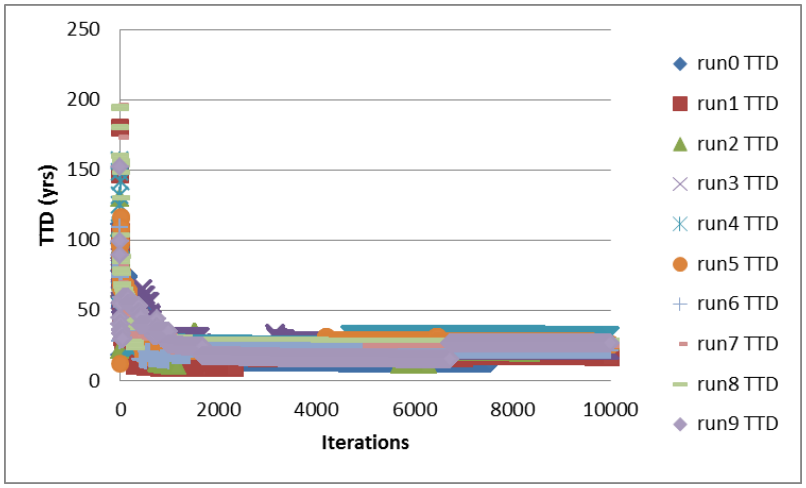


Figure 18: TTD performance for up to 12 sensors and 10,000 configurations.

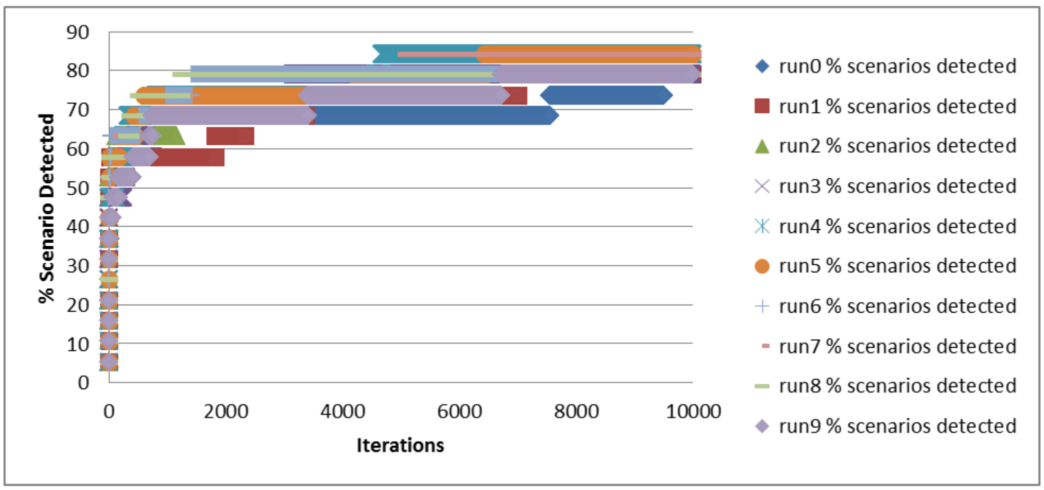
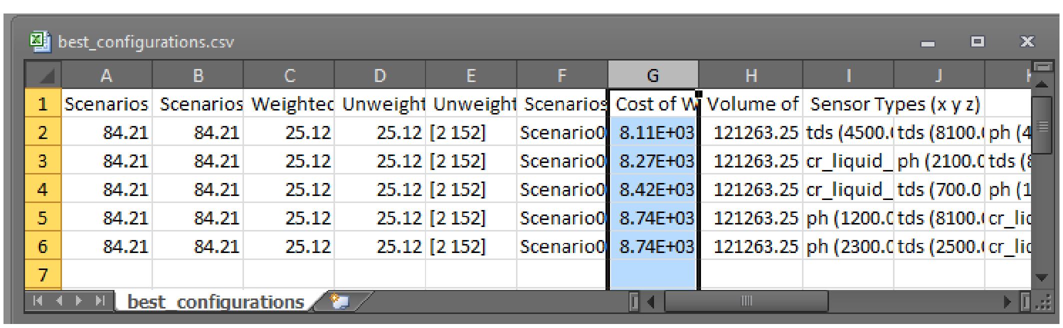


Figure 19: TTD performance for up to 12 sensors and 10,000 configurations.

The performance plots appear smooth and the 6 new solutions are all very close to the best possible solution. Note how they are ranked by "Cost of Well Configuration", where the top configurations require a shallower sampling configuration. In this case, the volume of aquifer degraded was the same across all of the best configurations.



best_configurations.csv

	A	B	C	D	E	F	G	H	I	J
1	Scenarios	Scenarios	Weightec	Unweight	Unweight	Scenarios	Cost of W	Volume of	Sensor Types (x y z)	
2	84.21	84.21	25.12	25.12	[2 152]	Scenario0	8.11E+03	121263.25	tds (4500.(	tds (8100.(ph (4
3	84.21	84.21	25.12	25.12	[2 152]	Scenario0	8.27E+03	121263.25	cr_liquid_	ph (2100.0 tds (8
4	84.21	84.21	25.12	25.12	[2 152]	Scenario0	8.42E+03	121263.25	cr_liquid_	tds (700.0 ph (1
5	84.21	84.21	25.12	25.12	[2 152]	Scenario0	8.74E+03	121263.25	ph (1200.0	tds (8100.(cr_lic
6	84.21	84.21	25.12	25.12	[2 152]	Scenario0	8.74E+03	121263.25	ph (2300.0	tds (2500.(cr_lic
7										

best_configurations

Figure 20: Best monitoring configurations for up to 12 sensors and 1,000 configurations.

3.2 PRE-PROCESSING DATA

DREAM comes with the DREAM HDF5 Converter tool (Fig. 23Figure 23: DREAM File Converter Tool), 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 realizations, or scenarios. Once the converter has translated all the ASCII files, the user is able to select the monitoring parameters of interest as well as the realizations and time steps of interest.

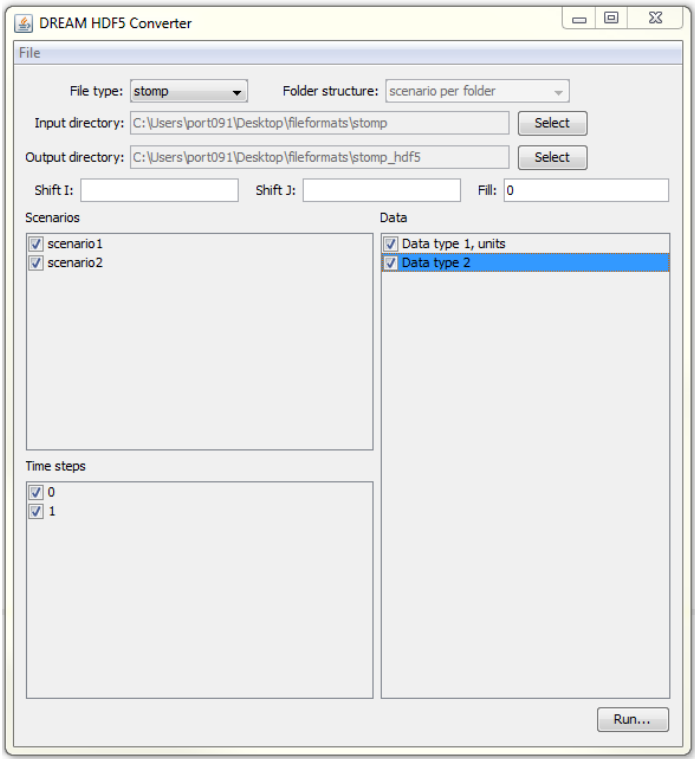


Figure 2**3:** DREAM File Converter Tool

3.2.1 <u>STOMP Data</u>

The DREAM file converter will accept most output types from STOMP. The required directory hierarchy is "input directory name\specific realizations\plot files". Detailed information follows.

Folder structure

For STOMP output we expect a folder with sub folders. 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_output/scenario1/plot.1
stomp_output/scenario1/plot.2
stomp_output/scenario2/plot.1
stomp_output/scenario2/plot.2

File example: stomp_output/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
4.5 4.5 4.5 4.5 4.5 4.5 4.5 4.5

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

3.2.2 NUFT/NTAB Data

The plot files must be sorted to directories containing like monitoring parameters across all realizations if the given plot files were generated by NUFT and given in NTAB format.

Folder Structure

In this case, the directory hierarchy is "input directory name\plot files for like parameters across all simulations," and the converter tool must be used multiple times (once for each parameter of interest). The NUFT HDF5 plot files must then be manually consolidated to one directory for DREAM to read.
ntab/scenario1.data_type_1.ntab
ntab/scenario1.data_type_2.ntab
ntab/scenario2.data_type_1.ntab
ntab/scenario2.data_type_2.ntab

File example: ntab/scenario1.data_type_1.ntab

This file contains data for all time steps of data type 1. All data including x, y, z is cell centered. **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

3.2.3 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/scenario1.tecplot
tecplot/scenario2.tecplot

File example: tecplot/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

3.2.4 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.

Folder structure:

/stomp

/stomp_hdf5/**Scenario1.h5**

/stomp_hdf5/**Scenario2.h5**

File example:

/stomp_hdf5/**Scenario1.h5**

The hdf5 files can be viewed with HDFView.

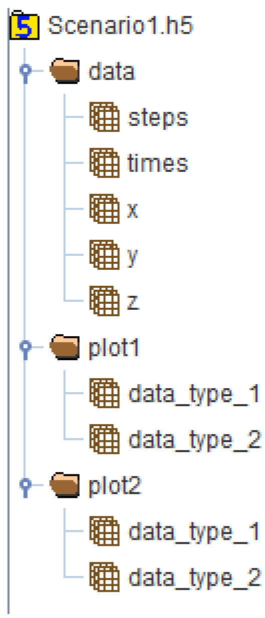


Figure 24: HDFView of DREAM input file structure.

Each scenario will contain an element called data that contains metadata about the scenario; the grids x, y, and z coordinates, the time steps and their matching times. There will also be an element for each time step containing data for each data type at that time step.

3.3 RANGE OF DREAM APPLICABILITY AND LIMITATIONS

DREAM version 1.0 is designed as a tool for additional analysis of subsurface CO_2 leakage simulations; however, it can be applied to any data set of the format 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.
- There is only one monitoring device, or sensor, per monitoring parameter. Similarly, there is only one monitoring parameter associated with each monitoring device.
- The cost of monitoring devices is treated as a one-time fee, as opposed to incurring costs during operation.
- The total cost of the monitoring configuration is set as a hard constraint. Future versions will minimize cost as a secondary objective.
- The monitoring configuration results produced by the simulated annealing algorithm are a function of the realizations provided to DREAM as well as the number of iterative procedures and number of configurations tested. Users are encouraged to vary each these parameters to determine the sensitivity of their results.
- DREAM was developed for use on PC; therefore the speed of the tool is dependent on the capability of the specific PC to handle the size of the datasets.
- The interactive map feature (Section 3.1.7) cannot work without an internet connection.

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4. REFERENCES

Carroll, S.A., Keating, E., Mansoor, K., Dai, Z., Sun, Y., Trainor-Guitton, W., Brown, C. and Bacon, D., 2014. Key factors for determining groundwater impacts due to leakage from geologic carbon sequestration reservoirs. *International Journal of Greenhouse Gas Control*, *29*, pp.153-168.

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

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

Yonkofski, C.M., Gastelum, J.A., Porter, E.A., Rodriguez, L.R., Bacon, D.H. and Brown, C.F., 2016. An optimization approach to design monitoring schemes for CO2 leakage detection. *International Journal of Greenhouse Gas Control*, *47*, pp.233-239.

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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).

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