

Final Scientific/Technical Report

Development of a Software Framework for System-Level
Carbon Sequestration Risk Assessment

Issued April 15, 2013
For the Period October 1, 2009 – February 28, 2013

WORK PERFORMED UNDER AGREEMENT

DE-FE0001164

SUBMITTED BY

GoldSim Technology Group LLC
22500 SE 64th Place, Suite 240
Issaquah, WA 98027

PRINCIPAL INVESTIGATOR

R. Ian Miller
Tel: 425-295-6985
Fax: 425-642-8073
imiller@goldsim.com

SUBMITTED TO

U.S. Department of Energy
National Energy Technology Laboratory

Program Manager: Brian Dressel
Brian.Dressel@NETL.DOE.GOV

Final Scientific/Technical Report

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

ABSTRACT

This report summarizes work carried out over the period from October, 2009 through February 2013. The work was carried out by GoldSim Technology Group LLC, supported by Los Alamos National Laboratory, under the US Department of Energy's National Energy Technology Laboratory (NETL) program.

The overall purpose of this project was to identify, evaluate, select, develop, and test a suite of enhancements to the GoldSim software program, in order to make it a better tool for use in support of Carbon Capture and Sequestration (CCS) projects. The GoldSim software is a foundational tool used by scientists at NETL and at other laboratories and research institutions to evaluate system-level risks of proposed CCS projects.

Four specific goals were identified, with each being addressed through one project task (project tasks 2 through 5, respectively):

- Task 2. Enhanced simulation of injection and release risks.
- Task 3. Enhanced comparison of alternative scenarios and approaches.
- Task 4. Enhanced modeling of programmatic risk.
- Task 5. Enhanced modeling of process flows.

The primary product of the project was a series of successively improved versions of the GoldSim software, supported by an extensive User's Guide. These enhancements were tested by scientists at Los Alamos National Laboratory, and several of the enhancements have already been incorporated into the CO₂-PENS sequestration model.

Final Scientific/Technical Report

TABLE OF CONTENTS

EXECUTIVE SUMMARY	4
A. INTRODUCTION	6
What is GoldSim?	6
Why Were Changes Needed?	6
B. TASK 2: NEW CAPABILITIES FOR HIGH PERFORMANCE COMPUTATIONS AND MANIPULATION OF LARGE MULTI-DIMENSIONAL ARRAYS	8
C. TASK 3: SCENARIO ANALYSIS AND MODEL REUSE CAPABILITIES	13
D. TASK 4: SIMULATION OF PROGRAMMATIC RISK	18
Monte Carlo Results Analysis	19
Bayesian Updating	20
Decision Analysis	21
Task 4 Accomplishments	23
E. TASK 5: MATERIAL BALANCE AND NETWORK FLOW SIMULATION	24
Proposed Solution Approach	24
Cell Element Media Store Option	24
User-Specified Media Amounts Option	25
Media Source Option	25
Media Sink Option	25
Media Router Option	26
“Clean” Flows	26
Flow Network Solution	27
F. LOS ALAMOS TESTING AND EVALUATION	28
G. SUMMARY AND CONCLUSIONS	29

Final Scientific/Technical Report

EXECUTIVE SUMMARY

This report summarizes work carried out over the period from October, 2009 through February 2013. The work was carried out by GoldSim Technology Group LLC, supported by Los Alamos National Laboratory, under the US Department of Energy's National Energy Technology Laboratory (NETL) program.

The overall purpose of this project was to identify, evaluate, select, develop, and test a suite of enhancements to the GoldSim software program, in order to make it a better tool for use in support of Carbon Capture and Sequestration (CCS) projects. The GoldSim software is a foundational tool used by scientists at NETL and at other laboratories and research institutions to evaluate system-level risks of proposed CCS projects.

Four specific goals were identified, with each being addressed through one project task (project tasks 2 through 5, respectively):

- Task 2. Enhanced simulation of injection and release risks.
- Task 3. Enhanced comparison of alternative scenarios and approaches.
- Task 4. Enhanced modeling of programmatic risk.
- Task 5. Enhanced modeling of process flows.

The primary product of the project was a series of successively improved versions of the GoldSim software, supported by an extensive User's Guide.

The following capabilities were developed under Task 2:

- Increased internal buffer sizes to support arbitrarily large result arrays.
- Auto-ID suggestion capability to assist users constructing complex equations.
- Improved ability to model date-time based projects.
- Improved integration with Excel.
- Addition of a programmable 'Script' element.
- Improved ability to control calculation sequence for complex models.

The following capabilities were developed under Task 3:

- A powerful capability for a user to define multiple 'Scenarios' for their model, to simulate these scenarios independently, and to compare and contract the results for the different scenarios..

The following capabilities were developed under Task 4:

- Enhanced presentation and reporting for calendar-based models.

Final Scientific/Technical Report

- Enhanced analysis tools for analyzing results of Monte Carlo simulations.
- Enhanced reporting of milestone success probabilities and of the probabilities of achieving milestones on time.
- Simulated Bayesian updating capability to represent project decisions as project uncertainties are reduced over time.
- Decision Analysis element providing Multiattribute utility analysis capabilities to compare outcomes of alternative project designs, including support for Monte Carlo model results.

The following capabilities were developed under Task 5:

- A powerful and flexible capability to simulate material flows through complex networks..

The primary product of the project was a series of successively improved versions of the GoldSim software, supported by an extensive User's Guide. All of the enhancements were tested by scientists at Los Alamos National Laboratory, and several of the enhancements have already been incorporated into the CO₂-PENS sequestration model.

Final Scientific/Technical Report

A. INTRODUCTION

This report summarizes work carried out GoldSim Technology Group LLC, supported by Los Alamos National Laboratory, under the US Department of Energy's National Energy Technology Laboratory (NETL) program.

The overall purpose of this project was to identify, evaluate, select, develop, and test a suite of enhancements to the GoldSim software program, in order to make it a better tool for use in support of CCS projects. Four specific goals were identified, with each being addressed through one project task (project tasks 2 through 5, respectively):

- Task 2. Enhanced simulation of injection and release risks.
- Task 3. Enhanced comparison of alternative scenarios and approaches.
- Task 4. Enhanced modeling of programmatic risk.
- Task 5. Enhanced modeling of process flows.

The primary product of the project was a series of successively improved versions of the GoldSim software, supported by an extensive User's Guide. This report documents the development process used for each of the four tasks, but does not document specific technical results as these are all described in the User's Guide.

The role of Los Alamos National Laboratory was to help identify useful enhancements and to evaluate prototype versions of the enhancements.

What is GoldSim?

GoldSim is a powerful and flexible platform for visualizing and dynamically simulating nearly any kind of physical, financial or organizational system. It is a graphical computer program for carrying out dynamic, probabilistic simulations. It is specifically designed to simulate risks and uncertainties in complex systems.

A model in GoldSim is built in an intuitive manner by drawing a picture (an influence diagram) of a system. In a sense, GoldSim is like a "visual spreadsheet" that allows you to graphically create and manipulate data and equations.

GoldSim software is built using a modular framework that allows each user to customize their GoldSim package to provide exactly the functionality they need. Various modules provide additional features or specialized functionality for particular applications.

Why Were Changes Needed?

GoldSim is a software application based on a generic framework that can be used to simulate almost any kind of system. While it is powerful and flexible it does not necessarily provide optimal tools for solving the specific challenges of system-level Carbon sequestration risk

Final Scientific/Technical Report

assessment. GoldSim was originally designed and developed for long-term safety analyses of nuclear waste disposal, and has subsequently been adapted to a wide range of engineering applications. The primary objective of this development effort was adapting and significantly extending the existing probabilistic simulation framework for the specifics of modeling and simulating carbon capture and storage.

Final Scientific/Technical Report

B. TASK 2: NEW CAPABILITIES FOR HIGH PERFORMANCE COMPUTATIONS AND MANIPULATION OF LARGE MULTI-DIMENSIONAL ARRAYS

Task Description:

The Recipient shall improve the ability of the GoldSim framework to model subsurface technical risks associated with the injection and subsequent release and transport of CO₂ in geologic formations. These modifications shall involve providing better support for intensive numerical computations and manipulation of large multidimensional arrays.

A preliminary review of GoldSim's capabilities for large models identified a potential for improvement in the following general areas:

- Large outputs: CCS models often “map” a model on geographical locations using 2d arrays with dozens or more grid points in each direction. In GoldSim they are represented as matrix type outputs that consist of hundreds, thousands or even more individual outputs. These require a significant amount of memory and processing, and potentially could be significantly simplified.
- Complex equations may require better formula editing capabilities, to assist the user in constructing and verifying their logic.
- Array type internal functions and expressions may be slow when solved sequentially.
- Solving many Monte Carlo realizations sequentially may be slow, yet distributed processing over a network may not be feasible. Locally distributed solutions using multi-core processors may be valuable.
- Large results: History results are (optionally) stored for each output at each plot point (designated time point at which the model is updated) in each history saving realization. For example: a single simulated result value (50x40 matrix output) of a Monte Carlo simulation running 100 realizations (saving all histories) on a monthly time step for 10 years requires about 96 MB of memory:
How best to manage results? How should the user select which results to save? How to report what is saved (i.e. how does the user know what has been selected)? What about result export, analysis, post-processing? Is more than 3 GB of model memory required (i.e. 64-bit GoldSim)?
- Generic data import (from spreadsheets into Data, Table and Time Series elements) may need to be optimized to be fast, automatic and on demand.
- External processing and interfacing capabilities may be limited by supported data types (most basic intrinsic types) and runtime requirements (native 32-bit/64-bit DLL).

Final Scientific/Technical Report

- GoldSim may not provide required mathematical functions or optimized algorithms that aid the specific technical requirements for CCS modeling.
- Some new algorithms or logic may best be packaged in new GoldSim elements.
- Is there a requirement for “Components”, which are user-defined GoldSim subsystems that could be ‘plugged into’ existing models?
- GoldSim may require new post-processing capabilities (i.e. contour plots).
- GoldSim’s Dashboard may require some new controls or capabilities.

In collaboration with our Los Alamos team partners each potential task was evaluated and categorized based on the following questions:

- What problem does it solve?
- What is the benefit of the feature?
- What are the implementation challenges?
- What is the estimated cost? Development effort (time to design, implement, test and document feature).

In addition the following attributes were determined for each potential task:

- **Enhancement category:** Must be one of the following:
 - Editing/Presentation (C-EP)
 - Process Integration (C-PI)
 - Simulation Performance (C-SP)
 - Logic (C-LC)
- **New feature (yes/no):** Does the task represent an entirely new feature, regardless of its size and impact, or is it an improvement of an existing capability?
- **Complexity rating (low/medium/high)?** Describes the estimated technical complexity of the task.
- **Potential for failure or no improvement (%)?** Estimates the likelihood of failure to accomplish the task or the chance that the task does not actually achieve an improvement (i.e. performance improvement).
- **Is prototyping or extensive investigation required (yes/no)?**
- **Are new technologies, software tools or libraries required (yes/no)?** Does the implementation of the task require use of a new technologies, API, software tool or libraries? If so, the (time) costs and risks may be higher.
- **What is the time estimate to design and code the task (days):** Roughly estimates the minimum number of developer days required to design and develops the task. Does not include time estimates for testing and documentation, which are expected to be approximately equal to 50% of the developer time.
- **What is the assumed benefit (0-10)?** Estimates the value of the feature to the user.
- **Value:** Expresses the expected value taking into account previously listed parameters.

Final Scientific/Technical Report

Following a thorough evaluation of all the potential tasks, including detailed discussions of end-user benefit, the inherent risk of failing to achieve the main objective of each task, and estimating the required design and development time the following features were short-listed for possible implementation, subject to resource constraints:

- **Increase internal buffer sizes**
- **Add auto ID suggestion to input fields**
- **Input find and replace capability**
- **Improved date-time capabilities**
- **Adjust browser search capability**
- **Add layered Excel interaction model**
- **Improve Excel integration**
- **Add Macro support to Spreadsheet element**
- **Support ‘massive’ outputs**
- **Locally distributed processing**
- **Script Expression element**
- **User-definable functions**
- **Sequencing improvements**

The task review indicated a high value and low cost for the first task (increased internal buffer sizes), and given these attributes it was decided to implement it immediately. The development was successful, and the new capability was made available in GoldSim version 10.11, release in March, 2010.

Not all of the short-listed tasks could be developed within the cost and time restriction of the project. In the end, the following items were developed. Of these, the development of the Script element (essentially a mini-programming language for GoldSim users) was the largest single task. The following table identifies some of the specific capabilities that were developed under Task 2.

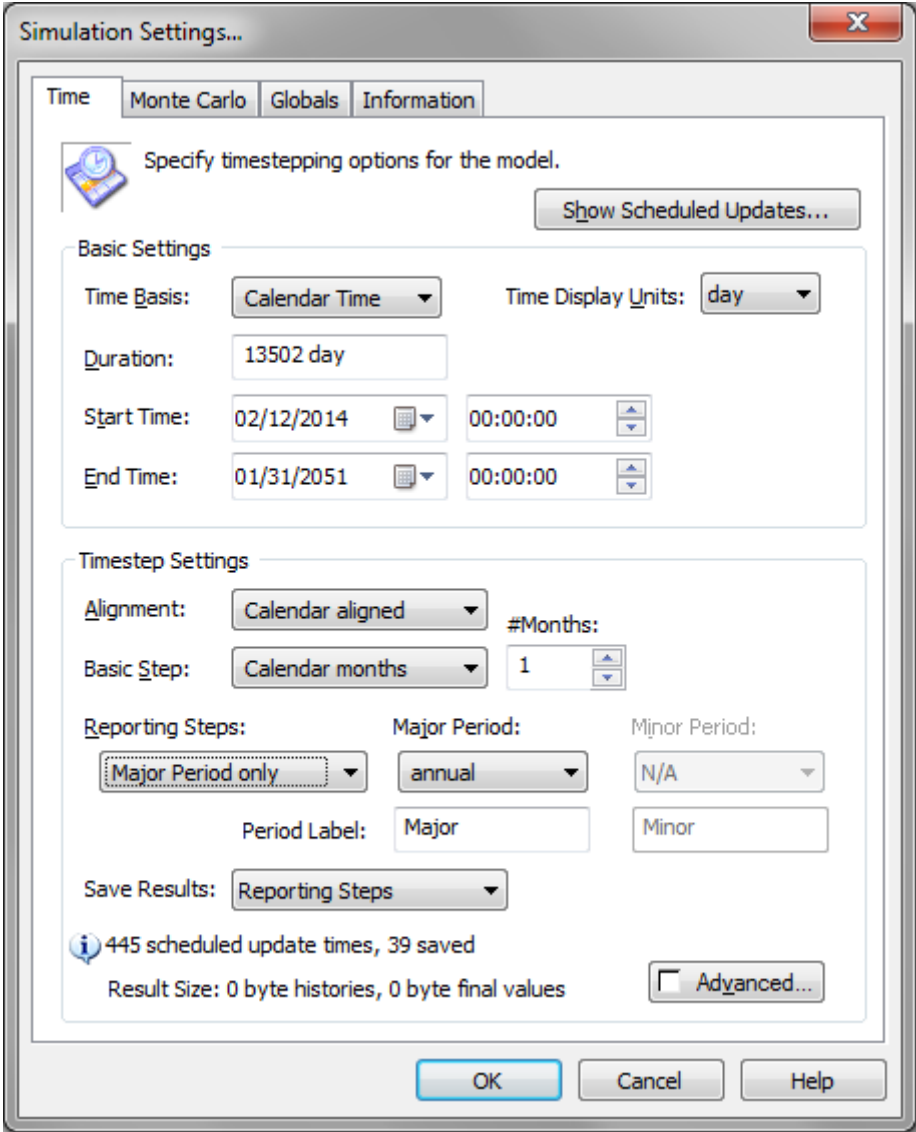
Task 2 Development Items	
Description	Comments
Increase internal buffer sizes, support ‘massive’ outputs.	This change allowed result items to be arbitrarily large in size, limited only by the computer’s memory capacity.
Add auto ID suggestion to input fields.	As a user types in an equation referencing different internal components of the model they are provided with interactive lists showing available components matching what they have typed so far.
Improve date-time capabilities.	A significantly enhanced user interface allows calendar-based selections of simulation start and end times, and of model timesteps. Model results can be calculated and aggregated based upon calendar periods while still using appropriately

Final Scientific/Technical Report

	sort time steps for generating accurate results..
Enhanced Units Management	GoldSim automatically converts any user units, and these changes provided an enhanced capability for units definition and management.
Improve Excel integration.	An ability to support extended worksheet sizes was added to GoldSim.
Script Expression element.	The new GoldSim element provides a ‘mini programming language’ whereby complex scripts can be embedded within a model in order to carry out specialized computations.
Sequencing improvements.	The dependency sequence for calculating results at a given time in the simulation can involve many thousands of calculations. This enhancement provided tools for the user to view and directly control this sequence when necessary.

The following screen-shot illustrates how calendar periods can be used to define and report the results of a simulation model:

Final Scientific/Technical Report



GoldSim 11 Simulation Settings Dialog

Final Scientific/Technical Report

C. TASK 3: SCENARIO ANALYSIS AND MODEL REUSE CAPABILITIES

Task Description:

The Recipient shall extend the GoldSim framework to improve the ability to rapidly create new models and to compare alternative scenarios and approaches. These changes shall focus on modifications to the overall GoldSim framework in two key areas: 1) the ability to create and reuse model components in order to facilitate rapid model construction for multiple sites; and 2) scenario management capabilities to make it easier to compare and contrast alternative scenarios, approaches and sites.

Many users have requested that GoldSim provide support for modeling, saving, and comparing results of multiple scenarios. However, there is no simple definition of a scenario.

In general, as used in GoldSim modeling a scenario represents either:

- An alternative set of external boundary conditions that is applied to test the behavior of a given GoldSim model,
- An alternative design of the system that is being modeled, to compare to other designs using the same external boundary conditions, or
- An alternative behavior of the system itself, which is directly specified by the user. For example, the scenario might represent a worst case where all components of a certain type are assumed to fail.

At the heart of the approach is an ability to centrally manage a set of saved scenarios for a model. There is a ‘central registry’ of scenario information, accessed by a Scenario Manager dialog, but the numeric input data and results for each scenario are stored within individual Data elements and dashboard controls, and Time History and Result Distribution elements.

A summary of the approach follows.

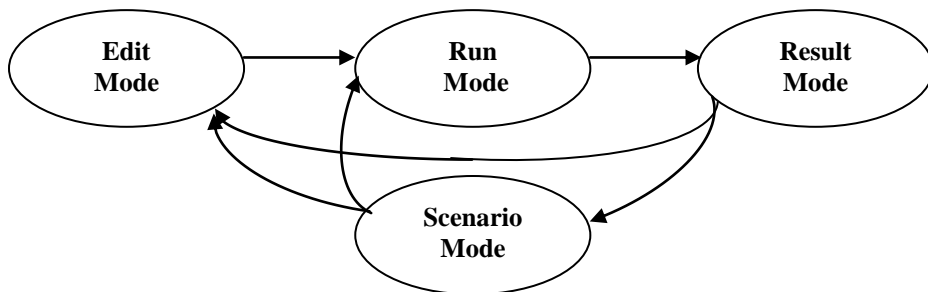
1. Apart from graphics and result elements, the only things that can differ between scenarios are specified fixed values for Data elements which may or may not be dashboard-controlled. For convenience, all Data elements that have no input links are referred to below as “**Fixed Elements**”.
2. Separate data-sets are kept for the “live model” and for each defined scenario. The live model represents the original GoldSim model data.
3. Data elements that have scenario-specific data values are referred to as “Scenario Data elements”. The presence of scenario data is indicated in the elements’ dialogs.
 - Scenario data can be added to/deleted from designated Data elements from within the Scenario Manager’s Scenario Data dialog.

Final Scientific/Technical Report

- Scenario data can be added/deleted for individual Data elements from within their editing dialog.
 - Scenario data are automatically added for dashboard-controlled Data elements when they are given unique values for specific scenarios, and are removed when they no longer have any scenario-unique values.
4. The user can ‘apply’ either a scenario or the live model (rather like putting on a set of clothes). Whatever is currently applied is displayed and modified in the affected Data elements and dashboard controls as the user edits their model. Running the model runs whatever is currently applied.
 5. Upon exiting Result Mode (F4) the user has an option to either go to Edit mode or to enter a new model state, “**Scenario Mode**”. This is a restricted model mode, similar to result mode, intended to allow the user to explore multiple scenarios for a model.

The color code for Scenario Mode is orange. In this mode:

- No normal output results are saved (like edit mode).
- One or more sets of scenario results have been saved, via Time History or Result Distribution elements and dashboard controls.
- No editing that affects model results or simulation settings can be performed (like result mode), except that **the user can modify the values of Fixed Elements for scenarios that don’t have saved results**.
- In the model is in Scenario or Edit mode then via the Scenario Manager dialog the user can define new scenarios, delete existing scenarios, modify existing ones, and run the new or modified scenarios.
- If the user chooses to exit Scenario Mode (F4 key also) in order to modify the simulation settings, or to add or modify other model elements, all existing scenario results are lost, but scenario definitions are saved.



State Transitions Diagram

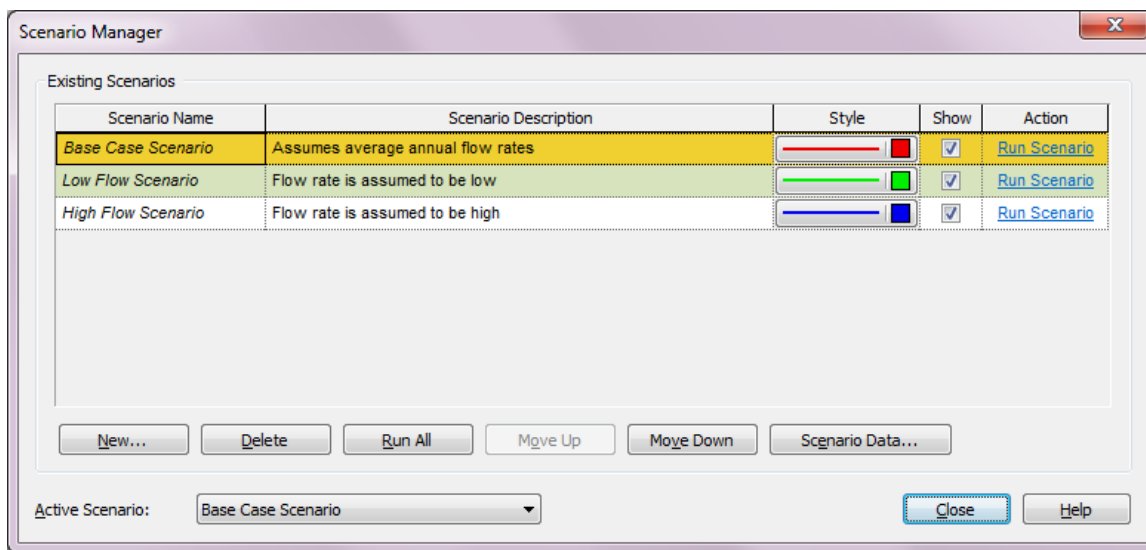
6. The model manages the information about the scenarios that it has stored, saving information about each scenario in the central registry. The user can view and manage their scenarios from the Scenario Manager.

Final Scientific/Technical Report

7. The user can define new scenarios in several ways:
 - The user who is experimenting with their model and who generates an interesting set of results can elect to save the current results as an *ad hoc* named scenario and enter Scenario Mode through an option in the ‘exit result mode’ dialog.
 - Through the Scenario Manager the user can manage the list of existing scenarios, define new scenarios and modify existing scenarios, or
 - Through a new dashboard control.
8. The Time History and Distribution result elements were given the ability to store the results of simulations, and associate those results with particular scenarios in the central scenario registry. While the model is in scenario mode these elements can display the recorded scenario data.
9. If the user elects to define a new *ad hoc* scenario when they exit result mode then all Fixed Elements, Time History, and Distribution result elements store their current results - there is no option to do such saving on an element-by-element basis. A new result element that is added to a model that has previously saved some scenario results will only contain results for subsequently-created scenarios.

Development of the scenarios capability for GoldSim was a massive effort, requiring well over a man-year of development time and affecting almost every aspect of the software. The result, however, is a powerful feature that is well integrated into the overall GoldSim architecture. It should provide significant benefits for comparing alternative designs for CCS systems.

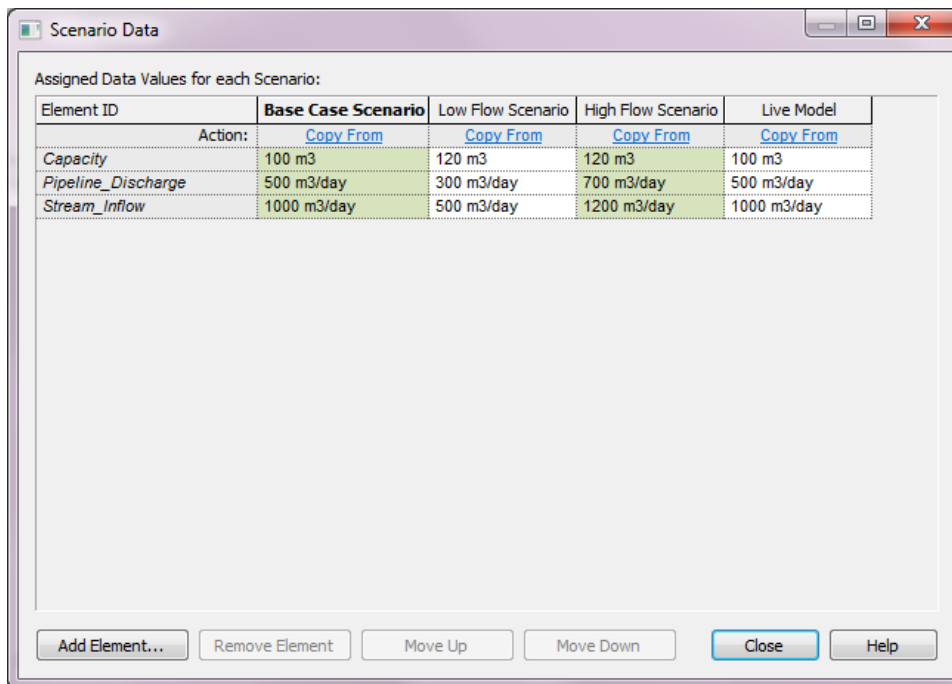
Scenarios are defined (and run) via the Scenario Manager dialog:



Using this dialog, users can create new scenarios, and delete existing ones. When they add a new scenario, they are prompted for a Scenario Name and Description. In the example shown above, three scenarios have been defined.

Final Scientific/Technical Report

Scenario Data are the Data elements that differentiate the various scenarios in your model. GoldSim provides several ways to specify Scenario Data. The most straightforward way to specify Scenario Data is to use the Scenario Manager, which provides a sub-dialog for specifying all of the Data elements defining the scenarios:



Assigned Data Values for each Scenario:

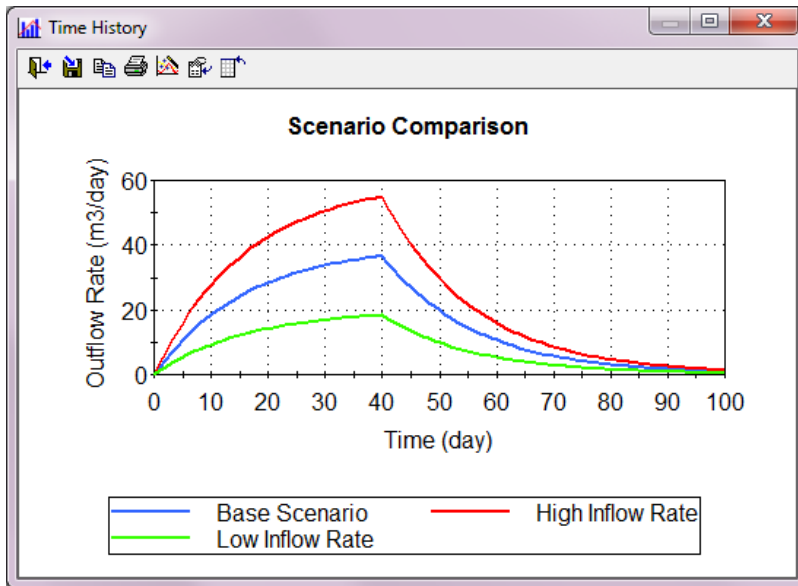
Element ID	Base Case Scenario	Low Flow Scenario	High Flow Scenario	Live Model
	Action: Copy From	Copy From	Copy From	Copy From
Capacity	100 m3	120 m3	120 m3	100 m3
Pipeline_Discharge	500 m3/day	300 m3/day	700 m3/day	500 m3/day
Stream_Inflow	1000 m3/day	500 m3/day	1200 m3/day	1000 m3/day

Buttons: Add Element..., Remove Element, Move Up, Move Down, Close, Help

Each row in this dialog represents a Scenario Data element. Each column represents a scenario. Users can add new Scenario Data using the Add Element... button. They can subsequently edit the value for any Scenario Data element in any defined scenario. This table is very convenient because it displays all Scenario Data values for all defined scenarios side-by-side.

In effect, when they use this capability, their model can store (and subsequently compare) multiple sets of outputs:

Final Scientific/Technical Report



This can be very useful for carrying out sensitivity analyses, testing and comparing alternative designs, and asking “what if” questions.

Final Scientific/Technical Report

D. TASK 4: SIMULATION OF PROGRAMMATIC RISK

Task Description:

The purpose of Task 4 is to extend the GoldSim framework to allow a better representation of programmatic risks. Many non-technical issues (e.g., financing, regulatory compliance, public acceptability, funding constraints) can impact project success and/or costs. Moreover, these risks are not independent of technical considerations. These changes shall extend the GoldSim framework to support detailed project simulation, which will facilitate decision-analysis for evaluation and comparison of alternative plans of activities, assessment of the impacts of alternative budget/funding scenarios, and representation of the consequences of identified risks that might affect project success and cost, including both technical and non-technical risk factors.

It was desired to extend the GoldSim framework to support detailed simulation of project or programs. This will allow using the power of GoldSim in order to:

- Facilitate decision analysis for evaluation and comparison of alternative plans of activities (strategies),
- Assess the impacts of alternative budget/funding scenarios, and/or
- Study the consequences of identified risks that might affect project success and cost, including both technical and non-technical risk factors.

Currently the more advanced commercial project management software programs can simulate the impacts of programmatic risk. Typically they do so by defining risk events that might occur during specific program activities, and associating with each event its likelihood of occurrence and its consequences, usually expressed in terms of delay and extra cost. This is a widely accepted approach, and is based on fundamental principles of risk analysis.

However, these software programs have a very limited scope- they only address the scheduling and costs of the planned program activities, along with associated resources required to conduct the activities. Compared to these programs the GoldSim software is far more versatile overall, and it has a greatly expanded repertoire of risk and simulation capabilities. It has also been used successfully to do project risk analyses, and to integrate project risk analysis with actual simulation of the associated physical activities and their consequences.

Although GoldSim can simulate programmatic risk it was not specifically designed to conduct project or programmatic risk analyses, and as a result it is cumbersome to use for this type of simulation. The purpose of this task was to enable GoldSim users to do more sophisticated analyses more easily.

Several work items in the previous tasks, specifically the enhanced calendar-based support and scenarios capability, have made a major improvement in GoldSim's ability to model

Final Scientific/Technical Report

programmatic risk. For Task 4 several significant additional items were selected for development:

1. Enhanced reporting based on calendar durations.
2. Enhanced analysis tools for Monte Carlo simulation results.
3. Enhanced reporting of Milestone success probabilities and of the probabilities of late or completely missed milestones.
4. Bayesian updating to represent knowledge gained through exploration, testing, or design activities.
5. Supporting decision analysis to help identify optimal strategies.

The requirements that were developed for these areas are discussed in more detail below.

Monte Carlo Results Analysis

The existing realization-selection approach (see screen-shot below) was replaced with a new, more general approach:

Realization Classification and Screening

Each Monte Carlo realization is assigned to the first category for which its final values satisfy the condition. Specify a condition for each category and select which categories to include in result analyses and displays.

Include	Label	Condition	Style	Gross %	Net %
<input type="checkbox"/>	Success	Success		78.8	78.8
<input checked="" type="checkbox"/>	Category 1	All realizations		100	21.2

The new approach:

- Is available in all model modes, via a “Result display” button on the simulation settings’ Monte Carlo tab. It is also available via Model/Options/Results.
- Consists of a user-defined “Result Classification” grid, similar to that of the Multivariate result element’s Classification dialog (see screen-shot below). Each row in the grid has:
 - An option whether to include the category in result displays and analyses,
 - A legend label (for charts),
 - A classification condition input field, which defines a subset of the remaining realizations,
 - A line-style selector button (for charts, and with its color used for scatter-plots and, possibly, tables), and
 - Two count displays, ‘Gross and ‘Net’ (only shown when in result mode).

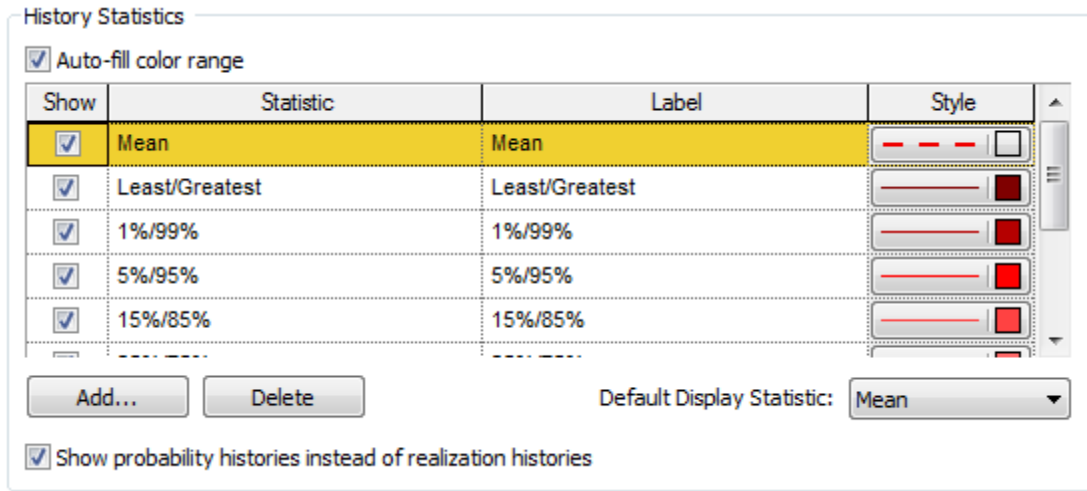
The last row’s selection definition is always fixed as “All realizations”.

When in result mode only the Included groups are used for realization screening and time history selection/charting. Whenever individual realizations are displayed the selected line style is used for the members of each classification group.

As part of this task the Multivariate element’s Classification tab was removed. Its scatter plots now use the specified line-style colors for each Included result classification group.

Final Scientific/Technical Report

The existing probability history options were migrated into this dialog as well, so all these options are more accessible for the user:



Bayesian Updating

In many projects items that are initially uncertain or vague become better known as the project progresses, and future project decisions will be based on the improved information that results. A simple example of this might be the development of a new product or process, where there may initially be significant uncertainty about its technical feasibility, cost, safety, or other important parameters. As the development process proceeds and additional information is generated these uncertainties will be reduced, and the project will face a number of go/no-go decision points.

The ability to model such projects would be valuable, and the GoldSim framework has the potential to perform the sophisticated calculations that are required. Such modeling would allow for improved understanding of the overall risks involved in such projects, and would help planners to design optimal programs and decision points.

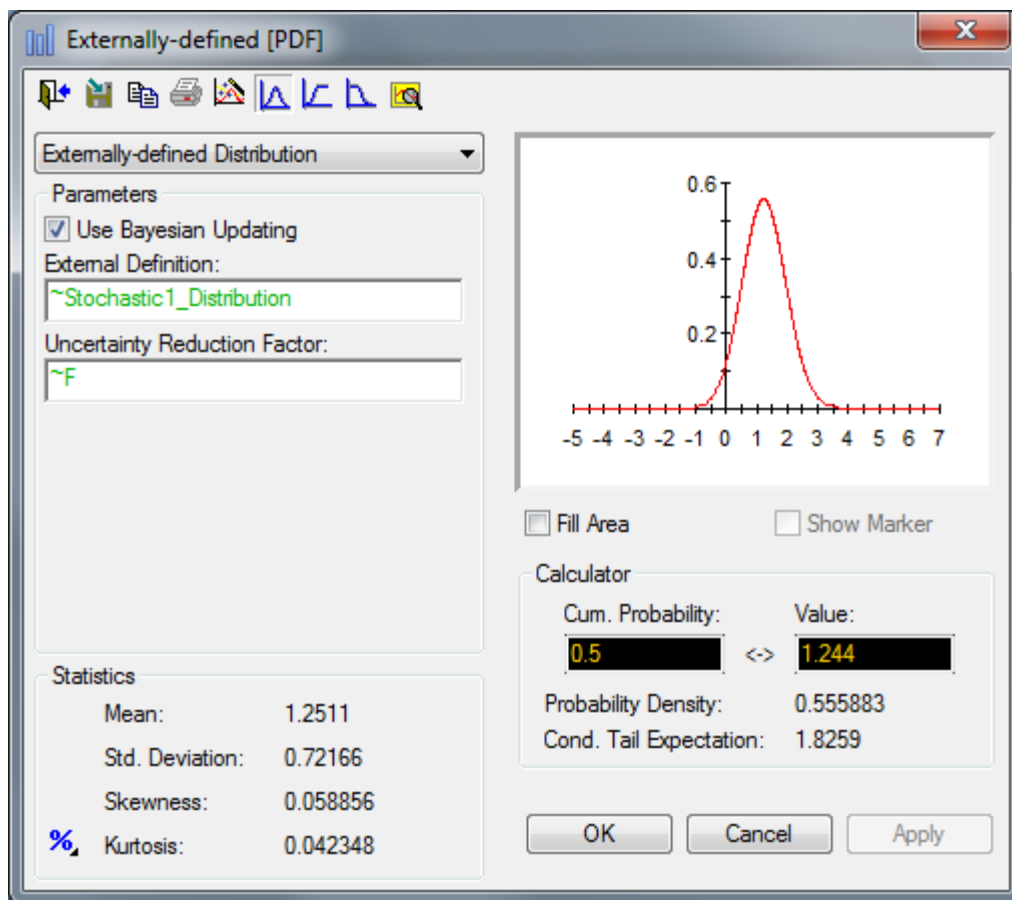
At its heart this approach requires giving GoldSim the ability to dynamically update probability distributions ('Bayesian updating') for uncertain parameters as a simulation progresses, and to simulate future decisions based on the improved understanding that is anticipated. Conceptually, the 'true' values of the unknowns are initially obscured, but with the passage of time and generation of additional information the uncertainties are reduced and the probability distributions converge towards their 'true' values.

For example, a new product might initially have a 50% likelihood of being cost-competitive, but in some Monte Carlo realizations it would gradually become clear that the cost would not be competitive, and at an appropriate time the project should be terminated. Exactly when, and under what circumstances, it should be terminated could be optimized based on the model's results.

Final Scientific/Technical Report

The simulated Bayesian updating capability that was developed required a number of new GoldSim capabilities:

- The ability to treat a probability distribution definition as a type of output.
- The ability to route probability distribution definitions into and out of SubModels.
- The ability to specify an “Uncertainty reduction Factor” for a prior probability distribution, and to generate an updated distribution based on that factor and the true value of the underlying variable (see screen-shot below).



Decision Analysis

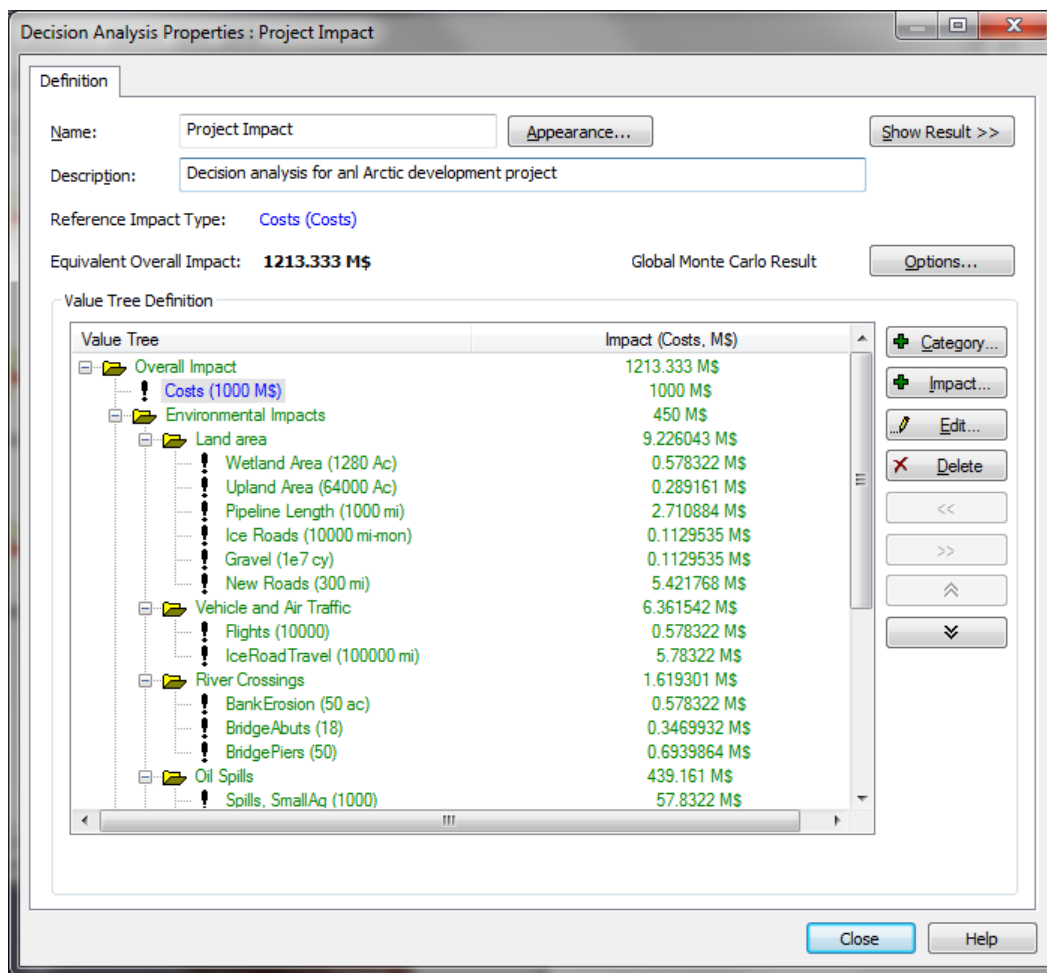
GoldSim project simulation models typically calculate a number of metrics of the project's performance. Overall success, cost and duration are nearly always computed, and numerous other metrics may also be calculated by the model, such as health and safety impacts, environmental impacts, public relations metrics, and more generally the overall quality of the project outcome.

Final Scientific/Technical Report

Given a multitude of probabilistic metrics how is a decision-maker to select (and defend) a particular project strategy, appropriately balancing all of the different metrics? Multiattribute utility theory (from the field of decision analysis) provides a theoretical foundation that allows combining all of the measured outcomes of a model into a single 'utility' value, and the expected value of the utility arising from a Monte Carlo calculation of a specific strategy is an appropriate single measurement of the strategy's overall value.

Accordingly, a decision analysis component should be added to GoldSim, to provide users with an effective way to specify the relative importance of the different metrics that the model produces, and to calculate an overall utility value for each alternative strategy that is studied.

Typically different stakeholders will have different priorities and values, so it may be useful for the decision analysis component to be designed in such a way that multiple stakeholder value systems can be represented.



Screen-Shot of Hypothetical Decision Analysis

Final Scientific/Technical Report

Task 4 Accomplishments

The Task 4 development activities were extensive, requiring significant design, development, and testing resources. The following Table summarizes the items that were developed under Task 4:

Task 4 Development Items	
Description	Comments
Enhanced reporting based on calendar durations	Results can be accumulated and presented as averages, changes, or rates of change over specified calendar periods such as days, weeks, months, quarters or calendar years.
Enhanced analysis tools for Monte Carlo simulation results	When Monte Carlo simulations have been carried out to study risks and/or uncertainties GoldSim provides a variety of analysis and display options. All of these were updated to provide support for separating out and reporting on subsets of the results, known as 'result categories'. Thus can provide very powerful insights into the meaning of results of complex models.
Enhanced reporting of Milestone success probabilities and of the probabilities of late or completely missed milestones	Project milestones can be specified with target achievement dates. Simulation results can then display the probability of achieving specific milestones, and for those that are achieved can display the likelihood of achieving them by the planned time and the probability distribution of achievement times.
Bayesian updating to represent knowledge gained through exploration, testing, or design activities	Where future project decisions will be based on new knowledge developed during early stages of a project GoldSim can simulate these decisions based on the evidence that would be available at any given time.
Supporting decision analysis to help identify optimal decisions or strategies	A Multiattribute decision analysis capability whereby any stakeholder group, or a decision-maker, can evaluate the results of a complex risk-based model in order to compare alternatives.

Final Scientific/Technical Report

E. TASK 5: MATERIAL BALANCE AND NETWORK FLOW SIMULATION

Task Description:

The Recipient shall conduct an analysis to identify requirements for providing basic material balance capabilities (e.g., an implicit flow network solver) that will enable users to model in detail the complex processes and risks associated with capturing, compressing, processing and transporting CO₂.

Specific capabilities that shall be addressed in Task 5.0 are:

- *Add an ability to solve the implicit flow equations for networks of connected components where CO₂ is stored, processed, and transported.*
- *Add logic to identify throughput bottlenecks in such systems, considering primary and backup components, their reliability, and operating rules.*
- *Add support for material balance accounting calculations, allowing for random and uncertain factors, in order to quantify the accuracy of the reported material balances.*

PROPOSED SOLUTION APPROACH

The heart of the proposed new approach is to enhance the CT module's Cell element so that it can solve for both media flows and contaminant transport. The key to its enhanced behavior is to add an option to the element to be a "**Media Store**". Additional new options will include "**Media Source**", "**Media Sink**", and "**Media Router**".

Cell Element Media Store Option



If this option is selected by the user the following things happen:

- The Cell's media quantity inputs are redefined to be the **initial** quantities in the Cell.
- At each new time point the media quantities in the Cell are automatically updated prior to solving the contaminant transport equations, with the media quantity rates of change being the sums of their inflow rates minus their outflow rates as of the **previous** time point.
- An optional "Maximum volume" input field is provided for the Cell.

Final Scientific/Technical Report

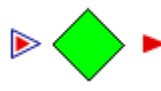
User-Specified Media Amounts Option



This represents the behavior of Cells in older GoldSim version, in that the user specified the amount of each medium. Unlike older versions, it requires that media inflow and outflow rates are consistent with any changed specified media quantities at each time step. A failure to match the media quantities will cause an error.

This will be the default behavior for Cells when importing older GoldSim models. Note that many older models will not satisfy media balances, as GoldSim has previously assumed ‘clean’ inflows or outflows existed wherever necessary. These older models will have to be modified by adding such flows before they will run in the new version. Typically a “**Media Source**” element will be required in order to provide the balance of media to the flow network, and an existing Cell will need to be converted to a **Media Sink** to define a termination point of media flows.

Media Source Option



If this option is selected the Cell will act as a source of media and contaminants, which is required in order to model inflows through the model boundary. There is no limit to the amount of media that can be removed from the source. Multiple Sources are allowed in a model. A Source outputs its cumulative produced amounts of media and species. For contaminant transport modeling, the user specifies contaminant concentrations in the reference fluid output by a **Media Source**.

Media Sink Option



If this option is selected the Cell will act as a sink for media and contaminants, which is required in order to model outflows through the model boundary. There is no limit to the amount of media that can flow into a sink. Multiple Sinks are allowed in a model. A Sink outputs its cumulative amounts of received media and species.

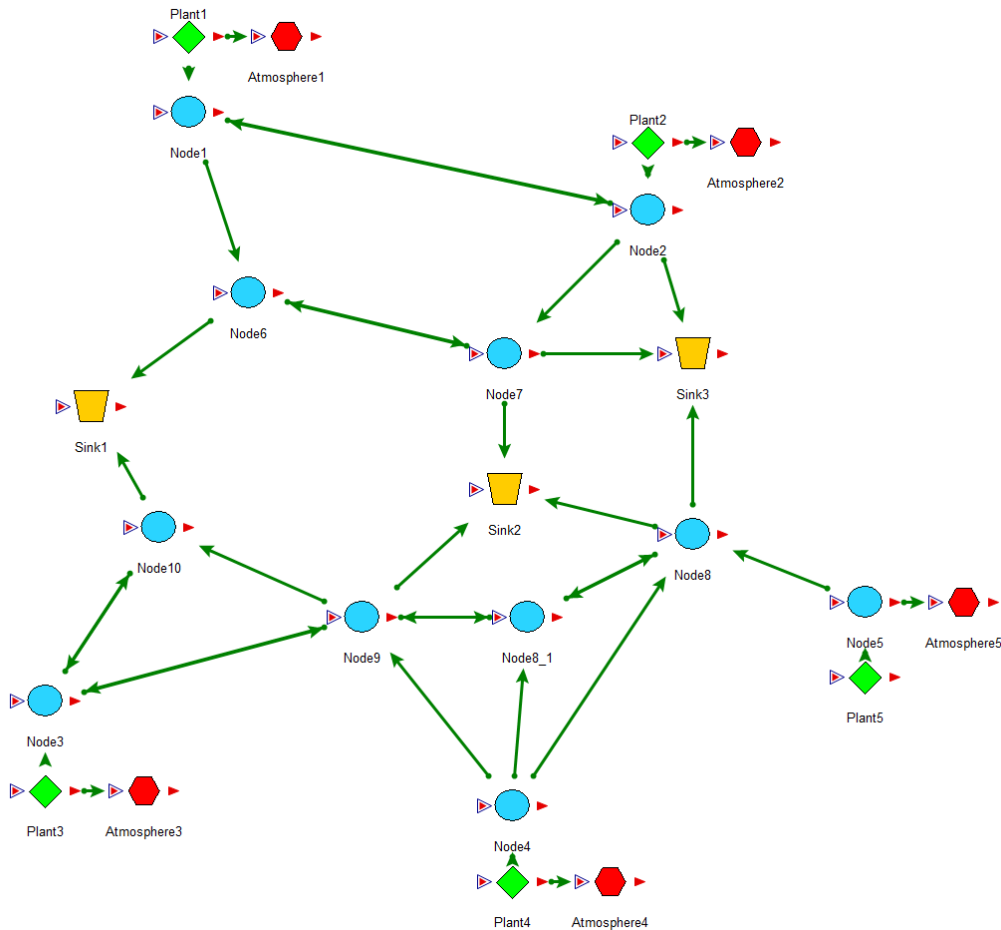
Final Scientific/Technical Report

Media Router Option



If this option is selected the Cell will hold zero amounts of its defined media, and only supports advective inflows and outflows. It is used to route media (and their contaminants) between other pathways. Multiple inflows can join at a **Media Router** and multiple outflows can split from it.

The figure below shows an overview of a LANL-developed simple network using media sources, routers, stores, and sinks. For clarity, each source (i.e., plant) is attached to its own sink (i.e., emissions to the atmosphere), though in reality each source can be attached to the same sink (creates overlapping lines):



“Clean” Flows

An additional “(clean)” media item will be added to the existing advective flux list of media types for Cell element outflows. This will be used to ensure no contaminant is

Final Scientific/Technical Report

present in the outflow, which is useful in representing processes like evaporation in contaminant transport models.

Flow Network Solution

It will be possible to use a network solver to find the media flow rates in a complex flow network. Where multiple solutions are possible the solver finds the flow rates that give the optimum solution for the system, using an approach based on linear programming. The user may optimize on the basis of costs ('least-cost') or relative priorities.

Note that the user can specify some of the flow rates while leaving the others to the network solver.

Priorities or costs can be associated with satisfying demands, increasing or decreasing stored amounts that are not at their optimal levels, and costs (but not priorities) can be associated with moving media through flow links and storage cells.

The prototype version of the Media Flows GoldSim capability was tested by Los Alamos, and the results are described in their final project report. Release of a final version, with accompanying documentation, is planned for late summer of 2013.

Final Scientific/Technical Report

F. LOS ALAMOS TESTING AND EVALUATION

Los Alamos National Laboratory (LANL) participated in this project, supported under agreement FWP FE-09-1006. The LANL team, headed by Dr. Philip Stauffer, had two main roles in the project:

- Provide suggestions and advice regarding useful enhancements to make to the GoldSim software.
- Review and evaluate prototypes of the enhancements.

The LANL team's participation was very effective. It is summarized in their final report describing their activities, dated October 6, 2012. The executive summary of their report is as follows:

The overall objective of this project was to provide a powerful and flexible framework that will allow system designers and/or regulators to build truly comprehensive, system-level risk assessments that realistically incorporate and couple all important aspects of an integrated carbon capture and storage (CCS) project. The Los Alamos National Laboratory (LANL) participation in this project involved application of LANL's CO2-PENS model. Over the past 3 years, LANL investigators worked with GoldSim Technology LLC (the project PI) to test new capabilities developed in the GoldSim framework through integration in the CO2-PENS model. New modules were created and existing modules modified. The applicability of the capabilities was tested by developing and applying CO2-PENS models for appropriate field sites. For the most recent Network Flows capability, example models were built to test the functionality in relation to pipeline routing and optimization. Finally, a graphical interface from CO2-PENS was created by LANL to allow visualization of model results, a function that was deemed more easily done outside of the GoldSim programming language after many discussions with the GoldSim development team. All of the improvements are now available and are being used by the National Risk Assessment Partnership (NRAP) to create the next generation risk models for CO2 sequestration.

Final Scientific/Technical Report

G. SUMMARY AND CONCLUSIONS

An extensive analysis was carried to identify ways to enhance the GoldSim software to make it a better tool for carrying out system-level risk assessment of proposed carbon sequestration projects. A number of individual development tasks were identified and carried out through a process of requirements analysis, design, development, testing, and documentation. The primary work product was a series of enhanced versions of the GoldSim software. The User's Guide for GoldSim version 11, the final version embodying all of these enhancements provides detailed documentation of all of these features.

The overall development process was difficult, as the enhancements are complex and required an investment of substantially more development resources than originally anticipated. The additional costs were covered by the contractor, GoldSim Technology Group LLC, rather than by NETL.

The final result of this development work is a significantly enhanced tool available to the CCS community to support risk-based total system models of sequestration projects.