GoldSim Contaminant Transport Module

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Chapter 1: Introduction

A journey of a thousand miles begins with
a single step.

Confucius

Chapter Overview

GoldSim is a user-friendly, highly graphical, object-oriented program for carrying out dynamic, probabilistic simulations to support management and decision-making in engineering, science and business.

The GoldSim Contaminant Transport Module is a program extension to GoldSim which allows you to probabilistically simulate the release, transport, and fate of mass (e.g., contaminants) within complex engineered and/or natural environmental systems.

Each of the GoldSim modules has a separate User's Guide describing its capabilities and features. This document provides a complete description of the features and use of the GoldSim Contaminant Transport Module.

Note: This document only describes the Contaminant Transport Module, and assumes that you are familiar with the basic capabilities of GoldSim (described in the **GoldSim User's Guide**).

In this Chapter

This introductory chapter discusses the following topics:

- What is the Contaminant Transport Module?
- What is the Difference Between GoldSim CT and GoldSim RT?
- Who Should Use the Contaminant Transport Module?
- How the GoldSim Documentation is Organized
- Learning to Use the Contaminant Transport Module
- Conventions Used in this Manual
- Activating the Contaminant Transport Module
- Using Help
- Technical Support, User Resources and Software Upgrades

What is the Contaminant Transport Module?

The GoldSim Contaminant Transport Module is a program extension to the GoldSim simulation framework that allows you to dynamically model mass transport within complex engineered and/or natural environmental systems. A *mass transport model* is a mathematical representation of an actual system (e.g., the subsurface environment near a waste disposal site) which can be used to simulate (and hence predict) the release, transport (movement) and ultimate fate of mass within the system. The "mass" that is typically simulated is that of chemical contaminants that have been accidentally released or intentionally disposed of within the system. As a result, such models are often referred to as *contaminant transport models*.

It is important to understand that unlike the basic GoldSim framework itself, which is quite generic, the Contaminant Transport Module was specifically designed to a be applied to a particular class of problems: those associated with modeling the transport (movement) of mass (typically contaminants) through a system (e.g., soils, surface water bodies, groundwater). As such, the fundamental output produced by the GoldSim Contaminant Transport Module consists of predicted masses and mass transfer rates at specified locations within the system, and predicted concentrations within environmental media (e.g., water, soil, air) throughout the system. If desired, concentrations in environmental media can be converted to doses and/or health risks to receptors by assigning appropriate conversion factors.

More specifically, the Contaminant Transport Module can be used to represent the following processes:

- **Release of mass (e.g., contaminants)** from specified sources, taking into account 1) the failure of engineered barriers and containers (if any) in which the contaminants are disposed; and 2) degradation of any materials in which the contaminants are bound (e.g., grout, metal, glass).

- **Transport of mass** through multiple transport pathways within an environmental system (e.g., aquifers, streams, lakes, soil atmosphere).

The transport pathways can consist of any number of transport and storage media (e.g., water, air, soil), and a variety of transport mechanisms can be directly simulated, including 1) advection via fluids (e.g., movement of dissolved constituents in water); 2) advection via solids (e.g., movement of constituents adsorbed to and/or mixed with solids via erosion and transport of contaminated soil); 3) diffusion through fluids; 4) advection and diffusion of contaminated particulates suspended in fluids; and 5) diffusion across boundary layers associated with adjacent fluids (e.g., transport across the air-water interface). Transport processes can incorporate solubility constraints and partitioning of contaminants between the media present in the system, and can include the effects of chemical reactions and decay processes.

In broad terms, you could use these capabilities to apply GoldSim and the Contaminant Transport Module to a wide variety of environmental problems, such as:

- investigation of the transport and fate of contaminants (or natural components) in aquifers, wetlands, lakes and other complex ecosystems;

- evaluation of the performance of existing or proposed disposal facilities and hazardous waste sites;

- investigation of the potential impact of engineered facilities such mines, power plants, and processing facilities on the environment; and

- simulation of the transport and fate of pharmaceuticals and other compounds within biological systems (e.g., physiologically-based pharmacokinetic modeling).

Having described the types of problems that it can be applied to, it is also important to highlight the manner in which GoldSim can represent these kinds of systems (and the limitations that imposes).

When environmental systems are modeled numerically, it is necessary to discretize space into finite volumes. For example, if you were modeling a lake, you could discretize the lake vertically (into layers) and horizontally (into areal sections), forming a three-dimensional grid of finite volumes. The question then becomes: how much discretization is appropriate? At one extreme, the lake could be represented using tens of layers and hundreds of areal sections (resulting in thousands of finite volumes). At the other extreme, the entire lake could be represented using a single finite volume.

The level of spatial discretization that is approproriate in such a case is a function of a number of things, the most important being the level of "mixing" that can be assumed. Representing the lake as a single finite volume is equivalent to assuming that the entire lake is always (instantaneously) well-mixed. Representing the lake as four vertical layers (four finite volumes) is equivalent to assuming that each layer is always (instantaneously) well-mixed.

When building a model, it is critical to give considered thought to the appropriate level of spatial discretization. For a case like a lake, it is often easy to do so (e.g., it is often quite appropriate to assume well-mixed conditions over a layer or even the entire water body). For other problems it is more difficult. For example, for systems involving advection and/or diffusion along a path (e.g, flow through an aquifer), a course level of discretization (e.g., representing an entire aquifer using a small number of finite volumes) can result in unrealistic spreading of the mass (a phenomenon known as numerical dispersion; as will be discussed, GoldSim has special features to deal with this specific issue.)

As a general rule, GoldSim is designed to represent systems at a relatively low level of discretization (tens or hundreds of finite volumes). That is, referring to the example above, a lake might be represented in GoldSim as two well-mixed layers (finite volumes), rather than many hundreds or thousands of finite volumes. This is not to say that GoldSim is not capable of representing systems at a higher level of spatial discretization. But it is not designed to be used in this way.

One other point is also important to understand regarding the Contaminant Transport Module. The Contaminant Transport Module itself is used to model the movement of mass through the system. This movement is typically the result of movement of media (e.g., water) through the system. This results in the advection of mass through the system (e.g., dissolved in the moving water). The key point here is that the Contaminant Transport Module requires the media flows through the system as input. That is, it solves equations based on specified media flow rates. It does not itself solve for the media flow rates. This means that you are required to create a flow model (using the basic GoldSim framework) that produces the media flow rates that can subsequently be used by the Contaminant Transport Module.

What Makes the Program Unique?

There are a variety of existing tools for simulating the transport and fate of contaminants in the environment. Because the Contaminant Transport Module utilizes all the capabilities of the GoldSim simulation framework, however, it has several unique features not present in traditional contaminant transport simulation tools:

- *The program is extremely flexible*, allowing it to be applied to nearly any kind of environmental system. The software is designed in a modular manner such that model details can be added by directly entering functional relationships or linking user-defined functions or subroutines (e.g., finite difference flow models) into the program. Hence, a GoldSim application can be very simple or extremely complex, and the complexity of the model can readily evolve as more knowledge regarding the system is obtained.

- *The program is highly graphical*, such that you can literally draw a picture of the environmental system that you wish to simulate. You can also add graphics, explanatory text, and hyperlinks to document your model.

- *Uncertainty in processes, parameters and future events can be explicitly represented.* Uncertainty in processes and parameters can be represented by specifying model inputs as probability distributions. The impact of uncertain events (e.g., earthquakes, floods, sabotage) can also be directly represented by specifying the occurrence rates and consequences of such "disruptive events".

These features, in combination with powerful contaminant transport capabilities, make the GoldSim Contaminant Transport Module a unique and powerful simulation tool.

What is the Difference Between GoldSim CT and GoldSim RT?

There are two versions of the Contaminant Transport Module that can be added to GoldSim: the CT Module and the RT Module. Your copy of GoldSim will have neither, one, or the other (but not both), depending on your license. The CT (Contaminant Transport) Module provides all of the features and capabilities that most contaminant transport modelers will need. The RT (Radionuclide Transport) Module includes all of the capabilities of CT, along with several additional features designed to facilitate simulation of radioactive waste disposal facilities and the fate and transport of radionuclides in the environment.

In particular, the RT module provides the following additional features:

- The RT Module allows decay chains (daughter products) to be simulated (one species can be specified to transform into one or more others). To support modeling of radioactive decay chains, the RT Module also allows you to link to an extensive database of radionuclide decay data (based on a standard reference provided by the Intenational Commission for Radiation Protection).

- The CT Module allows you to specify decay rates, but you cannot specify reaction (daughter) products.

- The RT Module provides a special element called a Source. The Source element can be used to simulate the complex release mechanisms of contaminants from engineered systems. This is particularly useful when simulating the behavior of proposed or

existing waste disposal facilities, which have as part of their design engineered packages or containers in which the waste is placed prior to disposal.

- The RT Module has a special type of pathway element called a Network Pathway. Network pathways provide a computationally efficient way to simulate large, complex networks of one-dimensional conduits in order to describe contaminant transport through fractured rock systems.

- The RT Module has a special type of element called a CellNet Generator. CellNet Generators provide an easy way to rapidly create two-dimensional Cell networks.

- The RT Module provides an option to utilize a large built-in database of radionuclide decay data (species, decay rates and daughter products). The data is based on the International Commission for Radiation Protection (ICRP)'s Publication 107. The feature allows you to view over 1300 radionuclides (along with their corresponding stable elements) and to selectively include some of these radionuclides in your simulation.

Who Should Use the Contaminant Transport Module?

The GoldSim Contaminant Transport Module is intended for use by engineers, scientists, researchers and students who are interested in understanding and predicting the migration of mass (e.g., contaminants) in environmental systems.

The software itself, although relatively complex, can be mastered by anyone familiar with the basic functions of a personal computer and the Windows operating system. The key requirements for applying the Contaminant Transport Module are a clear understanding of the physical system being modeled and a basic understanding of uncertainty analysis and probability theory:

- Because the software was designed to be extremely flexible, it intentionally imposes few constraints on the inputs that you define. Hence, it is your responsibility to ensure that the system being defined is consistent and realistic. As a result, the most important requirement for applying the program is that you have a clear understanding of the features, processes, and events controlling the behavior of the system to be modeled. This should include a good understanding of the fundamentals of contaminant transport modeling.

- Although GoldSim can be run in a deterministic manner (i.e., no specified uncertainty in input parameters), one of the key features of GoldSim is its ability to explicitly represent such uncertainty through the use of probability distributions. In order to do so, the user must have at least a basic understanding of the representation and propagation of uncertainty. Appendix A of the **GoldSim User's Guide** provides a brief primer on this topic, along with suggestions for further reading.

How the GoldSim Documentation is Organized

The GoldSim Documentation Suite

The Contaminant Transport Module is a specialized extension to the basic GoldSim simulation framework. The document you are reading only describes the GoldSim Contaminant Transport Module, and assumes that you are familiar with the basic capabilities of GoldSim.

The basic capabilities of GoldSim are described in the **GoldSim User's Guide**. That document provides a complete description of the features and capabilities of the GoldSim simulation framework.

How this Manual is Organized

This document is organized into seven chapters and five appendices. The chapters describe *what the program can do* and *how you make the program work*. Most users, however, will also want to understand *how the program carries out the calculations* (i.e., what equations are being solved, what are the basic assumption inherent in these equations, and what numerical techniques are being used to solve the equations). This information is provided in the appendices.

The seven chapters are as follows:

- **Chapter 1: Introduction**. The remainder of this chapter discusses the information required for you to get started using the GoldSim Contaminant Transport Module, including conventions used in the manual, activating the module, using online help, and obtaining technical support.

- **Chapter 2: Contaminant Transport Module Overview**. This chapter provides an overview of the features and capabilities of the Contaminant Transport Module, summarizes the specialized contaminant transport elements, and outlines the steps required to build a contaminant transport model in GoldSim.

- **Chapter 3: Species and Media**. This chapter describes how you define the basic building blocks of a contaminant transport simulation: 1) the contaminant species which are to be simulated; and 2) the environmental media (e.g., water, soil) in which these species are transported and stored.

- **Chapter 4: Transport Pathways**. This chapter describes the fundamental component of a contaminant transport simulation, the transport pathway. A contaminant transport model is constructed by defining multiple transport pathways and linking them together into a network.

- **Chapter 5: Contaminant Sources**. This chapter describes how you can introduce mass into a transport pathway network by defining one or more "sources", whose contaminant release rates are a function of a variety of user-defined properties.

- **Chapter 6: Receptors**. This chapter describes how concentrations in various media within transport pathways can be converted to impacts (e.g., health risk, dose) to specified receptor groups (e.g., adults, children, farmers).

- **Chapter 7: Advanced Modeling Concepts**. This chapter discusses a number of advanced contaminant transport topics, and will be of particular interest to experienced modelers. It includes discussions of

modeling complex (high-order) chemical reactions, nonlinear chemical partitioning , spatial variability, and the dynamic linking of GoldSim to external codes (e.g., flow models, geochemical equilibrium models).

The five appendices contain the following information:

- **Appendix A: Introduction to Environmental Simulation**. This appendix provides an overview of basic environmental simulation concepts, and is primarily intended for novice contaminant transport modelers.

- **Appendix B: Details of Pathway Computations**. This appendix presents the theoretical basis and mathematical details of the transport pathways.

- **Appendix C: Implementing External (DLL) Pathways**. This appendix provides instructions for those users who wish to directly link external contaminant transport codes into a GoldSim transport pathway network.

- **Appendix D: Network Pathway File Format.** This appendix describes the file format which can be used to import data from a discrete fracture network model into a specialized pathway in GoldSim that allows you to simulate complex pathways in fractured rock.

- **Appendix E: Details of Source Computations**. This appendix presents the theoretical basis and mathematical details of the contaminant sources.

The manual also includes a Glossary of Terms and an Index.

As will be discussed below, nearly all of the information available in the printed documentation can also be accessed via an extensive online help system.

Learning to Use the Contaminant Transport Module

Although GoldSim's intuitive interface will tempt you to simply dive in and start playing with the software, you are strongly discouraged from doing so, even if you are an experienced modeler. Spending some time up front (by following the steps outlined below) is the quickest and most effective way to understand the software's features and capabilities and start building models using the GoldSim Contaminant Transport Module.

1. **Learn how to use the basic GoldSim framework first**. In order to use the Contaminant Transport Module, you must first have a basic understanding of the GoldSim framework. You cannot learn the extension without first learning the basic concepts underlying framework. At a minimum, you should take the GoldSim Tutorial. The Tutorial is available from the GoldSim splash screen, and can also be accessed from the main GoldSim menu (**Help | Tutorial…**).

   In addition to the Tutorial, a free "hands-on" Online Training Course is available that will provide you with a thorough understanding of the key concepts on which GoldSim is based and all of the fundamentals required to build complex models of nearly any kind of system. (Note, however, that the Course only discusses basic GoldSim and does not discuss the Contaminant Transport Module). Because the Course is quite thorough, it will likely take as long as 40 hours to complete. Of course, if you are already somewhat familiar with simulation (and/or

have a strong quantitative background), you may in fact be able to cover the material in considerably less than 40 hours. You can find a link to the Course on the GoldSim website (https://www.goldsim.com/Web/Customers/Education/Training/).

2. **If you are not an experienced mass transport modeler, read Appendix A**. Appendix A of the Contaminant Transport Module User's Guide (Introduction to Environmental Simulation) provides an introduction to several basic mass transport concepts. Note that this appendix is not included in the Help system, and is only available in the User's Guide.

3. **Read "Contaminant Transport Module Overview"**. This section of GoldSim Help (equivalent to Chapter 2 of the Contaminant Transport Module User's Guide) provides an introduction to and a "quick tour" of the GoldSim Contaminant Transport Module. It presents the basic concepts of how contaminant transport is simulated in GoldSim, provides an overview of the features and capabilities of the program, summarizes the specialized elements associated with the module, and outlines the steps required to build a contaminant transport model for an environmental system.

4. **Request your free one hour web-based training session.** When you purchase GoldSim, you are entitled to a free one hour, live web-based training session in which one of our analysts provides an interactive training session via the Internet and telephone. You are strongly encouraged to take advantage of this free training, during which our analysts can provide an introduction to both the basic GoldSim framework and the Contaminant Transport Module.

5. **Open and explore the Example Files**. When you install GoldSim, a number of example models are installed with the program. (You can quickly access these files by selecting **File|Open Example…** from the main GoldSim menu, and look in a subfolder named Contaminant Transport Examples). This examples are referenced in the Help system and User's Guide where the element is introduced. These example model files are an excellent way to begin to experiment with the Contaminant Transport Module.

6. **Download Example Files from the Model Library**. The GoldSim website contains a Model Library with a number of models illustrating how GoldSim can be used for particular applications. The library includes a number of Contaminant Transport models. These models tend to be more complex than the simple example files found in the Contaminant Transport Examples folder, but are still relatively simple.

7. **Browse the User's Guide or Help System**. GoldSim has a large number of features, and you will not discover all of them by experimenting with simple example models. To fully utilize GoldSim's powerful features, browse through the User's Guide, using the index and table of contents as your guide. Each section of the User's Guide is heavily cross-referenced, so it is easy to just jump around. Note that the Help system contains all of the contents of the User's Guide, with the exception of the technical appendices.

8. **Contact us with questions**. When you purchase GoldSim, you are entitled to one year of free support. This does not include assistance in building and debugging your models, but it does include answering

questions on how to use GoldSim's features, so feel free to contact us! The best way to do so is through the GoldSim Help Center.

Conventions Used in this Manual

The following conventions are used in this manual:

Convention	Description
Important Terms	New and important terms are presented in *bold italics*. These terms all appear in the Glossary of Terms at the end of the document.
**File	Open…**	Menus and menu selections are separated by a vertical bar. File	Open… means "Access the File menu and choose Open"
CTRL+C	Key combinations are shown using a "+" sign.. CTRL+C means press the Control and C keys simultaneously.
	Warning: This means watch out! Warnings typically alert you to potential pitfalls and problems that may occur if you perform (or fail to perform) a certain action.
	Note: Notes highlight important information about a particular concept, topic or procedure, such as limitations on how a particular feature can be used, or alternative ways of carrying out an action.

In describing various mouse actions, the following conventions are used:

Mouse Action	Definition
Click	Press and release the left mouse button once.
Double-click	Press and release the left mouse button twice in rapid succession.
Right-click	Press and release the right mouse button once.
Drag	Press the left mouse button, and while keeping it depressed, move the cursor to another location, then release the button.

Activating the Contaminant Transport Module

In order to access the features and capabilities of the Contaminant Transport Module, either the CT Module or the RT Module must first be activated on your machine. Your copy of GoldSim will have neither, one, or the other (but not both), depending on your license.

Read more: What is the Difference Between GoldSim CT and GoldSim RT? (page 4).

You can determine which (if any) of the Contaminant Transport Modules is activated on your machine by selecting **Model**| **Options…** from the main menu, and selecting the **Modules** tab:
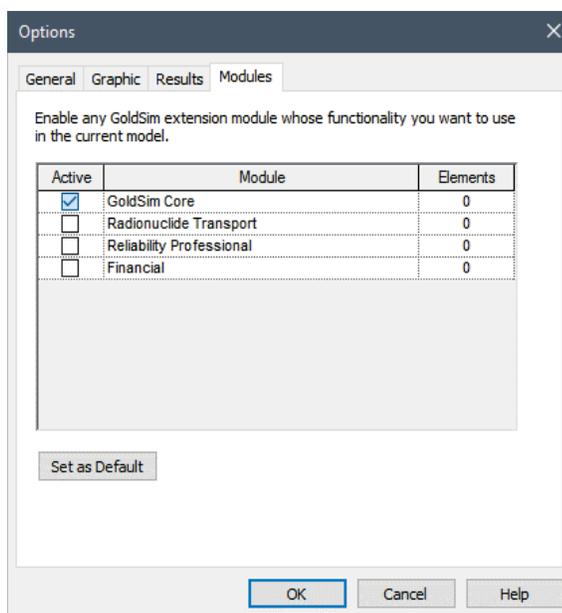
All extension modules that you are licensed to use appear in the dialog. If your license does not allow you to use a particular module, it will not be listed. You can activate and deactivate modules that you are licensed to use by clicking the **Active** checkbox. By default, whenever you activate GoldSim, none of the available extension modules allowed by your license will be activated. To use them, you must activate them using this dialog.

Note: If you try to open a file that contains elements associated with the CT or RT Module, and you are licensed to use that module but it is not currently active, GoldSim will automatically activate the module and open the file. If, however, you are not licensed to use the module, GoldSim will not open the file (and will display an error message).

If you deactivate a module (such ast CT or RT), the specialized elements associated with that module will be deleted from your model (if any are present) and any menu options will be removed in the current file. If you make a module active, the various options associated with that module are made available again. If you press the **Set as Default** button, the selected modules will be activated for all new models that are created.

Using Help

GoldSim has an extensive in-product help facility that describes the basic GoldSim features, which can be used to supplement this manual. The Help system can be accessed by selecting **Help | Help Topics** from the main GoldSim menu or the Help button (the question mark) on the standard toolbar. Pressing the **Help** button within any of the dialogs also provides access to Help (in a context-sensitive manner).

All of the information in the **GoldSim User's Guide**, the **GoldSim Contaminant Transport Module User's Guide**, and other extension module user guides (e.g., the **GoldSim Distributed Processing Module User Guide**) is accessible via GoldSim Help. Note, however, that information included in the appendices of the various user guides is not included in the Help system.

Technical Support, User Resources and Software Upgrades

The GoldSim Technology Group is dedicated to providing complete solutions for our customers. We pride ourselves in providing prompt and extensive support and resources to our users, and are committed to ensuring that each installation of our software is successful and adds value to the customer.

GoldSim Maintenance Program

When you purchase GoldSim software, you receive one year of Software Maintenance, entitling you to the following:

- Free software upgrades so that you always have the latest version of the GoldSim software.

- Basic Technical Support via email and phone. Basic support covers installation and licensing questions, as well as questions about GoldSim's features and capabilities.

After the first year, if you wish to continue to have access to new versions and technical support, Software Maintenance can be extended each year with payment of an annual fee.

Details regarding the GoldSim Maintenance Program can be found at www.goldsim.com/Web/Products/BuyGoldSim/Pricing/MaintenanceProgram/.

Getting Technical Support

Users with active Software Maintenance can submit questions directly to the GoldSim support team. Evaluation users are also welcome to contact us with questions on GoldSim functionality. The **GoldSim Help Center** (https://goldsim.zendesk.com) is the primary portal for technical support. You can submit your questions directly from the Help Center. If your register and log in through the Help Center, you will be able check the status and view a history of all of your support requests.

The Help Center also includes:

- The **GoldSim Forum**, where you can you can post questions to the GoldSim community, or just browse existing messages;

- Articles on licensing questions and modeling tips; and

- An archive of past webinars (which demonstrate GoldSim features and capabilities).

Although using the Help Center is the preferred way to access support, you can also contact us by phone at 1-425-295-6985 between the hours of 8AM and 5PM Pacific Time.

Free Basic Technical Support does <u>not</u> include consulting, model trouble-shooting or detailed assistance with applying GoldSim to a particular problem. Assistance of this nature is defined as Advanced Technical Support. Users may purchase Advanced Technical Support in pre-paid 10 hour blocks.

Details regarding Advanced Technical Support can be found at www.goldsim.com/Web/Resources/TechnicalSupport/.

Other GoldSim Resources

In addition to the GoldSim Help Center, additional resources are also available. These three resources can be accessed directly from the GoldSim website (www.goldsim.com):

- A free **Online Training Course** that will provide you with a thorough understanding of the key concepts on which GoldSim is based and all

of the fundamentals required to build complex models of nearly any kind of system.

- The **GoldSim Model Library**, which contains a collection of example models to allow you to see how specific features of GoldSim can be used and/or how GoldSim can be used for specific applications.

- The **GoldSim Blog**, which provides an informal mechanism for GoldSim staff to share their knowledge, point out some of the more advanced (and perhaps overlooked) GoldSim features, share and discuss common mistakes we see in GoldSim applications, discuss interesting applications, and keep you abreast of our plans for further GoldSim developments.

You can stay up to date on the latest GoldSim news through these resources:

- The GoldSim LinkedIn Group, which is primarily used for announcements (e.g., new versions, interesting applications). You can join the Group here: www.linkedin.com/groups/1798413)

- Periodic email newsletters are sent two to three times per year. To be added to the newsletter list, contact us via the GoldSim Help Center (https://goldsim.zendesk.com).

Note: When you purchase GoldSim, you are entitled to a free one hour, live web-based training session in which one of our analysts provides an interactive training session via the Internet and telephone. You are strongly encouraged to take advantage of this free training.

Chapter 2: Contaminant Transport Module Overview

A poet physicist once calculated how many atoms from Plato's body each of us has appropriated as our own - probably in excess of 10^{10}. Behind the vertigo of the multiple reincarnations and the comforting thought of all the great people each of us has been lies the profound and fundamental principle of the conservation of mass.

Francois M.M. Morel, *Principles of Aquatic Chemistry*

Chapter Overview

This chapter provides an introduction to and a "quick tour" of the GoldSim Contaminant Transport Module. It presents the basic concepts of how contaminant transport is simulated in GoldSim, provides an overview of the features and capabilities of the program, summarizes the specialized elements associated with the module, and outlines the steps required to build a contaminant transport model for an environmental system.

If you read nothing else in this manual before starting to use the Contaminant Transport Module, it is strongly recommended that you read this chapter, as it will tell you what the module is capable of doing, provide an overview of how to build a contaminant transport model, and direct you to those portions of the manual where you can obtain further information.

Warning: This chapter assumes that you are familiar with the basic capabilities of GoldSim. If not, you should refer to the **GoldSim User's Guide**.

In this Chapter

This chapter discusses the following:

- Top-Down Modeling Philosophy
- Modeling Contaminant Transport Using GoldSim: Basic Concepts
- Features and Capabilities of Transport Pathways
- What Does the Contaminant Transport Module Add to the GoldSim User Interface?

- Building a Contaminant Transport Model in GoldSim

- Using Features of the GoldSim Simulation Framework in Contaminant Transport Models

- Where Do I Go From Here?

Top-Down Modeling Philosophy

Before describing the GoldSim Contaminant Transport Module in detail, it is important to first discuss the underlying philosophy incorporated into its overall design.

In general terms, there are two ways to approach any kind of modeling problem: from the "***bottom-up***", or from the "***top-down***". Although the GoldSim Contaminant Transport Module can be readily used in a "bottom-up" manner, it was specifically designed to facilitate "top-down" modeling.

What is "Bottom-Up" Modeling?

"Bottom-up" modeling approaches attempt from the outset to acquire data and model the various controlling processes in great detail, and typically make use of complex ***process-level models*** for the various system components. The emphasis is on understanding and explaining the processes in great detail in order to eventually describe the behavior of the entire system.

While such an approach may seem at first glance to be "scientifically correct", for the following reasons it is generally not the best way to solve real world problems:

1. The level of detail in a model developed from the bottom-up often becomes inconsistent relative to the amount of available information. That is, a model is only as good as its inputs, and if you don't have much information, a detailed model is generally no better than a simple one.

2. It is often difficult to appropriately integrate and capture interdependencies among the various model components in a bottom-up model, since it is often impossible (or computationally impractical) to dynamically couple the various detailed process-level models used for the components of the system As a result, important interactions in the system are often intentionally or unintentionally ignored in a bottom-up model.

3. It is easy for a bottom-up modeling project to lose sight of the "big picture" (i.e., to "not see the forest for the trees"). As a result, such an approach can be very time-consuming and expensive, with much effort being spent on issues that prove to have little or no impact on the ultimate objective of the project.

4. Finally, and perhaps most importantly, such models tend to be very difficult to understand and explain (and hence be used) outside of the group of people who create them.

What is "Top-Down" Modeling?

"Top-down" modeling approaches, on the other hand, start from the top (i.e., the ultimate objective of the modeling exercise) and concentrate on the *integration* and coupling of all system components. The controlling processes may initially be represented by approximate high-level (i.e., less detailed or "abstracted") models and parameters.   The model can then evolve by adding detail (and reducing uncertainty) for specific components as more is learned about the system. Such an approach can help to keep a project focused on total system performance without getting lost in what may prove to be unnecessary details. Moreover, because a properly designed top-down model tends to be only as

complex as necessary, is well-organized, and is hierarchical, it is generally easier to understand and explain to others.

There are two key points in the application of a top down modeling approach:

1. Top-down models <u>must</u> incorporate an accurate representation of the *model and parameter uncertainty* resulting from the approximations.

2. As opposed to representing all processes with great detail from the outset, details are only added when justified (e.g., if additional data are available, and if simulation results indicate that performance is sensitive to a process that is currently represented in a simplified manner). That is, details are only added to those processes that are identified as being important with respect to system performance and where additional detail will reduce the uncertainty due to model simplifications.

It is important to understand that a top-down model does not have to be "simple". Whereas a "simple" model might completely *ignore* a key process, a well designed top down model *approximates* the process while explicitly incorporating the resulting uncertainty that is introduced. Hence, in a top-down approach to system simulation, the objective is not to *explain* the detailed behavior of all aspects of the system, but rather to be as comprehensive as possible by integrating the available information in an attempt to *describe* the possible range of system behavior. That is, the focus of a top-down approach is on the ultimate *performance* of the system, as opposed to understanding all the details of the *processes* contributing to that performance.

It is important to reiterate that for the reasons stated previously, the maximum predictive capability does not always lie in the most complex model. In fact, qualified expert judgment may be preferable to using any model at all in some cases (i.e., in cases where either the models or the available data are unreliable or do not represent the actual system). As a simple example, consider the case where one wishes to predict the temperature in Seattle on March 15 of next year. A "high-level" top-down approach to this problem might be to use an almanac to obtain average weather statistics in the month of March, and subjectively assess the degree of variability expected from day to day to obtain a probability distribution for the temperature on that date. A "low-level" bottom-up approach to this problem would be to use a global climate model computer program, and carry out simulations to obtain a probability distribution of the temperature on that date. Clearly, the top-down approach would be just as accurate (if not more accurate) than the bottom-up approach in this case. Although this is an extreme example, it does help to illustrate that complex models are not always technically better than "simple" models, a point often overlooked by scientists and engineers involved in complex modeling efforts.

Although detailed process-level models may not be directly implemented when using a top-down approach, this is not to say that detailed modeling is not required. Quite to the contrary, detailed process-models form the foundation for a top-down model and are always required to some extent in order to generate the appropriate input parameters, and to assess the degree of approximation involved in simplified approaches.

The figure below schematically illustrates the information flow within a top-down modeling approach. Note that information must flow in both directions. At the base of the system are process-level models and field and laboratory experiments. This information (i.e., what processes to include, what processes to ignore, what input values to use, what level of uncertainty to assume) is then assimilated by experts into a form that can be used in a top-down ***total system***

model. The downward flow of information from the total system model consists of identification of the processes and parameters to which system performance is sensitive, and requests for further information. With time, the total system model can expand down the pyramid as more details are added to it, and the degree of reliance on expert judgment will be reduced.
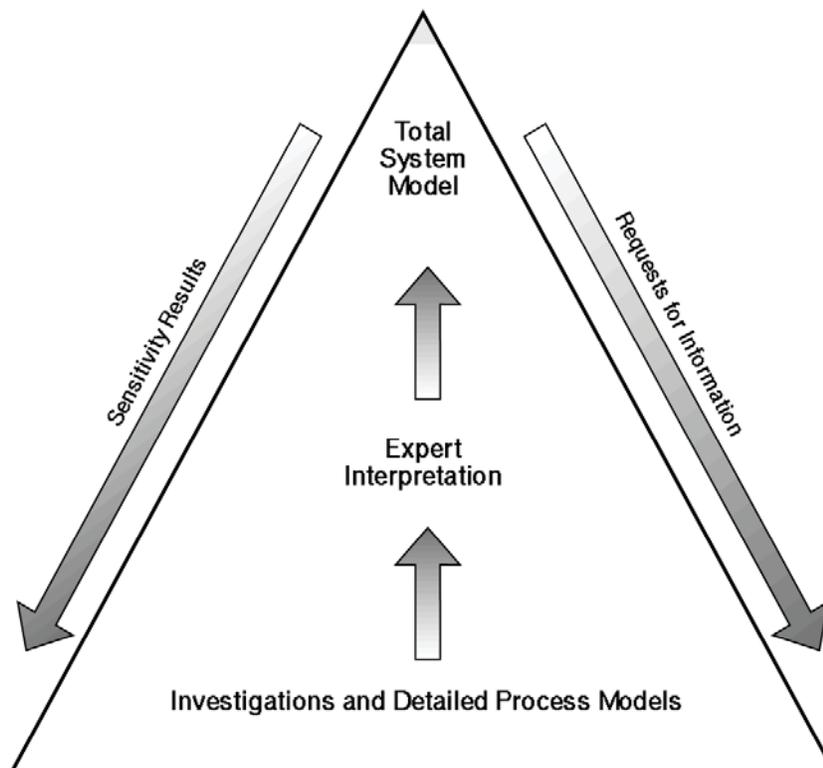
In summary, our view is that in almost all situations, you should design your models from the top-down, keeping them as simple as possible, and only adding complexity when it is warranted. As will be seen below and in the following chapters, the GoldSim Contaminant Transport Module can certainly be used in a bottom-up manner, and you can readily build very complex models. GoldSim was specifically designed, however, to facilitate top-down modeling, and we strongly encourage you to use the program in this way.

Modeling Contaminant Transport Using GoldSim: Basic Concepts

The GoldSim Contaminant Transport Module is a *mass transport model*. A mass transport model is a mathematical representation of an actual system (e.g., the subsurface environment near a waste disposal site) which can be used to simulate (and hence predict) the release, transport (movement) and ultimate fate of mass within the system. The "mass" that is typically simulated is that of chemical contaminants that have been accidentally released or intentionally disposed of within the system.

Contaminant Species

GoldSim allows you to simulate the transport of an unlimited number of species (types of chemical constituents) within an environmental system. The species can undergo complex user-specified chemical reactions as they are transported through the system. The species can be defined to behave independently, or can

be coupled by either being specified as part of a reaction (decay) chain or as isotopes of the same chemical element.

Note: Simulation of decay chains (reaction or daughter products) requires the RT Module. The CT Module can simulate decay, but cannot represent reaction products.

Note: Although the species in a GoldSim model will typically represent chemicals (man-made or naturally occurring), you can also use GoldSim to model the transport of other types of mass in an environmental system, such as bacteria, viruses or particulate matter such as dust or suspended sediments. You can even use GoldSim to simulate the transport of heat.

Read more: Creating and Editing Species (page 43); Simulating Non-Chemical Constituents (page 283).

Modeling Transport Pathways

The GoldSim Contaminant Transport Module allows you to simulate the transport of mass through an environmental system by providing a number of specialized GoldSim elements. The most important of these is the ***transport pathway*** (of which there are several types).

Transport pathways represent physical components through which contaminant species can move and/or be stored, such as aquifers, lakes, sediments, surface soil compartments, and the atmosphere.   You define the properties of the pathways, such as their geometry and which environmental ***media*** (e.g., water, soil, air) they contain. All pathways contain one or more environmental media. You define the general properties of each medium (e.g., its density) as well as the properties of each species in each medium (e.g., solubilities and partition coefficients).

You create an environmental system by defining a network of transport pathways, as shown below:
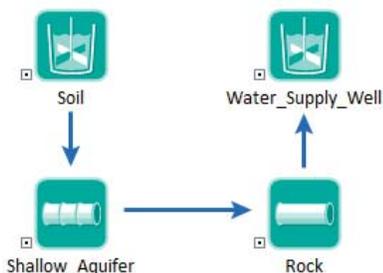
To create such a network, individual pathways are connected via mass flux links. A ***mass flux link*** defines the mechanisms by which species move between pathways. It represents a vector by species (i.e., it has one item for each species), since the flux will differ for each species being simulated, and has dimensions of mass/time.

Note: The Contaminant Transport Module relies heavily on GoldSim's ability to create and manipulate vectors. Therefore, in order to use the module, you must be comfortable with using vectors in GoldSim. If you are not familiar with this capability of GoldSim, refer to "Using Vectors and Matrices" in Chapter 10 of the **GoldSim User's Guide**.

Two major types of mass flux links and three special purpose mass flux links can be defined in GoldSim. In an ***advective mass flux link***, a quantity of a medium is specified to flow from one pathway to another, carrying dissolved, sorbed, and/or suspended species with it. In a ***diffusive mass flux link***, species diffuse between pathways according to a concentration gradient. Three special purpose mass flux links allow you to model processes that cannot be represented as using advection or diffusion. In a ***direct transfer mass flux link***, species are moved from one pathway to another based on a user-specified transfer rate. In a ***precipitate removal mass flux link***, species present as precipitated mass are moved from one pathway to another based on a specified transfer rate. In a ***treatment mass flux link***, species are treated or filtered and are moved to from one pathway to another based on a specified treatment efficiency (a fraction).

Note: The Contaminant Transport Module is a mass transport model, *not* a flow model. That is, it does not directly solve for the movement of media through the environmental system being modeled. Hence, you must directly enter the media flow rates associated with an advective flux link (or provide GoldSim with the equations for computing them).

Based on the properties of each pathway, the media in each pathway, the species, and the specified mass flux links, GoldSim computes the temporally varying concentrations in each pathway's media, as well as the mass fluxes between pathways. Hence, the fundamental output of a pathway element is a series of vectors:

- The mass (of each species) in the pathway;

- the concentration (of each species) within each environmental medium in the pathway; and

- the mass flux (of each species) to each of the pathways to which it is connected via mass flux links.

A typical pathway output is shown below:
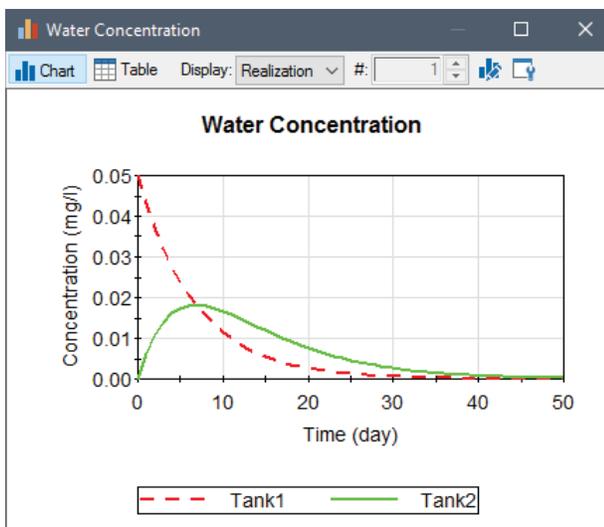
Read more: Features and Capabilities of Transport Pathways (page 20).

Modeling Contaminant Sources

Within GoldSim, there are two ways to introduce mass into the system:

- An initial mass or a rate of addition of mass can be directly specified for one or more pathways in the system; and

- When using the RT Module, the user can define the properties of one or more *sources*, and based on their properties, GoldSim will compute rates of release of mass from the source(s) to specified pathways. (Sources are not available in the CT Module.)

Often, you can use the former method to introduce mass into your model.   In many cases, however, direct specification of an initial mass or rate of release at various locations is not possible or appropriate, and explicit modeling of the source is necessary.

Note that the definition of what is meant by a "source" is completely determined by you. A "source" may represent an entire landfill, or a single buried drum; a group of leaking underground tanks or a complex engineered facility. The key point is that the source provides mass input to the pathways that then transport the mass through the system, as illustrated below.
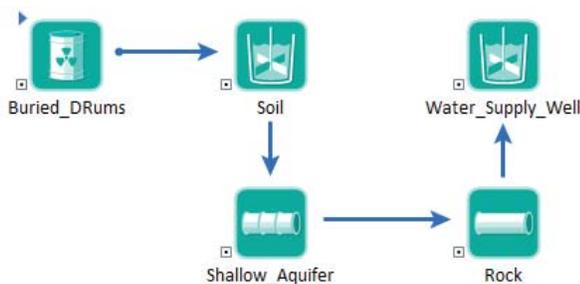
The Source element named "Buried_Drums" provides mass input to the Cell pathway named "Soil".

The properties of a source which you define consist of 1) the failure rate of any barriers (e.g., drums, boxes) which must fail before the species are released; and 2) the degradation rate of any matrix (e.g., cement, grout) in which the species are bound, which must degrade before the species are released.

Note: Sources are only available within the RT Module.

Modeling Impacts to Receptors

The objective of many contaminant transport studies is to not only compute contaminant concentrations or flux rates at various locations in the environment, but to also compute the impact of these contaminants on specific *receptors* (e.g., humans, wildlife, flora).

This is typically done by multiplying contaminant concentrations in environmental media (e.g., water, soil, air) by user-defined *impact conversion factors*. Impact conversion factors are species- and receptor-specific and have dimensions of impact per unit concentration.

GoldSim allows you to define specific receptors, and associate these with various pathways in your environmental system. The total impact to a receptor is then computed as the sum of the impacts associated with each pathway through which the receptor is exposed to the contaminant (e.g., drinking water from a well, breathing dust in the atmosphere, ingesting soil).

Impacts may be calculated as:

- *ratios* of contaminant concentrations to permissible limits (i.e., hazard quotients);

- health (e.g., cancer) *risks*; or

- radioactive *doses*.
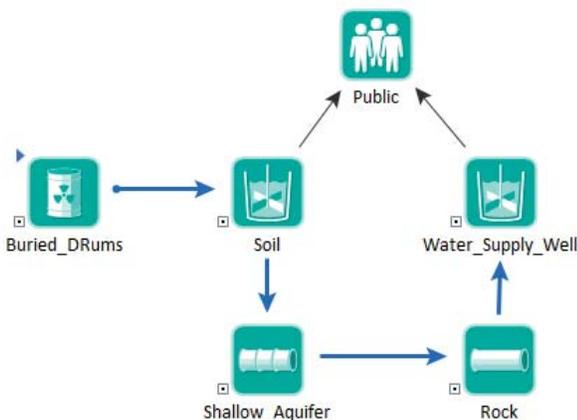
The Receptor named "Public" is exposed to contaminants via the Cell pathways "Water_Supply_Well" and "Soil".

Features and Capabilities of Transport Pathways

Having provided a quick overview of the basic components of the Contaminant Transport Module in the previous section, in this section the computational features of the primary component, the transport pathway, are outlined in somewhat greater detail, as this will provide an indication of the kinds of processes that can be simulated by GoldSim.

GoldSim transport pathways represent physical components through which contaminant species can move (and/or be stored) such as aquifers, lakes, sediments, surface soil compartments, and the atmosphere. In order to represent the wide variety of transport pathways that you may wish to simulate, GoldSim provides five different kinds of pathway elements:

- Cell pathways

- Aquifer pathways

- Pipe pathways

- External pathways

- Network pathways

These pathways can be used interchangeably within a model. Each of these four pathway elements is discussed briefly below.

Cell Pathway Features

A Cell pathway is mathematically equivalent to a mixing cell, and can explicitly represent the following processes:

- **Partitioning**. You can assign multiple fluid or solid media (e.g., water, oil, air, rock, soil) to a Cell, and define species partition coefficients between the various media. Contaminant mass is assumed to be instantaneously and completely mixed and equilibrated throughout the Cell, and contaminants are partitioned between the various media based on the partition coefficients and masses/volumes of the various media present.

- **Solubility constraints**. You can assign solubility limits for the contaminants in the fluids (typically water) present in the Cell. The dissolved concentration of the contaminants in the Cell cannot exceed the solubility limit. If you are simulating isotopes of the same element, GoldSim ensures that the sum of the concentrations of all isotopes does not exceed the solubility limit.

- **Mass transport**. You can define the processes and properties controlling the rate at which mass moves between pathways (e.g., from one Cell to another). Both advective and diffusive transport mechanisms can be explicitly represented. You must specify flow rates for advective transport and diffusion coefficients and geometric factors for diffusive transport. You must also specify the media which are being advected (both fluids and solids can be advected), and the media through which diffusion occurs (inter-media diffusion, such as across an air-water interface, can be specified). In addition, solids present in a Cell can be specified to be suspended in the Cell's fluid media, such that the transport of contaminants on suspended particulates (via advection or diffusion) can be explicitly modeled. For special situations, you can also simulate several transfer processes that cannot be described as either advection or diffusion (direct transfer, treatment, and precipitate removal).

When multiple Cells are linked together via advective and diffusive mechanisms, the behavior of the Cell network is mathematically described using a coupled system of differential equations. In effect, a network of Cells is mathematically equivalent to a finite difference network of nodes. GoldSim numerically solves the coupled system of equations to compute the contaminant mass present in each Cell (and the mass fluxes between Cells) as a function of time.

Cells are commonly applied to simulate discrete compartments in an environmental system (such as ponds, lakes, shallow soil compartments, or the atmosphere). In some situations, a series or network of Cells may also be the best way to simulate features such as aquifers and rivers.

Read more: Using Cell Pathways (page 116).

Aquifer Pathway Features

An Aquifer pathway is intended to represent a feature that essentially behaves as a *fluid conduit*. It provides a way to simulate processes such as vertical transport through an unsaturated (vadose) zone, and horizontal transport in aquifers, rivers, channels and pipelines.

Aquifer and Pipe pathways can be used for many of the same purposes. Depending on the system to be simulated, however, one is typically preferred over the other.

Read more: Comparing Pipes and Aquifers (page 87).

Unlike Cell pathways, Aquifer pathways can contain only a single fluid medium. They can, however, contain a solid medium which can impact transport (e.g., by modifying the porosity of the pathway and/or acting to sorb and hence retard species).

An Aquifer pathway actually performs its computations by creating a temporary set of linked Cell elements during the simulation, which are subsequently removed at the end of the simulation. In most cases, there is no need for you to be aware of how this is done, or to view the temporay Cell pathways that are created.

Because Aquifers internally use Cells to carry out their calculations, they can represent most of the same processes that can be represented by a Cell network. In particular, Aquifers can represent the following:

- **Partitioning**. Within each internal Cell contaminants are partitioned between the the Reference Fluid and the Infill Medium based on the partition coefficients and masses/volumes of the various media present.

- **Solubility constraints**. You can assign solubility limits for the contaminants in the Reference Fluid (typically water) present in the pathway. The dissolved concentrations of the contaminants in the pathway cannot exceed the solubility limits. If you are simulating isotopes of the same element, GoldSim ensures that the sum of the concentrations of all isotopes does not exceed the solubility limit.

- **Mass transport**. Advective, dispersive and diffusive transport mechanisms are explicitly represented within the pathway (using advective and diffusive mass flux links between the internal Cells).

- **Suspended Solids** can be specified to be present in the Aquifer. These Solids are assumed to be advected and dispersed along the Aquifer. Species which partition onto the suspended Solids are transported with them as they move through the Aquifer.

Because multiple Cells are linked together via advective and diffusive mechanisms, the behavior of the Cell network is mathematically described using a coupled system of differential equations. In effect, the network of Cells created within an Aquifer pathway is mathematically equivalent to a finite difference network. GoldSim numerically solves the coupled system of equations to compute the contaminant mass present in the pathway (and the mass fluxes leaving the pathway) as a function of time.

The geometry of the pathway is defined by specifying a length and a cross-sectional area. Conceptually, the pathway may be straight or curved. It simply represents a stream tube for the advecting medium.

Aquifer pathways are ideal for simulating processes such as vertical transport through an unsaturated (vadose) zone and horizontal transport in aquifers, rivers, channels and pipelines.

Read more: Using Aquifer Pathways (page 163).

Pipe Pathway Features

A Pipe pathway is intended to represent a feature which essentially behaves as a *fluid conduit*. Mass enters at one end of the conduit, advects through (and disperses within) the conduit, and then exits at the other end of the conduit.

Aquifer and Pipe pathways can be used for many of the same purposes. Depending on the system to be simulated, however, one is typically preferred over the other.

Read more: Comparing Pipes and Aquifers (page 87).

Unlike Cell pathways, Pipe pathways can contain only a single fluid medium. They can, however, contain solid media which can impact transport (e.g., by modifying the porosity of the pathway and/or acting to sorb and hence retard species).

Pipe pathways use a Laplace transform approach to provide analytical solutions to a broad range of advectively-dominated transport problems involving one-dimensional advection, longitudinal dispersion, retardation, decay and ingrowth, and exchanges with immobile storage zones (e.g., matrix diffusion).

Two types of simple contaminant retardation processes can be represented within a Pipe pathway:

- equilibrium partitioning between the fluid in the pathway and a user-specified infill material; and

- equilibrium partitioning between the fluid in the pathway and a user-specified coating material (around the perimeter of the pathway).

In addition to these linear retardation mechanisms mentioned above, Pipe pathways can also represent interchanges with two types of immobile storage zones along the length of the pathway:

- *matrix diffusion zones*, in which the transfer rate into and out of the zone is proportional to the concentration difference and the diffusive properties of the zone; and

- a *"stagnant" dispersive zone*, in which the transfer rate into and out of the zone is proportional to the concentration gradient and the flow rate in the pathway.

Finally, suspended Solids (e.g., colloids) can be specified to be present in a Pipe. These Solids are assumed to be advected and dispersed along the Pipe, but are not subject to retardation processes or interactions with storage zones. Species which partition onto the suspended Solids are transported with them as they move through the Pipe.

The geometry of the pathway is defined by specifying a length, a cross-sectional area, and a perimeter. Conceptually, the pathway may be straight or curved. It simply represents a stream tube for the advecting medium.

Pipe pathways may be used for simulating processes such as vertical transport through an unsaturated (vadose) zone, and horizontal transport in aquifers,

rivers, channels and pipelines. They are particularly valuable for simulating transport through fractured rock masses.

Read more: Using Pipe Pathways (page 179).

External Pathway Features

External pathways provide a mechanism by which external program modules for contaminant transport (e.g., analytical, finite element or finite difference transport models) can be directly integrated into GoldSim. These modules are linked into GoldSim as DLLs (Dynamic Link Libraries) at run time.

You determine the manner in which the External pathway operates on the contaminant mass it receives: the External pathway may be a simple one-dimensional representation, or could be a complex three-dimensional model.

You define the manner in which the External pathway is linked to the rest of the pathway network by specifying the input mass flux links (i.e., the pathway(s) which discharge mass to the External pathway) and the output mass flux links (i.e., the pathway(s) to which the External pathway discharges mass). GoldSim then automatically calls the function representing the External pathway at the appropriate times, passing the appropriate information back and forth between GoldSim and the function.

Integrating external contaminant transport modules into GoldSim requires that you develop a "wrapper" (or "shell") around your existing function, and in most cases, this will require only a limited number of programming modifications.

Read more: Using External Pathways (page 200).

Network Pathway Features

Network pathways provide a computationally efficient way to simulate large, complex networks of one-dimensional conduits in order to describe contaminant transport through fractured rock systems.

A Network pathway is made up of multiple "pipes". Each pipe has all the features and capabilities of the Pipe pathways discussed above. Hence, Network pathways are effectively large collections of Pipe pathways. The network, however, can be very large (e.g., 100,000 pipes). This allows complex and realistic fracture systems to be simulated.

Network pathways require specification of a *fracture network*, which can be entered by hand, but more likely, would be generated by a discrete fracture network generation and flow simulation code. The fracture network identifies all of the pipes in the network, the manner in which they are connected, and each pipe's geometry and flow rate. In addition, for each pipe, it specifies the *fracture set*, which identifies the transport properties of the pipe (e.g., porous infill material, coating material, properties of matrix diffusion zones, etc.).

GoldSim uses a Laplace transform algorithm to solve complex fracture networks in a very efficient manner. In fact, even large networks (100,000 pipes or more) can be solved relatively quickly.

To facilitate representation of uncertainty in the fracture network connectivity and flow properties, you have the option to define a number of separate fracture networks and instruct GoldSim to randomly select one of these every realization.

Note: Network pathways are only available within the RT Module.

Read more: Using Network Pathways (page 214); What is the Difference Between GoldSim CT and GoldSim RT? (page 4).

What Does the Contaminant Transport Module Add to the GoldSim User Interface?

The Contaminant Transport Module is a program extension to the GoldSim simulation framework. As such, it simply adds some additional features to the user interface. The user interface components which the Contaminant Transport Module adds can be summarized as follows:

- An additional item, **Contaminant Transport**, is added to the context-sensitive (right-click) menu in the graphics pane (shown below), to the context-sensitive menu for Containers, and to the **Model| Insert** menu on the menu bar:
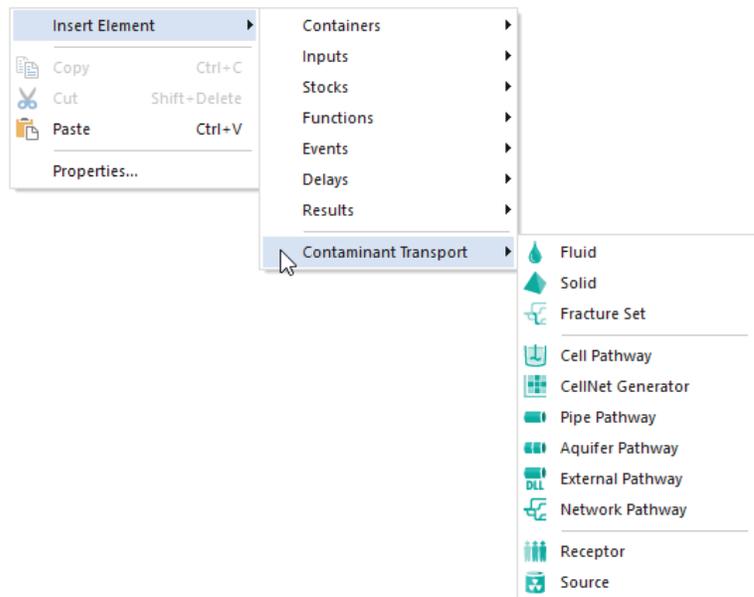
Note that "Fracture Set", "CellNet Generator", "Network Path", and "Source" only appear if you are using the RT Module. They are not present in the CT Module.

- Pressing the CT Element button in the Element toolbar provides access to a menu for inserting a CT Module element:
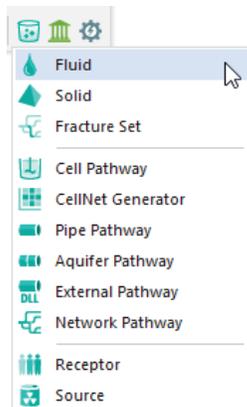
Note that "Fracture Set", "CellNet Generator", "Network Path", and "Source" only appear if you are using the RT Module. They are not present in the CT Module.

- When you create a new file, a Material Container is automatically placed in the Model Root. This Container contains a Species element and the Reference Fluid (named Water). These two elements can be moved, but cannot be deleted.

- The *Species* and *Elements* array label sets are added to the drop-down lists available when defining the output attributes for an element:
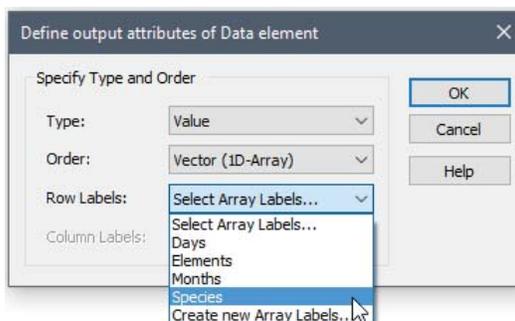
These sets of array labels are populated when you add species to your model (via a Species element).

- A **Contaminant Transport** tab is added to the Options dialog (accessed via **Model | Options**) for defining options which are specific to the Contaminant Transport Module:
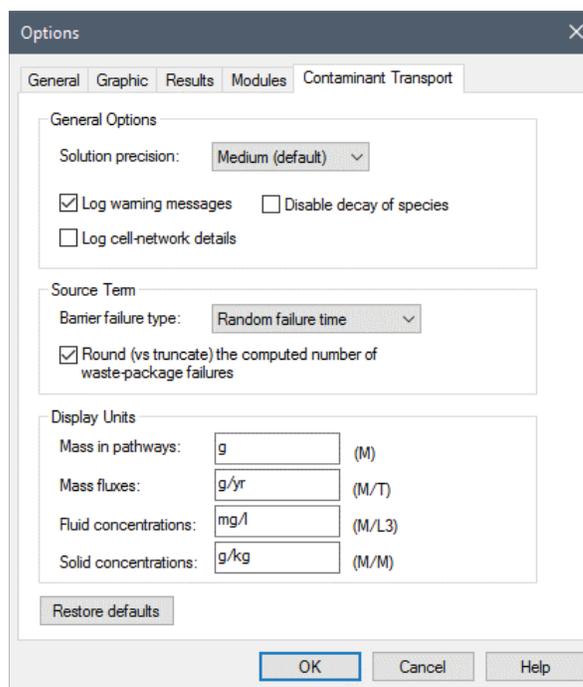
Building a Contaminant Transport Model in GoldSim

This section briefly outlines the steps required to create a contaminant transport model, and provides a quick tour of each of the GoldSim Contaminant Transport Module elements.

In general, you create a mass transport model of an environmental system within GoldSim in the sequence outlined below:

1. Specify the species to be included in the simulation;

2. Specify the transport and storage media within the environmental system;

3. Specify the transport pathways in the system;

4. Specify the manner in which the transport pathways are inter-connected via mass flux links;

5. Define the contaminant source terms for the system (if any);

6. Define the receptors who may be impacted by contaminants within the system; and

7. Specify the rate and consequences of any disruptive events that may occur.

Note: For all but the most simple models, the most important (and time-consuming) tasks in a contaminant transport modeling project are typically the development of a *conceptual model* and the quantification of the inputs for the system you are trying to simulate. Although the quantification of many of the inputs can be delayed until after you have represented the system in a numerical tool such as GoldSim, development of the conceptual model must, for the most part, occur beforehand. Development of a conceptual model and quantification of inputs are discussed further in Appendix A.

Read more: Appendix A: Introduction to Environmental Simulation (page 287).

Each of the seven steps listed above is outlined below. The intention of this section is to simply provide a quick overview of these seven steps, and introduce you to each of the Contaminant Transport Module elements. Each of the seven steps is discussed in greater detail in subsequent chapters.

Defining Species

GoldSim provides a specialized element for defining the contaminant species in a simulation. The *Species* element is located in the Material Container, which is automatically created in the Model Root whenever you create a new file with the Contaminant Transport Module. This element can be moved, but it cannot be deleted.

The Species element is used to add, delete, and edit species. Double-clicking on the Species element brings up the following dialog:
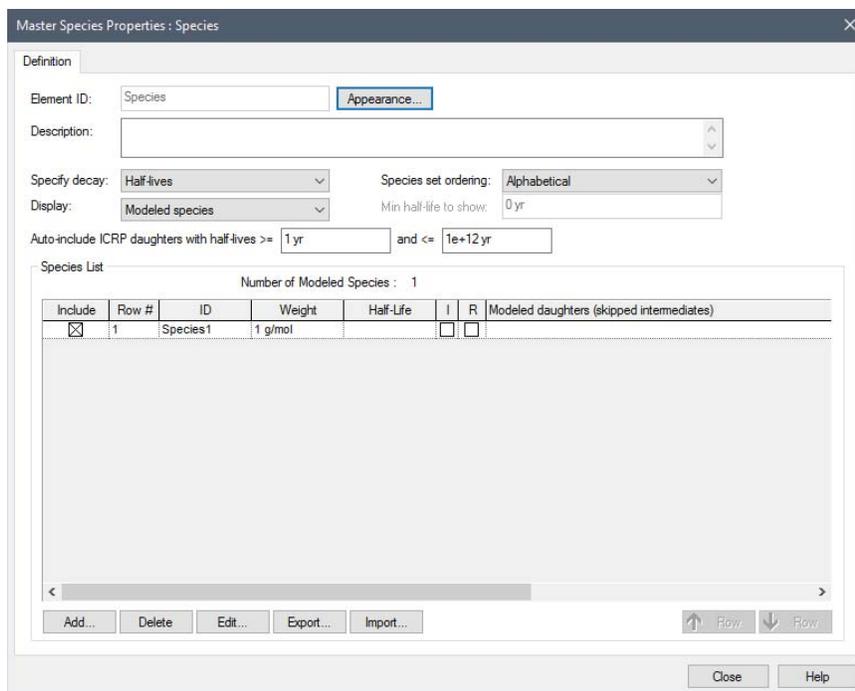
Because the RT Module allows decay chains (daughter products) to be simulated (and to support this, allows you to link to an extensive database of radionuclide decay data), the Species dialog is slightly different depending on whether you are using the RT Module or the CT Module. The screen above is from the RT Module. If you are using the CT Module, some of the fields will not be available.

Species are added (and deleted) using the **Add…** and **Delete…** buttons. (If you are using the RT Module, you also have access to a large database of radionuclide species that can be selected to be included in the model).

Read more: Displaying and Using Species from the ICRP Database (page 47).

Double-clicking on an existing species in the list, or adding a new species displays the Species editing dialog:

The fundamental properties of the species are defined in this window, including the rate at which the species decays (entered as either a half-life or a first-order decay rate), and whether it is part of a decay chain. Although GoldSim requires a first-order decay rate, by making the decay rate a function of the concentration of other species, or of other model parameters (e.g., temperature), nearly any complex reaction can be represented.

Note: Decay chains can only be specified in the RT Module.

Read more: Creating and Editing Species (page 43); Modeling Complex Chemical Reactions (page 279); What is the Difference Between GoldSim CT and GoldSim RT? (page 4)

Defining Media

Before you can define the transport pathways through which the species will be transported, you must first define the environmental media (e.g., water, air, soil) contained in those pathways.

You can define two types of media in GoldSim: *Fluids* and *Solids*. All models contain a *Reference Fluid*. Reference Fluids provide a basis for defining partition coefficients between media for the various species in the model (i.e., the ratio of the species' concentration in the medium to its concentration in the Reference Fluid at equilibrium).

For convenience, the Reference Fluid "Water" is automatically present in the Material Container (which is created in the Model Root whenever you create a new file with the Contaminant Transport Module). The editing dialog for the Reference Fluid looks like this:
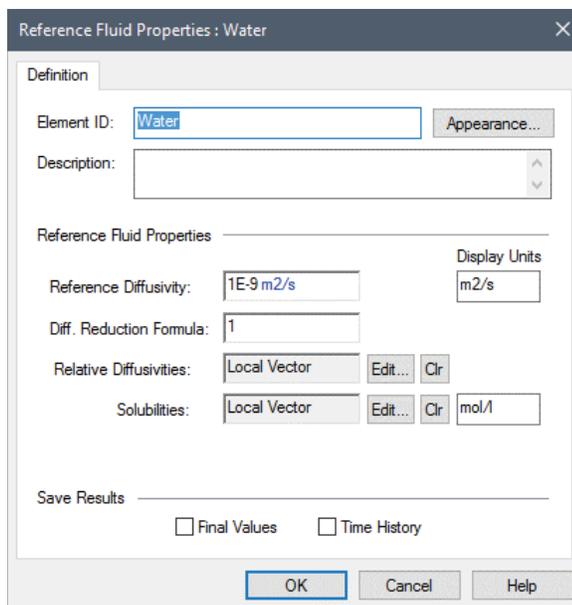
The default name for the Reference Fluid is Water, although you can change this if desired.
***Relative Diffusivities** and **Solubilities** are vectors, since the property must be defined separately for each species.*

You can add additional Fluids and Solids as required (and they can be placed in any Container in the model).

The dialog for other Fluids is similar to that of the Reference Fluid:
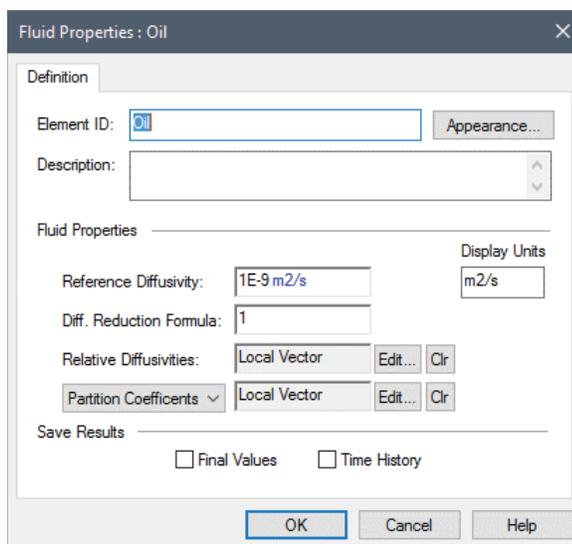
When defining a Fluid, you can choose to specify either Solubilities or Partition Coefficients. Partition coefficients are defined relative to the Reference Fluid. Because a partition coefficient is a ratio of concentrations, it is dimensionless for Fluids.

Solid elements require somewhat more information:

The partition coefficients for a Solid are defined relative to the Reference Fluid, and have dimensions of volume divided by mass.

The properties that you specify for Fluids and Solids are perhaps the most important group of inputs in your contaminant transport model. Because each pathway is defined in terms of these media (e.g., the volume of Water or the mass of Sand that exists in a particular pathway), these properties control the way that mass is transported and stored within the pathway network.

Because they represent the fundamental controlling properties of your system, quantifying these inputs in an appropriate manner is essential to producing defensible predictions of contaminant transport. This is discussed further in Appendix A.

Read more: Appendix A: Introduction to Environmental Simulation (page 287); Creating and Editing Environmental Media (page 63).

Defining Pathways

After having defined the species and media, you can start to build the network of transport pathways through which the species will be transported.

Because there are a variety of transport pathways that you may wish to simulate, GoldSim provides five different pathway elements that you can use interchangeably to build a pathway network. The two most commonly used pathway elements are discussed briefly below.

Defining Cell Pathways

The most versatile pathway element is the Cell pathway. Cell pathways would typically be applied to simulate discrete, well-mixed environmental compartments such as ponds, lakes, shallow soil compartments, or the atmosphere. In some cases, a series of Cells may also be the best way to simulate features such as aquifers and rivers.

The editing dialog for a Cell pathway looks like this:
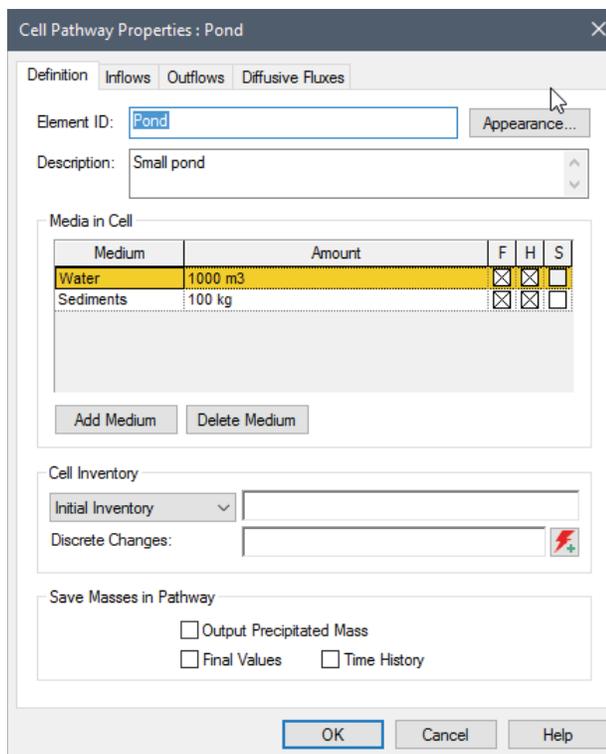
The primary input that must be defined for a Cell pathway is the quantity of each medium that is present in the pathway. The Reference Fluid is automatically present in each new Cell. Media are added and deleted using the **Add Medium** and **Delete Medium** buttons. The number of separate media present in a pathway is unlimited, but most Cell pathways will typically include no more than two or three.

The output of a Cell pathway element includes the total mass of each species in the pathway, and the concentration of each species in each medium in the pathway.

Read more: Using Cell Pathways (page 116).

Defining Aquifer Pathways

Aquifer pathways are intended to represent environmental features that behave as fluid conduits, such as aquifers, rivers, channels and pipelines.

An Aquifer pathway actually performs its computations by creating a temporary set of linked Cell elements during the simulation, which are subsequently removed at the end of the simulation.

The editing dialog looks like this:

The Fluid flowing through the Aquifer pathway is always the Reference Fluid. The geometry of the pathway is defined by specifying an Aquifer Length and an Aquifer Area. You must also define the Number of Cells to be used to discretize the system. Based on this, GoldSim internally creates a series of linked Cell pathways. The specified Infill Medium and Fluid Saturation are used to determine the quantity of media in each Cell. A pathway Dispersivity is also specified. Advective and diffusive flux links are automatically created by GoldSim to appropriately model advection, dispersion and diffusion through the linked Cells.

The output of an Aquifer pathway element consists of the total mass of each species in the pathway, and the concentration of each species in the flowing Reference Fluid exiting the pathway (i.e., in the last Cell).

Read more: Using Aquifer Pathways (page 163).

Interconnecting Transport Pathways

A mass transport model simulates the movement of species between pathways. Hence, the pathways that you create must be interconnected into a pathway network before you can simulate contaminant transport.

Pathways are connected together into a network by creating *mass flux links* between pathways. Mass flux links control the rate at which each species is transported between pathways. Mass flux links are created from tabs (**Inflows**, **Outflows**, and **Diffusive Fluxes**) in the pathway editing dialogs. There are two primary types of mass flux links: *advective* and *diffusive,* and 3 special purpose mass flux links: *direct transfer, precipitate removal,* and *treatment.*

For most applications, mass transfer between pathways can be represented as a combination of advective and diffusive processes. In some specialized cases (e.g., uptake of contaminants by plants, removal due to treatment processes),

however, it may be necessary to utilize one of the three special purpose flux links to properly represent the kinetics of the mass transfer.

Advective mass flux links (as well as the three special purpose mass flux links) are created from the **Inflows** and **Outflows** tabs, which are nearly identical in appearance. The **Outflows** tab is used to create an advective (or special purpose flux link) *from* the current pathway *to* another pathway. The **Inflows** tab is used to create an advective flux link (or special purpose flux link) *to* the current pathway *from* another pathway.

The **Outflows** tab looks like this:
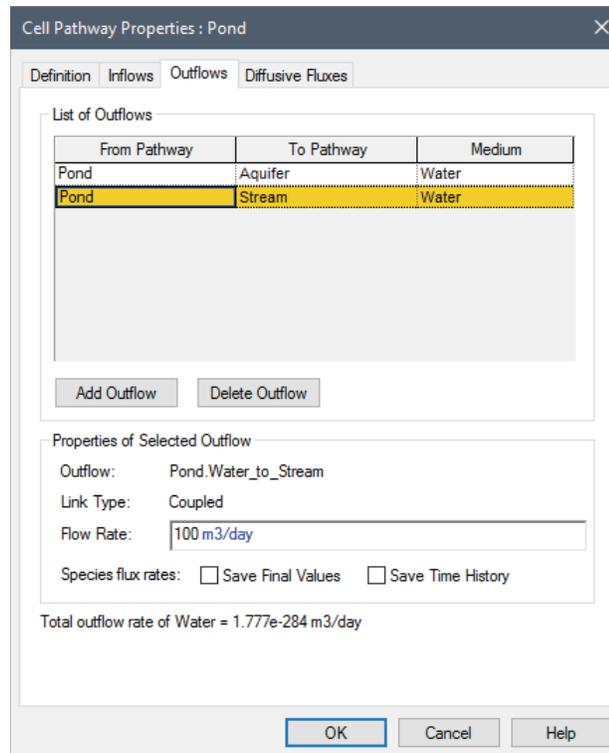
For each advective mass flux link, you must specify the pathway to which you are connecting, the medium that is flowing, and the flow rate.

You can create as many advective (and special purpose) outflows (or inflows) as desired in order to build your pathway network. Note that advective and special purpose mass flux links are unidirectional (the flow rate cannot be negative).

Diffusive mass flux links are created from the **Diffusive Fluxes** tab. Whereas advective fluxes can be defined between all types of pathways, all diffusive fluxes must originate in a Cell pathway.

The **Diffusive Fluxes** tab looks like this:
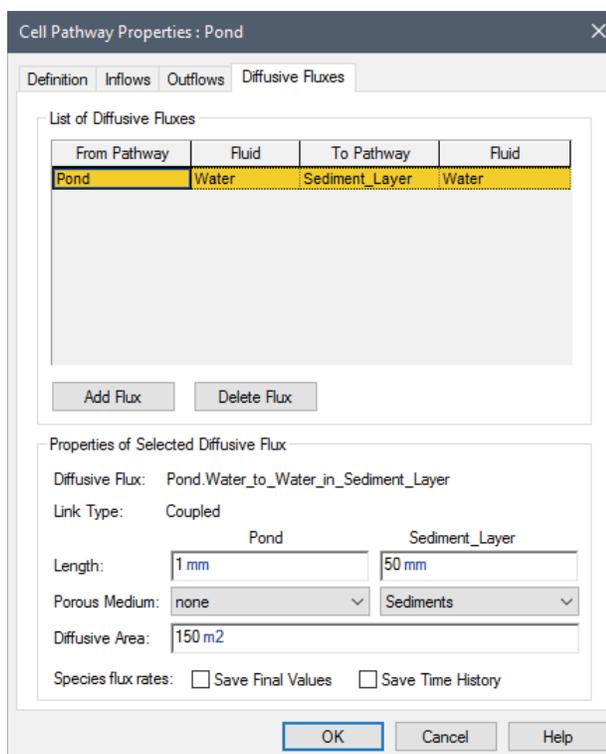
For each diffusive flux link, you must specify the pathway to which you are connecting, the Fluid through which the species are diffusing, and the properties of the diffusive link. The properties of the diffusive link include the geometry of the link and whether the diffusion takes place through a porous medium.

Unlike advective mass flux links, diffusive mass fluxes can be bi-directional. That is, species can be transported in either direction.

Although in most cases, the mass flux between two pathways will be dominated by either advection (e.g., advection in flowing water) or diffusion (e.g., diffusion through stagnant water), in some situations it will be appropriate for pathways to be simultaneously connected by both advective and diffusive links (e.g., advection and diffusion in slowly flowing water).

Read more: Creating Mass Flux Links (page 88).

The assumptions and mathematical details upon which the transport pathway elements are based are described in Appendix B.

Read more: Appendix B: Details of Pathway Computations (page 295).

Defining Sources

One way to specify a source of contamination in a contaminant transport model is to simply specify an initial mass of contaminant or a rate of addition of mass for one or more transport pathways. In many cases, however, it may be necessary to explicitly model a source such that the effect of the barriers (such as drums or boxes) and/or waste matrix (e.g., cement) in which the species are initially contained can be more accurately represented.

This is particularly important when simulating the behavior of proposed or existing waste disposal facilities which have, as part of their design, engineered packages or containers in which the waste is placed prior to disposal.

GoldSim provides a Source element that allows you to accomplish this. The editing dialog for a Source looks like this:
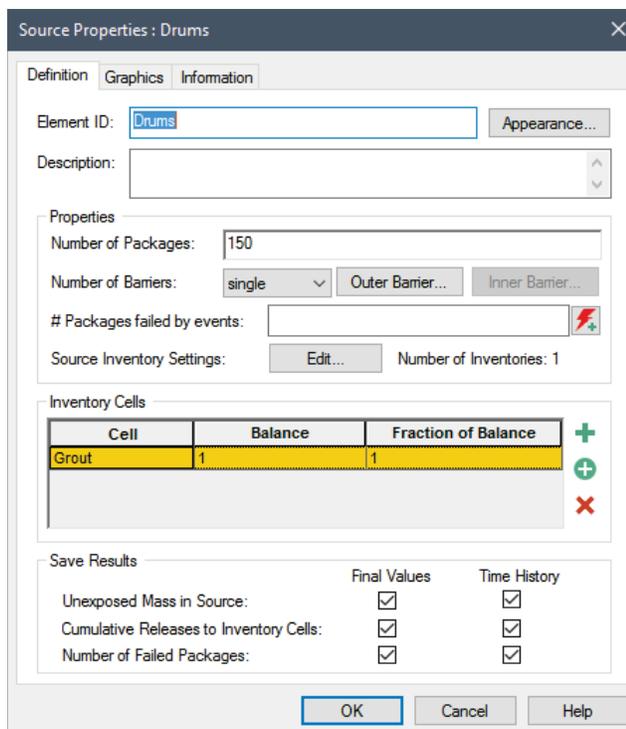
Inputs to a Source element include the rate at which the packages containing the waste fail, the amount of initial mass of each species (the inventory),the location of the inventory (with respect to the barriers), the degradation rate of any matrix material in which the inventory is initially contained, and the pathways to which the mass from the Source will be released.

Note: Source elements are only available in the RT Module.

Read more: What is the Difference Between GoldSim CT and GoldSim RT? (page 4).

The outputs from the Source include the amount of mass of each species remaining in the Source, the cumulative amount of mass of each species which has been released, and the number of failed packages.

Read more: Chapter 5: Contaminant Sources (page 239).

The assumptions and mathematical details upon which the Source element is based are described in Appendix E.

Read more: Appendix E: Details of Source Computations (page 355).

Defining Impacts to Receptors

The objective of many contaminant transport calculations is to not only compute contaminant concentrations or flux rates at various locations in the environment, but to also compute the impact of these contaminants on specific *receptors* (e.g., humans, wildlife, flora).

Impacts may be calculated as:

- ratios of contaminant concentrations to permissible limits (i.e., hazard quotients);

- health (e.g., cancer) risks; or

- radioactive doses.

Impacts such as these are typically computed by multiplying the concentrations in an environmental medium to which the receptor is exposed (e.g., water in a well) by a set of *impact conversion factors*. Impact conversion factors are species- and receptor-specific, and have dimensions of impact per unit concentration.

> **Note:** Computing the impact to a receptor always involves carrying out a term-by-term multiplication of a concentration vector and an impact conversion factor vector. As described in "Using Vectors and Matrices" in the **GoldSim User's Guide**, you can carry out a term-by-term multiplication of two vectors using the * operator.

Within GoldSim, you could compute an impact by using an Expression element to carry out a term-by-term multiplication of the species concentration vector for a particular medium in a pathway by a vector of impact conversion factors. For convenience, the Contaminant Transport Module provides a specialized version of an Expression element (a Receptor element) to facilitate this calculation. The dialog for this element looks like this:

*The **Impact Type** determines the dimensions of the impact which is computed. The equation computing the impact is entered directly below the type. The output of this equation must be a vector by species, with the dimensions being consistent with the specified impact type.*

Typically, the impact to a receptor will be a sum of several term-by-term vector multiplications, since the receptor is likely to interact with multiple contaminated media (e.g., water in a well, soil, dust).

Read more: Chapter 6: Receptors (page 269).

Defining Disruptive Events

The final step in creating your contaminant transport model is to define the occurrence and consequence of any disruptive events that may impact your system.

GoldSim provides the ability to model the occurrence and consequences of discrete events (see "Simulating Discrete Events" in the **GoldSim User's Guide**). For example, you could simulate an event such as an earthquake which

has the consequence of instantaneously changing the value of some parameters in the model (e.g., increasing the flow rate in a pathway) when the event occurs.

In addition to changing parameter values, the GoldSim Contaminant Transport Module allows you to use events and consequences to instantaneously move mass from one pathway (or Source) to another pathway, and/or to disrupt packages in a Source in response to an event such as an earthquake or an industrial accident.

Read more:

Using Basic GoldSim Features in Contaminant Transport Models

It is important to keep in mind the basic features of the GoldSim simulation framework as you build your contaminant transport model, as these greatly expand the power and flexibility of the tool. Three key of these basic features are highlighted below.

Utilizing the Basic GoldSim Elements in a Contaminant Transport Model

Nearly all of the inputs to the GoldSim Contaminant Transport Module elements accept links from other GoldSim elements (with compatible data type and dimension). For example, you could define the length of a pathway using an Expression, or the partition coefficient of a species for a particular medium using a Look-Up Table.

If necessary, you can even link an external DLL to your model using GoldSim's External element. This, for example, would allow you to dynamically define the solubilities using a geochemical equilibrium code.

GoldSim's Extrema element is also likely to be useful when carrying out contaminant transport simulations. The Extrema element allows you to compute the highest or lowest value achieved by a particular output over the course of a simulation. For example, you could use an Extrema element to compute the peak concentration in a particular medium in a pathway, or the peak impact to a receptor.

Perhaps the most powerful feature of the GoldSim simulation framework is the ability to describe inputs as probability distributions using Stochastic elements. This is particularly appropriate when simulating contaminant transport through the subsurface, as many of the controlling parameters will necessarily be uncertain. If you describe your inputs using probability distributions, the output of your model will be in the form of probabilistic contaminant transport predictions (e.g., the probability distribution of the peak concentration in a particular pathway).

Note: Chapter 4 of the **GoldSim User's Guide**, "Using the GoldSim Elements", describes all of the basic GoldSim elements in detail.

Representing Variability in the Contaminant Transport Module

All real environmental systems are variable to some extent. For example, aquifers are generally heterogeneous with respect to flow and transport properties, chemical conditions vary spatially throughout the environment, and flow rates vary spatially within a stream. Such variability can have a large influence on the behavior of the system, and it is therefore very important to represent this in your model.

Much of this variability can be directly represented within GoldSim using the basic structure and features of transport pathways and sources. For example, variability in transport pathways can be represented by defining multiple pathways with differing properties, and barrier failure distributions in contaminant sources typically reflect spatial variability in chemical and/or hydrologic conditions.

How would one represent, however, the fact that the decay rate or partition coefficient for a contaminant is spatially variable? In this case, the solution is to define separate Solid, Fluid or Species elements in each location where the properties vary. GoldSim provides some advanced capabilities to facilitate this (localizing Containers and cloning elements). These two features are discussed in detail in Chapter 10 of the **GoldSim User's Guide.**

Read more: Representing Spatial Variability (page 274).

Utilizing GoldSim's Graphical Features in a Contaminant Transport Model

A powerful feature of the GoldSim simulation framework is its ability to incorporate graphics, text, images and hyperlinks into a model. By using these tools, you can create more than just a contaminant transport model of your system - you can create a visual information management system in which the model, the model documentation, and the presentation of results are one and the same.

GoldSim's ability to create top-down, hierarchical models (by using Containers), coupled with these presentation and documentation capabilities allows you to present your model at different (and appropriate) levels of detail to different audiences.

Note: These documentation and graphical features are discussed in detail in Chapter 9 of the **GoldSim User's Guide**, "Documenting and Presenting Your Model".

Where Do I Go from Here?

If you are in a hurry to get started with building a contaminant transport model, you can "dive in" to the GoldSim Contaminant Transport Module now. Using the information presented in this chapter, coupled with the context-sensitive online help (and/or occasional reference to the index or table of contents of this document), you should be able to begin to experiment with the program and build some simple contaminant transport models. Experimenting with the GoldSim Contaminant Transport Module in this way prior to proceeding will be a worthwhile exercise for most users.

Contaminant Transport Example Models

The remaining chapters utilize and discuss examples that are relevant to each chapter. When you install GoldSim, a number of examples are installed with the program. These example model files are mentioned in the text, and provide an excellent way to begin to experiment with GoldSim. Each example is internally documented with comments regarding the way the model was implemented.

Note: You can quickly access these files by selecting **File|Open Example…** from the main GoldSim menu. They are all located in ia subfolder named Contaminant Transport Examples.

Note: Additional (and generally more detailed) example models are available in the Model Library on the GoldSim web site.

While these example problems will provide an excellent introduction, in order to build more complex models, sooner or later you will likely have to read most of the remainder of this manual. In particular, many users may not feel comfortable using the program until they understand the assumptions and mathematical basis for the Contaminant Transport Module elements. This information is provided (in great detail!) in the remaining chapters and appendices.

Regardless of which of these routes you choose to take, before proceeding it is critical that you first have a solid understanding of the basic functionality of the GoldSim simulation framework. Therefore, if you have not already done so, you should refer to the **GoldSim User's Guide**.

Similarly, if you are new to contaminant transport modeling and have not already done so, it is strongly recommended that you read Appendix A, "Introduction to Environmental Simulation" before proceeding further with the Contaminant Transport Module.

Read more: