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A User's Guide to the GoldSim/BLT-MS Integrated Software Package: A Low-Level Radioactive Waste Disposal Performance Assessment Model

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Abstract

Sandia National Laboratories (Sandia), a U.S. Department of Energy National Laboratory, has over 30 years experience in the assessment of radioactive waste disposal and at the time of this publication is providing assistance internationally in a number of areas relevant to the safety assessment of radioactive waste disposal systems. In countries with small radioactive waste programs, international technology transfer program efforts are often hampered by small budgets, schedule constraints, and a lack of experienced personnel. In an effort to surmount these difficulties, Sandia has developed a system that utilizes a combination of commercially available software codes and existing legacy codes for probabilistic safety assessment modeling that facilitates the technology transfer and maximizes limited available funding. Numerous codes developed and endorsed by the United States Nuclear Regulatory Commission (NRC) and codes developed and maintained by United States Department of Energy are generally available to foreign countries after addressing import/export control and copyright requirements. From a programmatic view, it is easier to utilize existing codes than to develop new codes. From an economic perspective, it is not possible for most countries with small radioactive waste disposal programs to maintain complex software, which meets the rigors of both domestic regulatory requirements and international peer review. Therefore, re-vitalization of deterministic legacy codes, as well as an adaptation of contemporary deterministic codes, provides a credible and solid computational platform for constructing probabilistic safety assessment models. This document is a reference users guide for the GoldSim/BLT-MS integrated modeling software package developed as part of a cooperative technology transfer project between Sandia National Laboratories and the Institute of Nuclear Energy Research (INER) in Taiwan for the preliminary assessment of several candidate low-level waste repository sites. Breach, Leach, and Transport-Multiple Species (BLT-MS) is a U.S. NRC sponsored code which simulates release and transport of contaminants from a subsurface low-level waste disposal facility. GoldSim is commercially available probabilistic software package that has radionclide transport capabilities. The following report guides a user through the steps necessary to use the integrated model and presents a successful application of the paradigm of renewing legacy codes for contempary application.

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A number of people at Sandia National Laboratories including, Hong-Nian Jow (Org.6773) (Project Lead), F. Joseph Schelling (Org. 6772), Cedric Sallaberry (Org.6784), and John C. Cochran (Org. 6793), have made significant contributions to the technology transfer program which either directly or indirectly supported the development of this integrated software package documented in this report. In addition, Jerry McNeish (Org. 6784) provided an internal technical review of this report.

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NOMENCLATURE

ACM	Alternative Conceptual Model
BLT-MS	Breach, Leach, and Transport - Multiple Species code
CFR	U.S. Code of Federal Regulations
Ci	Curies
DCF	dose conversion factor
DOE	Department of Energy
IAEA	International Atomic Energy Agency
ICRP	International Commission on Radiological Protection
INER	Institute of Nuclear Energy Research
LAN	Local Area Network
LHS	Latin Hypercube Sampling
LLW	Low-Level Radioactive Waste
NRC	U.S. Nuclear Regulatory Commission
SNL	Sandia National Laboratories
SZ	Saturated Zone
UZ	Unsaturated Zone

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1. INTRODUCTION

Sandia National Laboratories (SNL) has developed a model paradigm for probabilistic performance assessment analyses of potential low-level radioactive waste (LLW) disposal sites that utilizes legacy United States Nuclear Regulatory Commission (NRC) sponsored software coupled with contemporary software in a Monte Carlo framework. The SNL model package presented in this document utilizes the Breach, Leach, and Transport – Multiple Species (BLT-MS) code (NRC, 1989) to evaluate potential releases from a disposal facility. The BLT-MS code was developed by Brookhaven National Laboratory (BNL) for the U.S. NRC specifically for LLW compliance analyses. The BLT-MS code was coupled with GoldSim™ to create the framework for a probabilistic model capable of evaluating uncertainties in a potential LLW repository system. This document is intended as a user's guide for the probabilistic model package comprised of BLT-MS and GoldSim™.

Background

An evaluation was conducted of available codes potentially suitable for the source-term release and far-field transport of radionuclides from proposed LLW repositories. Two codes developed for the U.S. Nuclear Regulatory Agency (NRC) have the capability to simulate source-term releases as well as far-field transport of radionuclides. These codes are the Disposal Unit Source Term (DUST) code and the Breach, Leach, and Transport – Multiple Species (BLT-MS) code. The DUST code is one-dimensional, whereas the BLT-MS code is two-dimensional. Because of the multi-dimensional analysis capabilities, BLT-MS was selected for the performance assessment model.

BLT-MS has the following functionality:

- The code is able to simulate the degradation of waste containers in the source term for two types of processes:
    - Localized corrosion, where pitting occurs and the rate of water contact with the waste form is proportional to the extent of corrosion of the container; and
    - Generalized corrosion, where the container fails instantaneously once a breach time is achieved.
- The code includes four types of waste-form release, or leaching, mechanisms, including:
    - Rinse release, where the groundwater comes in contact with the waste and radionuclides are solubilized into the groundwater;
    - Diffusion release, which is the dominant release mechanism for stabilized waste, the code has several analytical models to choose from as well as a numerical solution;
    - Degradation release, where the waste form is depleted by dissolution linearly over a set time-frame; and
    - Solubility-limited release.
- The code incorporates a finite element-based transport solver for the far-field movement of radionuclides, which includes the following processes:
    - Advection;

- Dispersion;
- Sorption;
- Ingrowth and decay;
- Sources and sinks; and
- Boundary conditions, including Neumann, Cauchy, and Dirichlet type conditions.

The BLT-MS code was developed in the mid-1990s. It is a FORTRAN code that has been compiled to run under DOS or a DOS-emulator. SNL did not modify any of the code's functionality relative to the process models incorporated in the code. However, modifications to the input/output constructs of the model were necessary to integrate the code with GoldSim™.

In addition, computers at the time BLT-MS was developed did not have the processing or storage capacity of today's computers. Several iterations during the development of the radionuclide release and transport model domain revealed that the BLT-MS code had some limitations relative to the number of finite-element nodes, the number of waste containers allowed, and the number of time steps. To accurately simulate the proposed sites, arrays in the code associated with these attributes were increased to accommodate models having up to 30,000 nodes, 5000 waste containers, and 5000 time steps. Dr. Terry Sullivan, of Brookhaven National Laboratory, helped modify the code for the new requirements. Dr. Sullivan was the lead developer of the BLT-MS code when it was first developed for the NRC.

Summary

This manual is divided into six chapters with one appendix. Chapter 2 is a detailed user's guide for the integrated model for probabilistic analyses with BLT-MS, including an introduction to the concepts and integration strategy considered for coupling legacy software and the probabilistic contemporary software available today. Chapter 3 presents a 1-D transport model developed as an alternative conceptual model, which was used to validate the 2-D transport solution in BLT-MS. Chapter 4 discusses the dose model logic and implementation included in the model. Chapter 5 discusses the functionality of the codes that are part of the software package. Chapter 6 is a summary and Appendix A lists the source codes contained on the attached CD for the software developed as part of this model package.

2. GOLDSIM™ BLT-MS INTEGRATED MODEL

To implement a probabilistic version of BLT-MS, decisions need to be made regarding what input will be considered to be uncertain. Theoretically, each realization of a probabilistic analysis could have a unique finite-element mesh, source term configuration, and set of parameter uncertainties. The input/output requirements, as well as the computational burden, could become prohibitive if this much flexibility were built into the tool. Therefore, simplifying assumptions were made to make the code integration more practical.

In probabilistic analysis involving spatial variability, it is common to fix the physical aspects of the problem, such as the model boundaries and finite-element mesh configuration. If there uncertainty in the design of the finite-element mesh and the boundary conditions, then this may require additional model configurations to address this uncertainty explicitly. A fixed, deterministic approach was taken for the design of the finite-element mesh and the specification of boundary node types (i.e., Cauchy, Neumann, or Dirichlet) for this model.

In addition to the overall configuration of the finite-element mesh and boundary conditions, it is also advantageous to fix the locations of the source term containers. If the elements containing containers are allowed to vary with each realization of a probabilistic analysis, then the dependent specifications for container types, waste form types and breach/leach processes become much more intensive in terms of data configuration and formatting. In practice, any given site under consideration will have a proposed engineering design layout of the disposal area, and the physical configuration of the source term could be fixed based on this design. This still allows the user flexibility with the specifications of container types and waste form types for any of the specified containers. For the GoldSim BLT-MS integrated model, the physical source-term configuration (e.g., finite-element locations containing containers) is fixed or deterministic for any given probabilistic analysis, but the characteristics of each of the containers may be uncertain.

The input parameters that are fixed, or deterministic in the GoldSim BLT-MS Integrated Model, are:

- Finite-element mesh design parameters/specifications;
- Material property assignments within the finite element mesh (although the characteristics of each material may be uncertain, the element assignments will remain fixed for a given material type);
- Finite element nodes for boundary conditions, including keeping the type of boundary condition fixed for a given node (i.e., Cauchy vs Neumann vs Dirichlet);
- Number of isotopic species;
- Number of decay chains and branching fractions;
- Number of container types; and
- Number of waste types.

In general, the parameter sets that will be considered uncertain include (the names of specific parameters will follow):

- Initial concentrations within the source term;
- Boundary flux/concentration quantities;
- Breaching characteristics for any given container type;
- Leaching characteristics for any given waste type;
- Transport characteristics of the host rock/soil; and
- Darcy flux and moisture content distributions within the host rock/soil.

Input parameters that will be explicitly considered for uncertain parameter distributions (Note: these parameter definitions are taken from the BLT-MS User's Guide (NRC 1989)):

CSAT(iso)	Solubility limit for contaminant iso (g/cm^3).
prop(1,i)	molecular diffusion coefficient (cm^2/s) of material i.
prop(2,i)	bulk density of the soil (g/cm^3) of material i
prop(3,i)	longitudinal dispersivity (cm) of material i.
prop(4,i)	transverse dispersivity (cm) of material i.
prop(5,i)	porosity of material i.
prop1(1,k,i)	distribution coefficient (cm^3/g) of material k and contaminant i.
QCBF(j,i,iso)	Specified flux value of the j^{th} data point in the i^{th} profile for contaminant, iso ($mass/cm^2/year$).
QNBF(j,i,iso)	Specified dispersive flux value of the j^{th} data point in the ith profile for isotope, iso ($mass/cm^2/year$).
CDBF(j,i,iso)	Specified concentration value of the j^{th} data point in the i^{th} profile for contaminant, iso ($mass/cm^3$).
THICK(J)	Thickness of the J^{th} container (cm). 55 gallon drums are typically 0.127 - 0.152 cm thick.
PITN(J)	Pitting parameter n for the J^{th} container (dimensionless). If PITN(J) = 0, a value for PITN is estimated by the code based on input parameters for clay content (CLAY), soil aeration (IAER), and the moisture content. Measured values for PITN range from 0 - 1.
PITK(J)	Pitting parameter k for the J^{th} container (cm/yr). If PITK is input as zero, a value is estimated based on the soil pH. Measured values for PITK range from 0.03 - 0.15. If soil pH is input as zero, PITK is set to 0.0737, the average for all soils.
AREA(J)	Area of the J^{th} waste container (cm^2). The area of a 55 gallon drum is 21,000 cm^2. The value is used to calculate the maximum pit depth and the area breached by pitting.
ASCALE(J)	Area scaling exponent (dimensionless) for container J.

PITS(J) — Number of penetrating pits in the container (dimensionless) for container J. The total area breached is linearly proportional to the number of pits that penetrate the container, PITS(J). The default value used by BLT-MS is 1000.

GRATE(J) — The general corrosion rate (cm/s) of container J. If the input values of GRATE(J) are zero, then a default value of 3E-10 cm/s is used.

CLAY(J) — Clay fraction of the soil ($0 \leq$ CLAY(J) $\leq$. 1) around container J. If PITN is input as zero, PITN is calculated as a function of clay and moisture content as well as the degree of aeration (IAER).

SPH(J) — Soil pH. If PITK is input as zero, PITK is calculated as a function of pH. If SPH(J) is input as zero, a default value of 7.0 is used.

IAER(J) — Aeration index for the soil around container J. Used in calculating PITN, the values of J are: 1 = good, 2 = fair, 3 = poor, and 4 = very poor. If PITN and IAER are input as zero, PITN is set equal to 0.26, 0.39, 0.44, 0.59 for IAER = 1, 2, 3, 4 respectively. Most soils considered for low-level waste disposal will have good or fair aeration.

SFRACT(J,ISO) — Fraction of the mass in the J^{th} waste form that is available for surface wash-off in the rinse release model for contaminant iso. Useful for surface contaminated waste forms such as lab trash ($0 \leq$ SFRACT(J) $\leq$ 1.). The user must exercise caution such that (SFRACT + PFRACT + BFRACT) = 1 for any given model realization in the probabilistic framework.

PFRACT(J,ISO) — Fraction of the mass in the J^{th} waste form that is available for diffusion controlled release for contaminant iso. Useful for cement solidified waste forms (0. $\leq$ PFRACT(J) $\leq$ 1.). The user must exercise caution such that (SFRACT + PFRACT + BFRACT) = 1 for any given model realization in the probabilistic framework.

BFRACT(J,ISO) — Fraction of the mass in the J^{th} waste form that is available for release due to dissolution of the waste form for contaminant iso. Useful for waste forms such as activated metals or when modeling a constant release rate in time. ($0 \leq$ BFRACT $\leq$ 1.) The user must exercise caution such that (SFRACT + PFRACT + BFRACT) = 1 for any given model realization in the probabilistic framework.

DEFF(J,ISO) — J^{th} waste form effective diffusion coefficient for contaminant iso (cm^2/s). Used only if PFRACT(J,ISO) > 0.

DISOL(J,ISO) — J^{th} waste form fractional release rate (1/yr) for contaminant iso. Used only if BFRACT(J,ISO) > 0.

PARTKO(J,ISO) — J^{th} waste form partition coefficient for contaminant iso (cm^3/g) at time t = 0. Used only if SFRACT > 0.

PARTKI(J,ISO) — J^{th} waste form partition coefficient for contaminant iso (cm^3/g) at time t = ∞.

PARTD(J,ISO)	J^{th} waste form partition coefficient degradation rate constant for contaminant iso (1/yr). PARTD(J,ISO) must be greater than or equal to 0.
POREL(J)	Radius or half-length of waste form J (cm). Used in calculating diffusion and dissolution controlled release (PFRACT > 0).
VOLWF(J)	Volume of waste form J (cm^3). Used in calculating the height of cylindrical waste forms and initial concentrations within the waste form.
VRATIO(J)	Ratio of the volume of waste form J to the finite element in which it is located. (0 ≤ VRATIO(J)). Used in the rinse with partitioning model.
WTINIT(J,ISO)	Initial inventory of contaminant iso in waste form J. If IACT = 0, WTINIT is input in grams. If IACT = 1, WTINIT is input in Curies.
VX(I)	Darcy velocity in the X-direction at node I (cm/s).
VZ(I)	Darcy velocity in the Z-direction at node I (cm/s). It is recommended to define the lower left hand corner of the modeled domain as the minimum value for X and Z. In this case, a negative Z velocity implies downward flow.
TH(IQ,J)	Moisture content at nodal point IQ, in element J. Moisture content is defined at each nodal point in the finite element grid. In quadrilateral elements there are four moisture content values associated with each element.

2.1 Model Overview

Figure 1 shows the flow chart for the GoldSim/BLT-MS integrated model. Model development starts with the generation of a BLT-MS model using the BLT-MS preprocessor (Section 5.1). The analyst defines the problem and sets up a stand alone deterministic BLT-MS simulation. The GoldSim/BLT-MS Integration Model is designed to require a ***pre-existing*** BLT-MS input file. The GoldSim/BLT-MS Integration Model reads this 'master' input file and writes a new set of input files, replacing selected parameters with uncertain values sampled from pre-defined distributions within the GoldSim model file. The GoldSim/BLT-MS Integration Model executes BLT-MS.exe sequentially for each realization over the set of corresponding input files. Selected BLT-MS output from each realization is saved within the GoldSim/BLT-MS Integration Model.

Integration of the BLT-MS code with GoldSim software was accomplished though the use of two separate program modules written in FORTRAN and directly coupled to the GoldSim software. These codes are linked to GoldSim model file using a predefined interface and compiling the program modules as dynamic linked libraries (DLL). The GoldSim software interfaces with the DLL using an external element inserted in the GoldSim model file(GoldSim User's Manual, page 451 and Appendix C, GoldSim Technology Group LLC, 2006). The GoldSim model file discussed in this manual has been designated as open-source and is freely available. It can be accessed on a Sandia National Laboratories website at the following URL: http://www.sandia.gov/icp/.

The basic operation of the GoldSim/BLT-MS Integration Model is summarized in Figure 1 and outlined in the following steps. The analyst first:

1) constructs a BLT-MS Model using the BLT-MS preprocessor to generate a 'master' input file called: bltmsin.inp,
2) specifies the uncertain distributions and selects which parameters to make uncertain in the GoldSim Model (Some user specified controls are required and are detailed in the following sections.),
3) specifies the duration of the simulation and number of realizations desired in the GoldSim Model,
4) saves the GoldSim/BLT-MS Integration Model, and
5) runs the GoldSim/BLT-MS Integration Model.

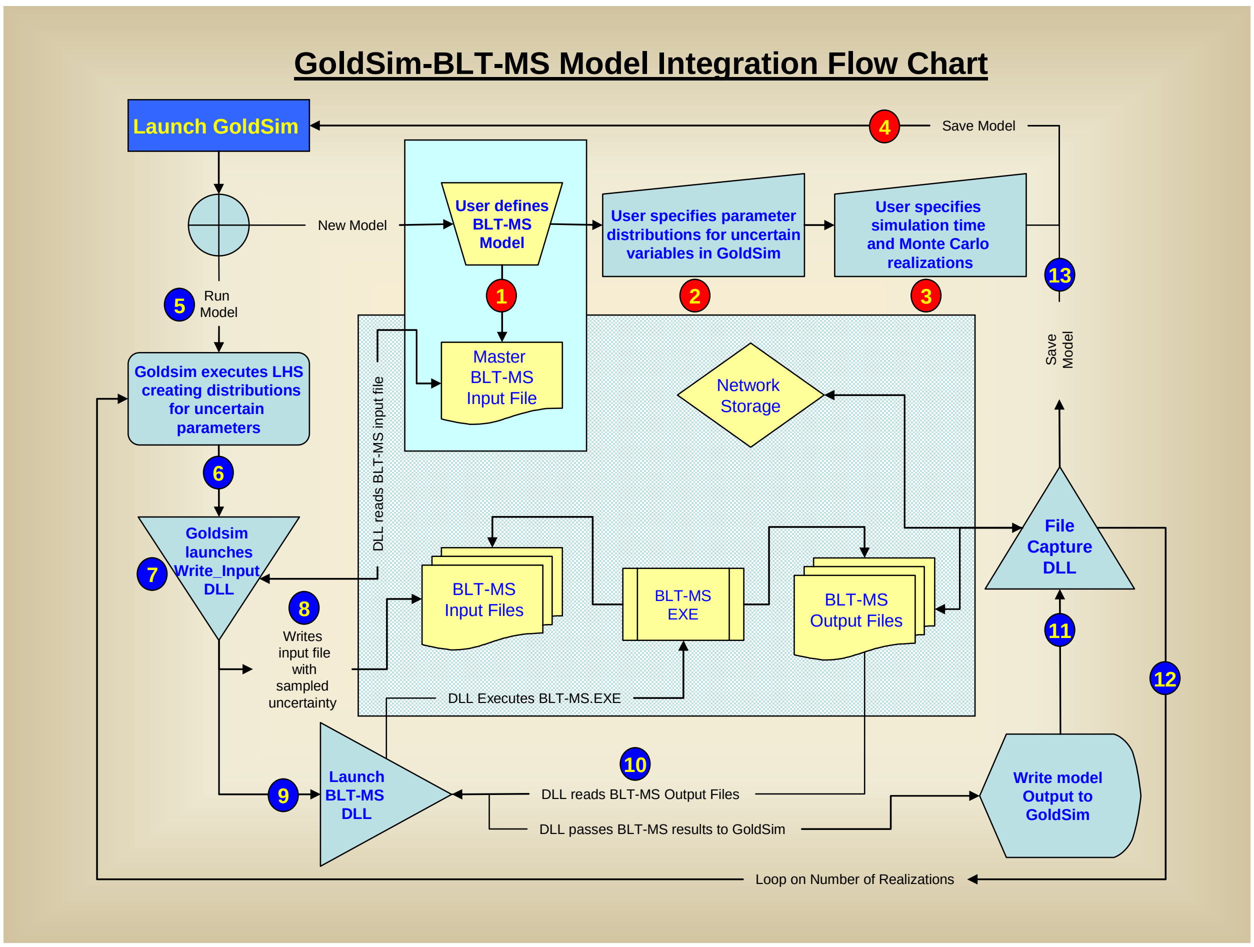

Figure 1. Flow Chart for GoldSim/BLT-MS Integration Model

Running the GoldSim/BLT-MS Integration executes the following actions:

6) Upon execution, GoldSim samples all the uncertain distributions using Latin Hypercube Sampling (LHS).
7) The first realization is started by calling the Read_BLT.DLL. GoldSim passes the uncertain values to the DLL using predefined arrays.
8) The Read_BLT.DLL code reads the bltmsin.inp file first (This is the file already generated using the preprocessor for BLT-MS, Section 5.1.), and writes a new input

file called BLTMS0000*.inp (* = the realization number). The new input file has deterministic values for selected parameters replaced with sampled values from the predefined uncertain distributions.

9) Upon successful completion of the Read_BLT.DLL, GoldSim then launches the Launch_BLTMS.DLL, which executes BLTMS.EXE for the BLTMS0000*.inp input file.
10) Upon successful completion of BLTMS.EXE, the Launch_BLTMS.DLL extracts selected data from the output files (TRACECN*.dat and LEACHRL*.dat) and passes the output to the GoldSim/BLT-MS Integration Model for storage and use in downstream calculations.
11) To save copies of BLTMS.EXE output files during local or networked runs using GoldSim's Distributed Processing Module, the FileCapture.DLL is used to copy selected output files to a central location on a local area network (LAN).
12) Steps 7-11 are repeated until all the realizations have been executed.
13) Upon successful completion of the simulation, the GoldSim/BLT-MS Integration Model is saved and the analyst can begin review of the results.

Specific steps required for the successful execution of the GoldSim/BLT-MS Integration Model are discussed in four parts below: 1) Input File Set, 2) Upper Level Model Structure and Simulation Settings, 3) Defining Model Uncertainty, and 4) Capturing Model Output.

In addition following that discussion, Section 3.0 presents an example alternative conceptual model for 1-D transport, which is included in the model. Section 4.0 details a simplified dose model calculation embedded in the integrated model. This guide assumes the analyst generates the BLT-MS model and input file using the BLT-MS preprocessor (Section 5.1) and therefore does not include instructions for those steps.

2.2 Input File Set

The GoldSim/BLT-MS Integration Model utilizes a set of files to execute the BLT-MS code and the GoldSim software with its associated DLL's. Table 1 lists the set of files necessary to run the Integration Model and includes a brief description of each file. The file set consists of the GoldSim model file (.gsm file), which is compatible with GoldSim™ Version 9.2. To execute the GoldSim model file, the analyst must have a current licensed version of GoldSim™ with the Radionuclide Transport Module enabled (GoldSim Technology Group LLC, 2006). In addition, three DLL's and BLTMS.exe must be present in the directory in which the GoldSim/BLT-MS Integration Model file is executed. The DLL's and BLTMS.EXE were compiled using Compaq Visual Fortran, Professional Edition 6.0.A, on an Intel compatible operating system. The source code for Read_BLT.DLL version 1.0, Launch_BLTMS.DLL version 1.1, and FileCapture.DLL version 1.0 is distributed with this user guide. As mentioned previously, a 'master' BLTMS input file is required to execute the integrated model. The logic programmed in the GoldSim model file and associated DLL's require information obtained from the bltmsin.inp file.

Table 1. File Set Required for the GoldSim/BLT-MS Integration Model

File Name	Description
BLTMS_GS9.21_v1.4.1.gsm	GoldSim model file that contains the elements and logic necessary to execute a probabilistic simulation of a BLTMS model. (This file can be re-named if desired.)
Read_BLTv1.1.002.dll	DLL accessed by GoldSim during simulation to create BLTMS input files with uncertain samples for selected parameters.
Launch_BLTMSv1.1.011.dll	DLL accessed by GoldSim during simulation to execute BLTMS.EXE, read a selected output file, and pass the data back to GoldSim.
Bltmsin.inp	Master BLTMS input file used by the Read_BLT.dll to create the new input files with deterministic values replaced by sampled values from GoldSim for selected parameters.
BLTMS.EXE	BLTMS executable used to calculate radionuclide release and transport.
FileCapture_v1.0.dll	DLL used to copy output files from BLTMS.EXE for each realization.
Fcapture.in	Input file listing the output files and location of the directory where they are copied.

2.3 Upper Level Model Structure and Simulation Settings

Error! Reference source not found. outlines the upper level model structure for the GoldSim/BLTMS Integration Model. Table 2 lists the upper level containers and level 2 model containers within each upper level container. As can be seen in Error! Reference source not found. and Table 2, the basic structure of the integration model is broken into two main parts (or upper level containers):

1) BLT-MS Model
2) 1-D Pipe-Pathway Transport Alternative Conceptual Model (ACM) (Section 3.0)

Each container includes the logic necessary to implement its respective parts of the model. In the *BLTMS* container, generation of the input files for BLTMS and uncertainty sampling is defined within the *BLT_MS_Input_File* container (Table 2). The execution of BLTMS.EXE and extraction of BTLMS model results is contained within the *Launch_BLTMS* container. The *Pipe Model* container has the logic and implementation for the 1-D transport ACM. Each of these areas is discussed in further detail below. The analyst must ensure that the model conditions are correctly defined within the *BLT_MS_Input_File* container before the simulation is launched.

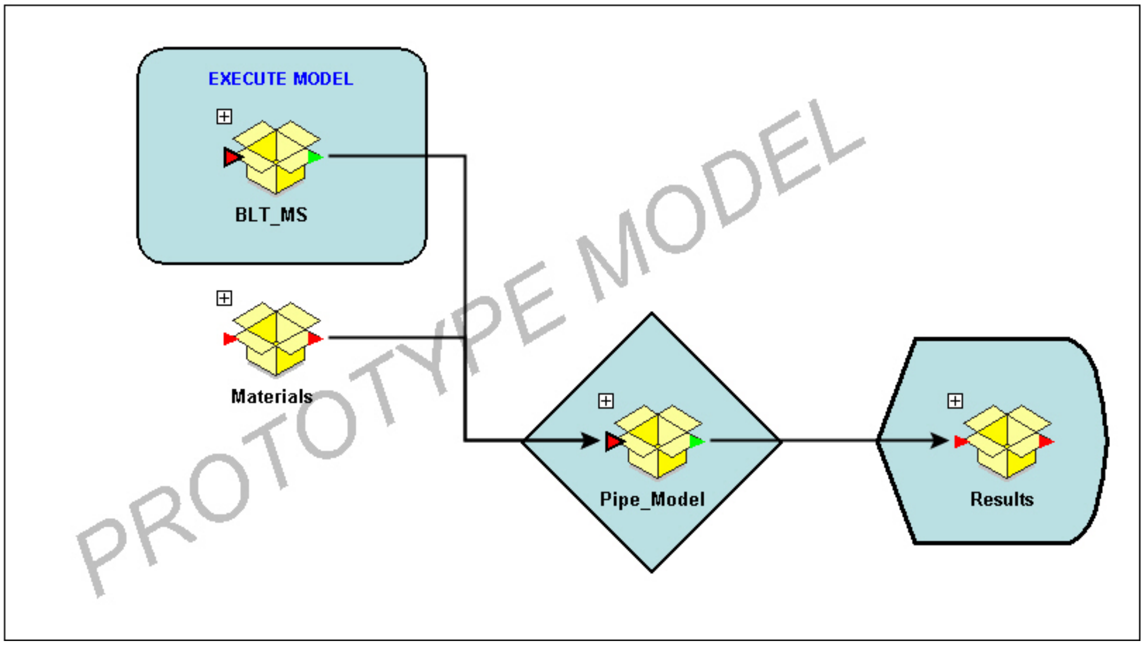

Figure 2. Upper Level Model Structure

Table 2. Upper Level Hierarchy for BLTMS/GoldSim Integration Model

Upper Level Container	Description	Level 2 Container	Description
BLT_MS	Contains Model Linking BLTMS.EXE with GoldSim. Allows the user to add uncertainty to the model by selecting from 36 BLTMS input parameters. Selected BLTMS output data is passed to GoldSim to record multiple realization data.	BLT_MS_Input_File	Contains the Read_ BLTMS.DLL. Contains the elements used to substitute uncertainty for deterministic values in BLTMS Model.
		Launch_BLTMS	Contains the Launch_BLTMS.DLL and elements used to capture the selected output.
		BLTMS_Results	Contains predefined plot of BLTMS concentration traces and selected output.
Pipe_Model	1-D Transport Model using GoldSim transport equations and source term from BLTMS.	Source_Term_Zone1	Contains the elements used to calculate the source term release from Zone 1 containers. User must identify which containers, by BLTMS element number, for this zone.
		Source_Term_Zone2	Contains the elements used to calculate the source term release from Zone 2 containers.
		Source_Term_Zone3	Contains the elements used to calculate the source term release from Zone3 containers.
Results	Plots of the output from BLTMS Model and 1-D GoldSim transport Model	Dose_Conversion_Factors	Contains the input data used in the simplified dose model.
		Dose	Contains the calculation used in the simplified dose model and the plots for the dose calculated from BLT-MS and the 1-D model.

Running the Model

The basic steps for running the GoldSim/BLT-MS Integration Model are defined as follows:

1) Open the ***Simulation Settings*** and set the run time, number of time steps, and total number of realizations. The Latin Hypercube Sampling check box should be selected. The number of time steps and simulation time should be the same as defined within the BLTMS input file (Note: time steps can be smaller or larger than BLT-MS uses, but GoldSim will employ a linear interpolation of the data).
2) Define physical properties for isotopes (ISO) listed in the BLT-MS input file in the GoldSim ***Species*** element.

3) Open the ***BLT_MS_Uncertain_Param_Switch*** element located in the ***BLT_MS_Input_File*** container Select which parameters will be made uncertain. (See section below for details and Figure 3**,** Figure 5 and Table 3).
4) Open the ***BLT_MS_Uncertain_Arrays*** container (Figure 4, Table 3). Define the uncertainty using stochastic elements for each of the parameters sets selected in step 2 above (see section below for details and Table 4).
5) Open the ***Control_Values*** container and edit the following two arrays: ***NELCON_LIST***, listing the element numbers that are associated with containers for each of the zones used in the 1-D Pipe model, and ***NTRCEC_LIST***, listing the element numbers where concentration trace data is to be used to calculate the biosphere dose (Section 4.0).
6) In the ***Control_Values*** container, indicate whether or not the BLTMS input file will be saved for multiple realizations and if it is desirable to capture input/output with the FileCapture DLL using the elements ***BLTMS_INPUT_OUTPUT_SWITCH*** and ***FileCapture_Switch,*** respectively.
7) Save the Model.
8) Run the GoldSim Model.
9) Save the Model when the simulation is complete.

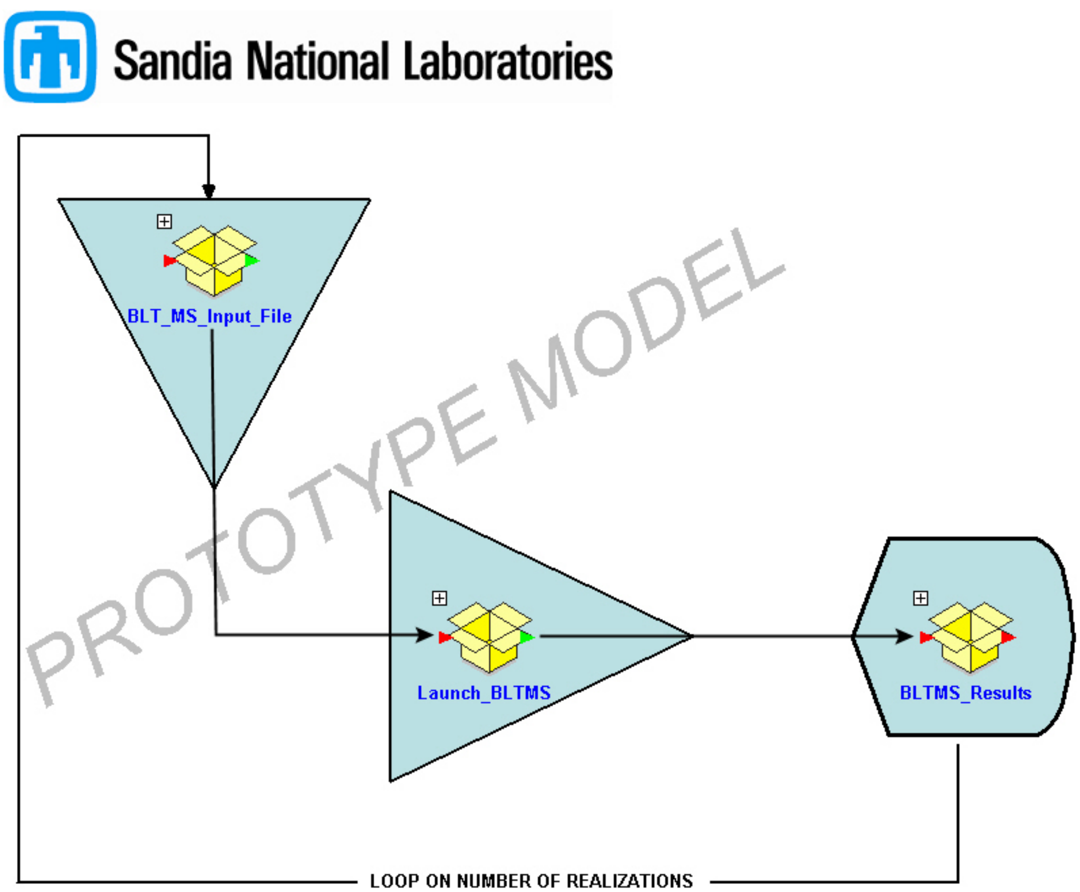

Figure 3. Level 2 Container Structure

Table 3. GoldSim/BLT-MS Integration Model Level 2 Containers

Level 2 Container	Level 3	Description
BLT_MS_Input_File	BLT_MS_Uncertain_Array_Sizes	Array that passes the DLL the maximum size of each uncertain array. DO NOT ADJUST THIS ARRAY.
	BLT_MS_Uncertain_Param_Switch	Array that passes the DLL which parameters are intended to be uncertain – ANALYST MUST SELECT UNCERTAIN PARAMETERS.
	BLT_MS_Uncertain_Arrays	Contains the BLTMS parameters by data set that can be replaced with uncertain values - ANALYST MUST INPUT UNCERTAIN VALUES HERE.
	Read_BLTMS_DLL	DLL that writes uncertain values to the input file and passes control values to Launch_BLTMS_DLL
Launch_BLTMS	BLTMS	DLL that launches BLT-MS and passes selected output data back to GoldSim.
	Control_Values	Parameters used to process output from BLTMS-
	CONC_TRACE_FILE_OUTPUT	Contains the output data read from BLTMS concentration trace files and passed by the DLL to GoldSim.
	LEACHMS_FILE_OUTPUT	Contains the output data read from BLTMS LEACHRL* files and passed by the DLL to GoldSim.
BLTMS_Results	None	Container for selected BLTMS output.

In the following sections, key parameters will be discussed in detail. However, each individual element contained in the GoldSim/BLT-MS Integration Model is not discussed. It is assumed the analyst has a basic proficiency with GoldSim and the necessary understanding of the features of the GoldSim code to implement this coupled model. The GoldSim model file itself should be considered as part of the model documentation. A description is embedded within each model element in the GoldSim model file. Additionally, the GoldSim software allows the user to browse influence traces that graphically show the links between elements both upstream and downstream for each element in the model. The analyst is encouraged to review the GoldSim User's Manual (GoldSim Technology Group LLC, 2006) for specific details of the model elements used in this implementation.

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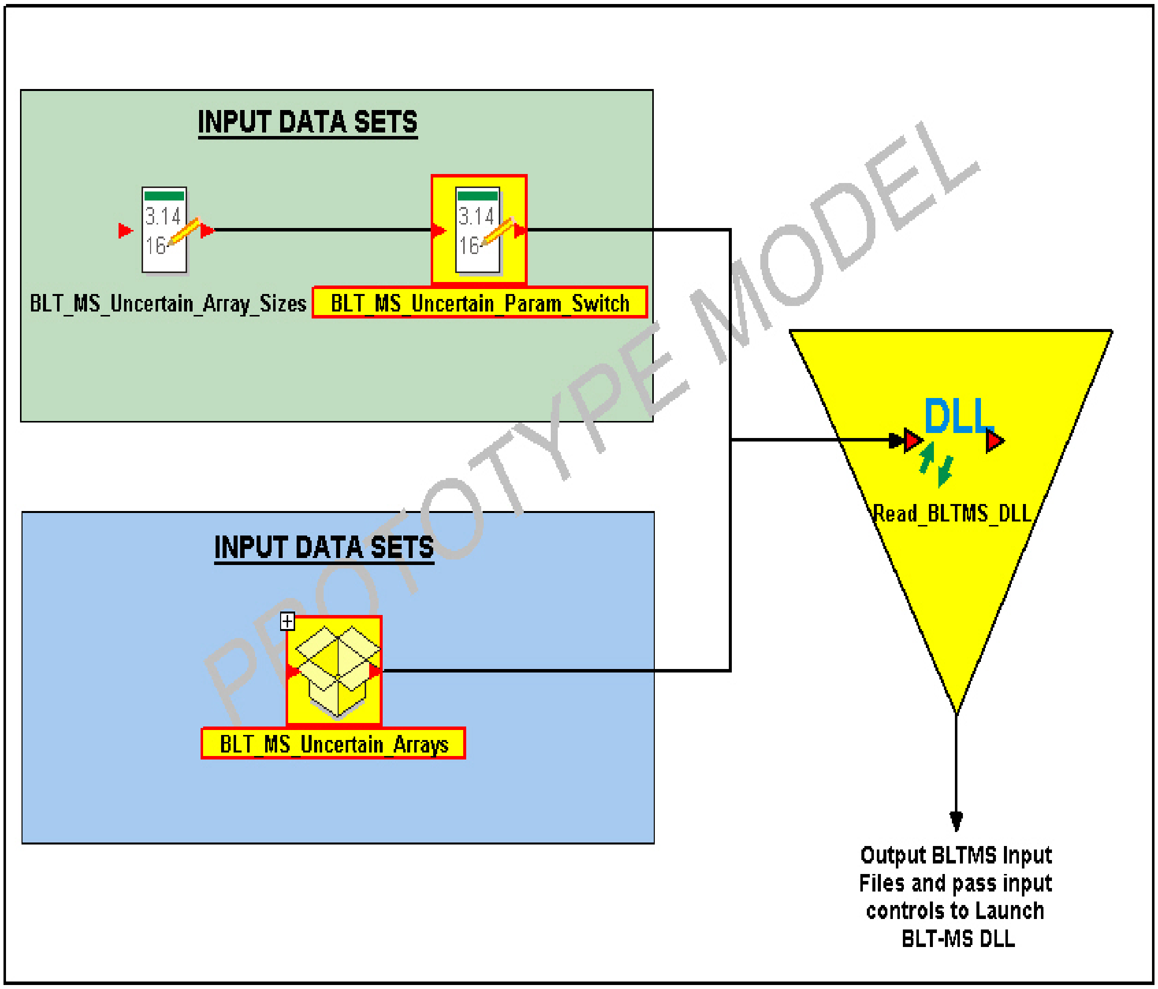


Figure 4. BLT_MS_Input_File Container Structure

2.4 Defining Model Uncertainty

Figure 4 outlines the structure for *BLT_MS_Input_File* container. This container contains the logic used to select which BLTMS parameters will be uncertain for a given model and to define the uncertain distributions with stochastic elements. The first step in this process is to select the uncertain parameters using the *BLT_MS_Uncertain_Param_Switch* Array Element (Figure 4**)**. The *BLT_MS_Uncertain_Param_Switch* is a vector of 35 inputs, one for each BLT-MS parameter available. The analyst must edit this vector (see Figure 5). Entering a 1 indicates that the deterministic value (or data set) will be replaced with a sampled distribution defined within the GoldSim model file. The default value of 0 indicates that the original deterministic values from the master BLTMS input file (bltmsin.inp) will be used over all realizations. In the example shown in Figure 5, CSAT, prop2i, CLAY, and the velocity terms, Vx and Vz, have been selected as uncertain. Each time the GoldSim/BLTMS Integration model is used, the analyst should review the *BLT_MS_Uncertain_Param_Switch* array elements to ensure that the correct parameters are selected as uncertain.

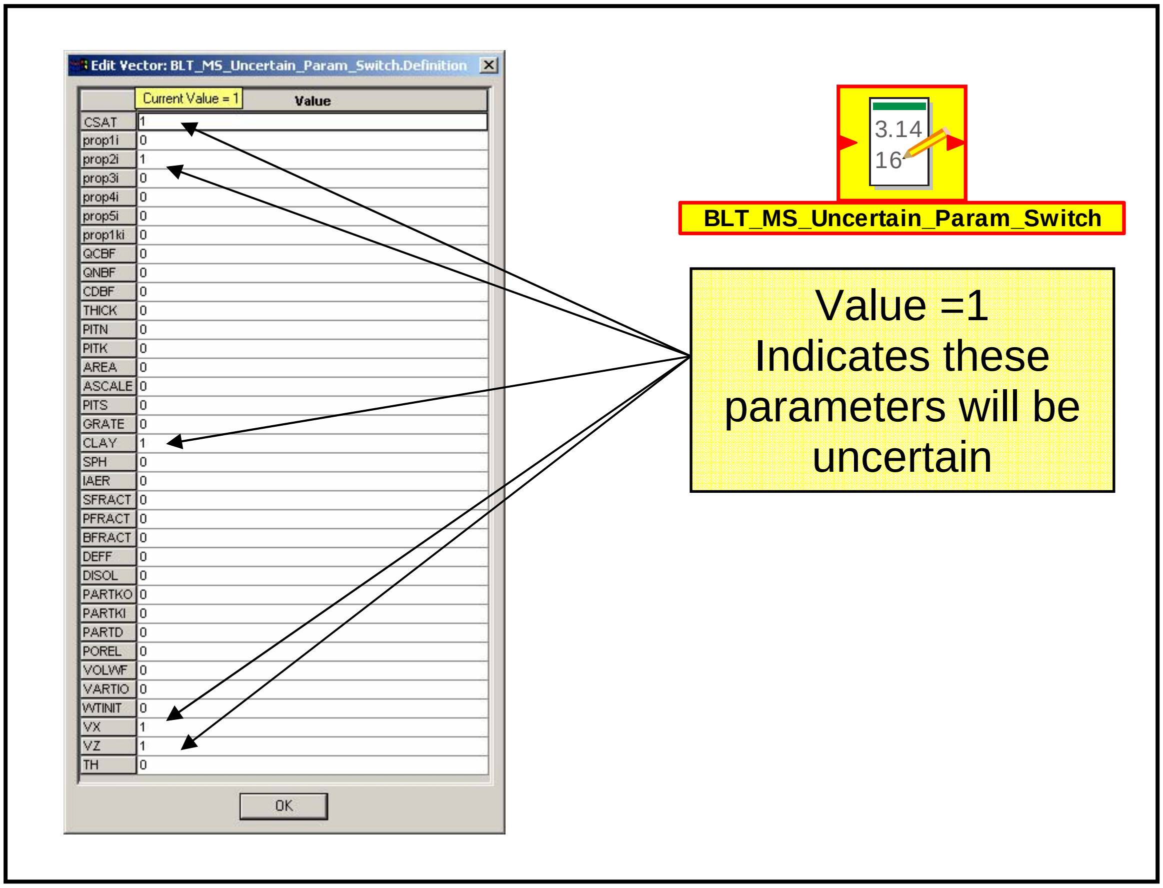


Figure 5. BLT_MS_Uncertain_Param_Switch Array Element Example

The *BLT_MS_Uncertain_Array_Sizes* element defines the size of each of the 35 arrays passed to the DLL. Currently, the array is set for the maximum size for each input parameter. Figure 6 shows the array and default values. An integer value is required. The maximum value for each of the 35 arrays corresponds to the maximum number of ISOTOPES ($1 \leq$ NISO ≤ 10), WASTE FORMS (NWTYPE ≤ 20), MATERIAL ($1 \leq$ NMAT ≤ 5), and TYPES OF CONTAINERS (NCTYPE ≤ 20).

In the default example, there are ten isotopes (ISO) defined in the bltmsin.inp file, and therefore CSAT has a value of 10. CSAT is an array by isotopes. BLT-MS accepts a maximum of five materials. As seen in Figure 6, prop1i through prop5i are arrays by NMAT, so their values are set to 5, THICK through IAER are arrays by NCTYPE, so their values are set to 20, and SFRACT through PARTD are matrixes defined by ISO and NWTYPE, therefore their values are set equal to 200. The uncertainty input arrays in GoldSim are set to fixed values equal to the maximum sizes. The DLL expects a fixed size of the input array (in(*)) equal to 2249. This array should not be changed, because the DLL uses the values of NISO, NWTYPE, NMAT, and NCTYPE from the bltmsin.inp file to read only the data needed from the array, and the values from the *BLT_MS_Uncertain_Array_Sizes* element are used only to index to location in the in(*) array at the beginning of each parameter's input values. If there are fewer isotopes, waste forms, materials or container types, the DLL will automatically skip over the array locations that are not used.

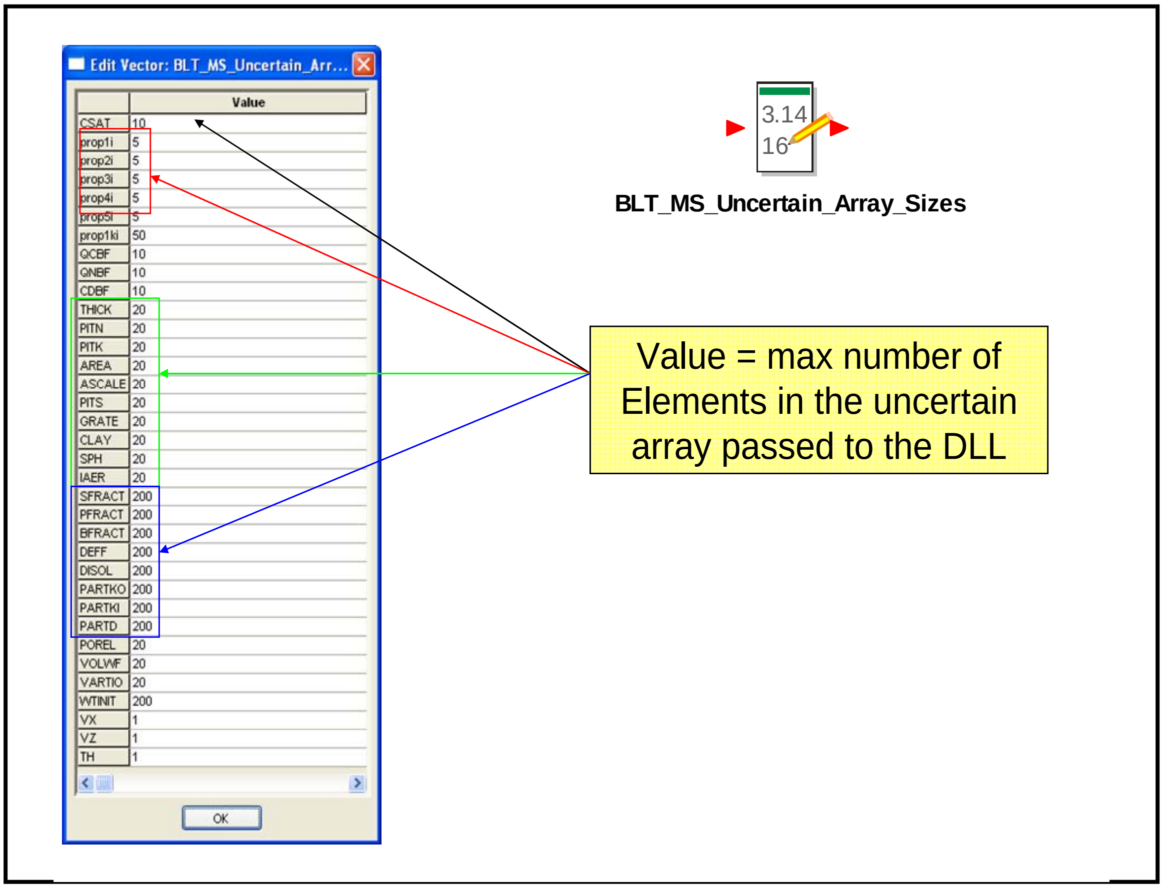


Figure 6. BLT-MS Uncertain Array Sizes Parameter

The next step is to define the uncertainty ranges for the selected parameters using GoldSim's stochastic elements. The input data is defined within the *BTL_MS_Uncertain_Arrays* container, Figure 5. The BLTMS parameters are organized by BLTMS data sets, as shown in Table 4. Each data set container includes the parameter data array and stochastic elements used to define the uncertainty. In the example, CSAT has been selected to be uncertain. Opening the *DATA_SET_9* container,

[\BLT_MS_Integration_Model\Open_Model\BLT_MS\BLT_MS_Input_File\BLT_MS_Uncertain_Arrays\DATA_SET_9],

reveals the input array for CSAT, labeled *CSAT*, and the stochastic elements that contain the uncertainty data for this parameter (Figure 7). Since CSAT can be defined for each ISO defined in the BLTMS model, it is necessary to define up to ten distributions, one for each ISO, as seen in Figure 7. If the model contains less then ten ISO's, extra data will be ignored. However, it is important to note that if it is intended to make CSAT uncertain for only some of the isotopes, the analyst must still define the CSAT values for all of them. For example, if a BLTMS master input file contains five ISO's and the GoldSim/BLTMS Integration Model *BTL_MS_Uncertain_Arrays* element has a value of 1 for CSAT, then all five ISO values will be replaced with the values defined in GoldSim. Therefore, the analyst must edit the array *CSAT* in GoldSim to define the deterministic values as well as the uncertain values. In the example shown in Figure 7, ISO2 and ISO3 have deterministic values of 2.75 and 1.45 respectively, whereas ISO1, ISO4, and ISO5 are uncertain. The remaining ISO's are ignored if only five have been defined in the master input file (bltmsin.inp).

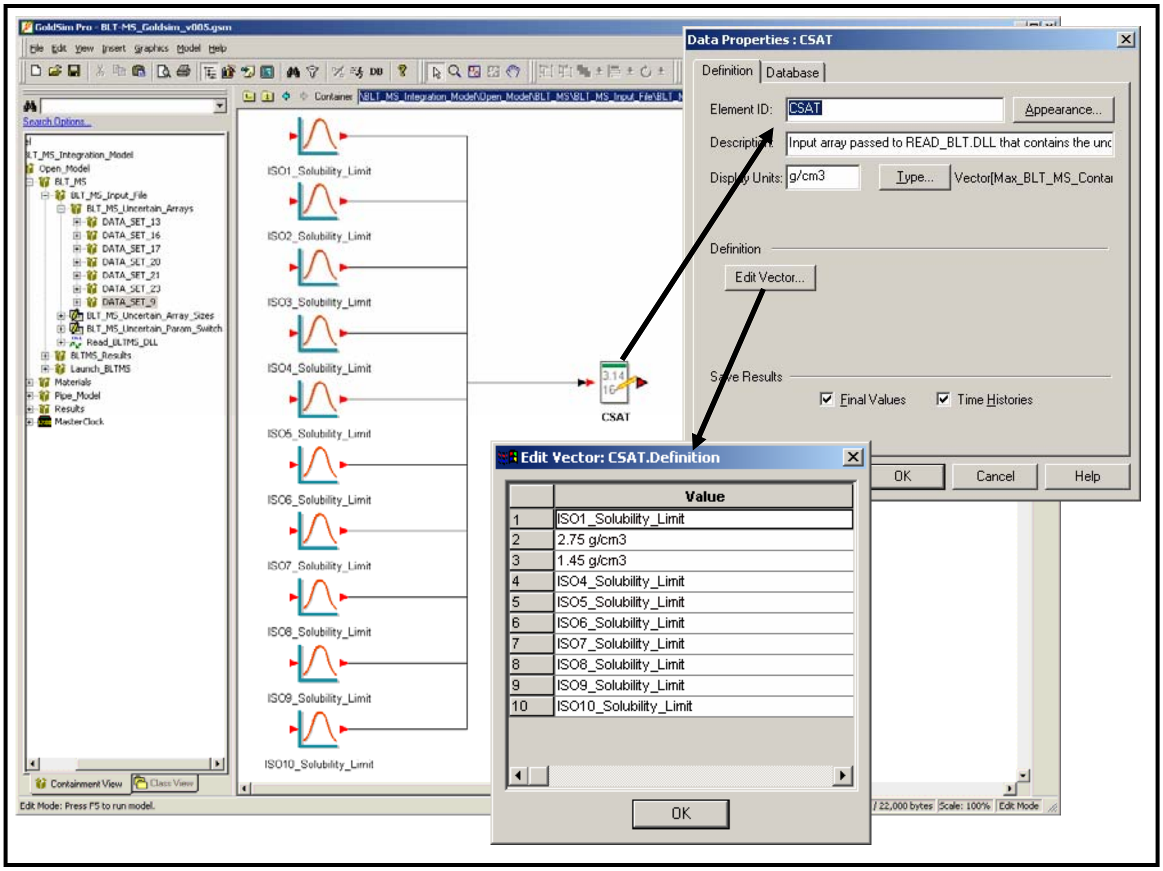


Figure 7. CSAT array and stochastic elements, \BLT_MS_Integration_Model\Open_Model\BLT_MS\BLT_MS_Input_File\BLT_MS_Uncertain_Arrays\DATA_SET_9

In contrast to CSAT, the input arrays for prop2i and CLAY are defined by material type and container type, respectively (Figure 8**)**. BLTMS allows up to five material types and up to 20 container types; therefore, a distribution (or deterministic value) must be supplied for each material and container defined in the bltmsin.inp file.

The last parameters selected to be uncertain in this example input array, shown in Figure 5, are the velocity terms, Vx and Vz (Data Set 23). These two terms represent the Darcy velocity in the x and z directions. The uncertainty factor for these parameters is applied to all nodes as a multiplier term. Therefore, only one stochastic element is needed for Vx and one for Vz. The sampled values are passed to the DLL (Read_BLT.DLL), and the BLTMS input terms VXNI and VZNI are scaled by multiplying the sampled value with the value read from the bltmsin.inp file.

In summary, the analyst needs to select the BLTMS parameters that will be uncertain in the *BLT_MS_Uncertain_Param_Switch* file, define the appropriate uncertainty distributions using stochastic elements or deterministic values, and link these data to the parameter input array. Close attention should be paid to the different input array sizes for each parameter. In some cases, they represent a matrix that is dependent upon ISO and waste form type (e.g. *partk0_j*). The input arrays represent the data values that the DLL will use to replace the deterministic values of parameters selected in *BLT_MS_Uncertain_Param_Switch* array element.

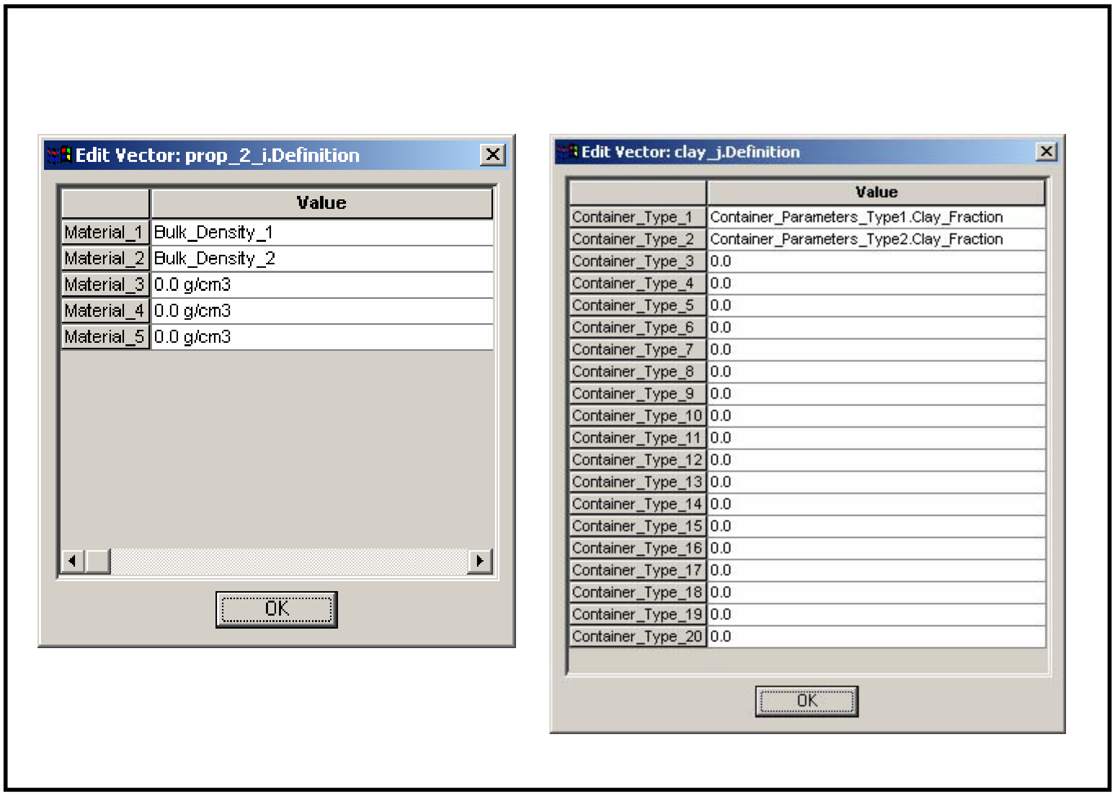


Figure 8. prop_2_i and clay_i input arrays

Table 4. Level 3 Containers and BLT_MS Uncertain Array Elements

Level 3 Container	Container	Element	Description
BLT_MS_Uncertain_Arrays ANALYST MUST INPUT UNCERTAIN VALUES	DATA_SET_9	CSAT	Input array passed to READ_BLT.DLL, which contains the uncertain values for solubility.
		ISO1_Solubility_Limit **to** ISO10_Solubility_Limit	Stochastic elements that can be used to define uncertainty distributions for the solubility of selected ISOs in the BLTMS model.
	DATA_SET_13	prop_1_i	Property 1 Array: Uncertainty distributions of molecular diffusion coefficient of material (i)
		prop_2_i	Property 2 Array : Uncertainty distributions of bulk soil density of material (i)
		prop_3_i	Property 3 Array: Uncertainty distributions of longitudinal dispersivity of material (i)
		prop_4_i	Property 4 Array: Uncertainty distributions of transverse dispersivity of material (i)
		prop_5_i	Property 5 Array: Uncertainty distributions of porosity of material (i)
		prop1_1_k_i	Property matrix of uncertainty distributions for distribution coefficient of material (k) for ISO (i)
		Material_Property_Uncertainty	Contains stochastic elements that can be used to define distributions of uncertainty for the material properties used in the BLTMS model.

Table 4: Continued

Level 3 Container	Container	Element	Description
BLT_MS_Uncertain_Arrays continued	DATA_SET_16	QCBF	Array of specified flux value for Cauchy nodal points for ISO(i) (all profiles)
		Cauchy_Boundary_Uncertainty	Contains ISO(i) stochastic elements used in array for Cauchy boundary conditions (QCBF)
		QNBF	Array of specified dispersive flux value for Neumann nodal points for ISO(i) (all profiles)
		Neumann_Boundary_Uncertainty	Contains ISO(i) stochastic elements used in array for Neumann boundary conditions (QNBF)
	DATA_SET_17	CDBF	Array of specified concentration value for Dirichlet nodal points for ISO(i) (all profiles)
		Dirichlet_Boundary_Uncertainty	Contains ISO(i) stochastic elements used in array of specified concentration values for Dirichlet nodal points (CDBF)
	DATA_SET_20	thick_j	Array of thickness of container type j
		pitn_j	Array of pitting parameter of container type j
		pitk_j	Array of pitting parameter of container type j
		area_j	Array of area of container type j
		ascale_j	Array of area scaling exponent parameter of container type j

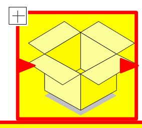
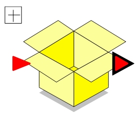
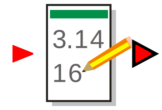
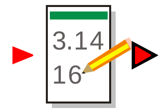
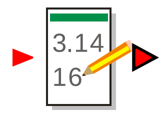
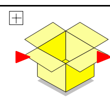
Table 4: Continued

Level 3 Container	Container	Element	Description
BLT_MS_Uncertain_Arrays continued	DATA_SET_20 continued	pits_j	Array of number of penetrating pits for container type j
		grate_j	Array of general corrosion rate of container type j
		clay_j	Array of clay fraction of soil around container type j
		spH_j	Array of pH of soil around container type j
		iaer_j	Array of aeration index of soil around container type j
		Container_Parameters_Type1	Contains uncertainty parameters for Waste Container Type(i) – ANALYST HAS THE OPTION TO DEFINE UNCERTAINY SPECIFIC TO EACH WASTE CONTAINER TYPE (20 Maximum)
	DATA_SET_21	sfract_j	Matrix of mass fraction values for j^{th} waste form available for surface wash off in the rinse model for contaminant ISO(i)
		disol_j	Matrix of j^{th} waste form fractional release rates for contaminant ISO(i)
		porel_j	Array of radius or half length of j^{th} waste form
		volwf_j	Array of volume of j^{th} waste form

Table 4: Continued

Level 3 Container	Container	Element	Description
BLT_MS_Uncertain_Arrays continued	DATA_SET_21 continued	partk0_j	Matrix of j^{th} waste form partition coefficient for contaminant ISO(i) at time t=0 yr
		vartio_j	Array of ratios for the volume of the j^{th} waste form to the finite element in which it is located.
		pfract_j	Matrix of mass fraction values for j^{th} waste form available for diffusion controlled release for contaminant ISO(i)
		partki_j	Matrix of j^{th} waste form partition coefficient for contaminant ISO(i) at time t=∞ yr
		bfract_j	Matrix of mass fraction values for j^{th} waste form available for dissolution controlled release for contaminant ISO(i)
		partd_j	Matrix of j^{th} waste form partition coefficient degradation rate constant for contaminant ISO(i)
		wtinit_j	Matrix of j^{th} waste form initial inventory for contaminant ISO(i)
		deff_j	Matrix of j^{th} waste form effective diffusion coefficient for contaminant ISO(i)
		Waste_Form_Leaching_Uncert	Contains stochastic elements used to populate Data Set 21 parameters

Table 4: Continued

Level 3 Container	Container	Element	Description
 BLT_MS_Uncertain_Arrays **continued**	 DATA_SET_23	 **vxni_j**	Multiplier for Darcy velocity in the x-direction. Allows the analyst to vary the velocity each realization over a specified range over all nodes.
		 **vzni_j**	Multiplier for Darcy velocity in the z-direction. Allows the analyst to vary the velocity each realization over a specified range over all nodes.
		 **thni_j**	Multiplier for moisture content. Allows the analyst to vary the moisture content each realization over a specified range over all nodes.
		 Velocity_and_Moisture_Uncert	Contains the stochastic parameters used to simulate a range of multipliers for vxni_j, vzni_j, and thni_j

2.5 Capturing Model Output

The Launch_BLTMS.DLL (Section 5.5) executes the BLTMS.EXE and captures selected output for each realization. The concentration trace files (see BLT-MS User's Guide, NRC 1989) produced by BLT-MS and the mass release data are captured and saved in the GoldSim model file using the Launch_BLTMS.DLL. Figure 9 outlines the structure for the *Launch_BLTMS* container. Table 5 lists the contents for each output data container. The data contained within the BLTMS output files TRACECN*.dat and LEACHRL*.dat are read by the Launch_BLTMS.DLL, and the data is passed to the GoldSim model file for storage via links to table elements.

For the concentration trace data contained in the TRACEN*.dat file, one table is defined in the GoldSim model file to store the output data; *BLT_Concentration _Trace_Sum*. Each layer of the table represents a zone that is defined by selecting a set of BLTMS finite element grid nodes. This set of nodes are used to calculate an average concentration for that zone. For example, to simulate a well intersecting the water table 100 meters down stream from a source, a zone is defined by selecting the BLTMS finite-element grid locations that represent a vertical cross section of nodes below the water table 100 m from the source. Each column in the table is a number representing the ISO for which concentration data was saved. This table is linked to *BLTMS_Concentration_Trace_Data*, which is used by the biosphere dose calculation. A maximum of only 100 concentration traces can be saved by the BLTMS code, and a maximum of 10 zones can be defined in the *NTRCEC_LIST* array element defeined in the GoldSim model file. The *NTRCEC_LIST* array element is a list begins with a value of -1 to indicate the first zone, which is followed by a list of element numbers in the TRACECN*.dat file that will be used to define the average concentration for that zone. Next, a value of -2 indicates a second zone, and is followed by a list the element numbers used to define zone 2. Up to 10 zones may be defined, and the list is terminated by a value of -99. Only one zone is required; multiple zones are optional.

For example, consider a BLTMS model in which the master input file bltmsin.inp has defined output concentration traces for element numbers 10, 62, and 442, that represent a vertical slice down gradient from the waste containers at some distance from the source. The Launch_BLTMS.DLL will pass the *NTRCEC_LIST* data (-1, 10, 62, 442, -99) for this zone. The output table (*BLT_Concentration_Data_Table*), defined by ISO, will be automatically populated with the average concentration data versus time from these elements. For the LEACHRL*.dat output data, CUMR and BAREA, a set of GoldSim 3-D tables are utilized to store the extracted data (Table 5). Similar to the concentration data table, for *Cumr_Sum* each layer represents a zone, whereas each column represents an ISO. Each column is a sum of the cumulative releases for the node numbers listed for each zone. The LEACHRL*.dat file contains only the node locations that are associated with a waste container at that location. The *NELCON_LIST* vector needs to be defined listing the node numbers where the waste containers are located. This vector (node list) can be divided into one or more zones. Given an example configuration divided into three zones, the *NELCON_LIST* vector may be [-1, 316, 317, 338, -2, 162, 163, 184, -3, 8, 9, 30, -99], where the waste container locations defined in DATA SET 20 of the bltmsin.inp file are divided into three zones. The final switch is the *BLTMS_INPUT_OUTPUT_SWITCH*. If a value of 1 is passed to Launch_BLTMS.DLL, the input file (bltms.inp) will be renamed as bltms####.inp, # equal to the realization number, and likewise for the bltms.out file. This option is only necessary when a history of the input and output files is desired and the FileCapture.DLL is not used to keep a copy of them.

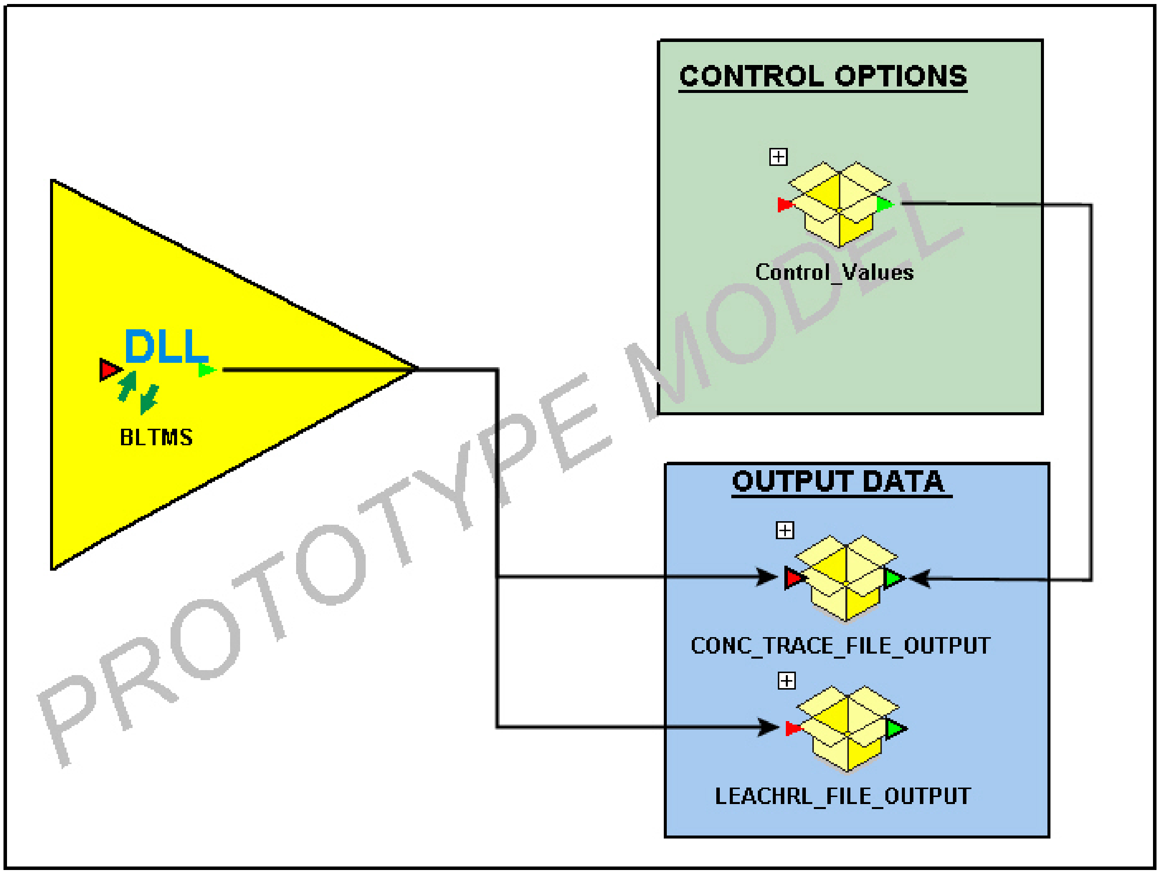


Figure 9. Launch_BLTMS Container Structure

Table 5. Level 3 Containers and Launch_BLTMS Output Elements

Level 3 Container	Element	Description
Control_Values	NTRCEC_LIST	Vector listing element locations used for the calculation of the average concentration for one or more zones.
	NELCON_LIST	Vector listing element locations used for the calculation of the cumulative mass released from waste containers defined in one or more zones.
	BLTMS_INPUT_OUTPUT_SWITCH	Switch passed to Launch_BLT.DLL to indicate whether or not to save a copy of the bltmsin.inp and bltms.out file for every realization.
	FileCapture_Switch	Switch used to turn on and off the FileCapture.DLL [Discussed in further detail below].
CONC_TRACE_FILE_OUTPUT	BLT_Concentration_Data	ISO concentration for specificed nodal locations from TRACECN*.DAT FILES.
	BLTMS_Concentration_Trace_Data	Array of concentration trace data [extracted from BLT_Concentration_Data table].
LEACHMS_FILE_OUTPUT	Cumr_Sum	Total cumulative mass released from source term elements for ISO(1) to ISO(i).
	Barea	Container breached area at each source term element.

3. 1-D TRANSPORT MODEL

3.1 Model Overview

A one-dimensional transport model was implemented within the GoldSim software using the "pipe" pathway option in GoldSim. The pipe pathway represents a fluid conduit in which advection, dispersion, and sorption of radionuclides can occur and from which diffusion into the immobile groundwater of the rock matrix can occur. The numerical solution of transport through the pipe is solved using the computationally efficient Laplace transform method. The important characteristics of each pipe include the cross sectional area, the volumetric flow rate into the pipe, the length, the properties of any infill medium, and the diffusive characteristics of the rock matrix outside the pipe. The design of the GoldSim 1-D model is a function of the proposed repository design and geologic features. This basic implementation is discretized into three parts: Drift Transport, UZ transport, and SZ transport. This 1-D model implementation may require a site specific reconfiguration.

Three flow pathways were specified, with each flow path consisting of a pipe for unsaturated flow beneath the disposal cell and a pipe for saturated flow, connected in series. The number of pipe pathways and properties of the pipes used in this one-dimensional transport model can be adjusted to represent the system being modeled appropriately accounting for; cross sectional area (m^2), volumetric flow rate (m^3/yr) and length (m). Other material properties such as porosity, dispersivity, and sorption coefficients should be assigned within the one-dimensional transport model to match the values used in the corresponding BLT-MS transport models. For the fractured rock units, the matrix diffusion coefficient and fracture spacing are also specified. A simplified conceptual model for matrix diffusion is employed in the pipe pathway, in which there are multiple equally spaced parallel fractures. It should be noted that in the fractured medium the pipes are conceptualized to represent only the open fractures. Consequently, the cross sectional area specified in the GoldSim model is the total cross sectional multiplied by the fracture porosity, and the porosity within the pipe is set to a value of 1.0.

3.2 Using the 1-D Transport Model

The hypothetical pipe-pathway is an alternative conceptual model from the 2-D transport embeded in BLTMS with both an unsaturated zone and saturated zone component is depicted in Error! Reference source not found.. The model is setup to automatically feed the cumulative mass release from the source term containers defined in the BLT-MS model into an example alternative conceptual model for SZ transport using GoldSim 1-D pipes. Two steps are required for the successful invocation of the 1-D Pipe Model: 1) assign physical constants to the GoldSim Species list (found in the *\BLT_MS_Integration_Model\ Open_Model\Materials* container, see Figure 1; and 2) define each source term zone by listing the finite-element locations (by number) for each container in each source term zone using the *NELCON_LIST* vector. This example 1-D transport can be modified to reflect site specific characteristics of a potential LLW repository under consideration.

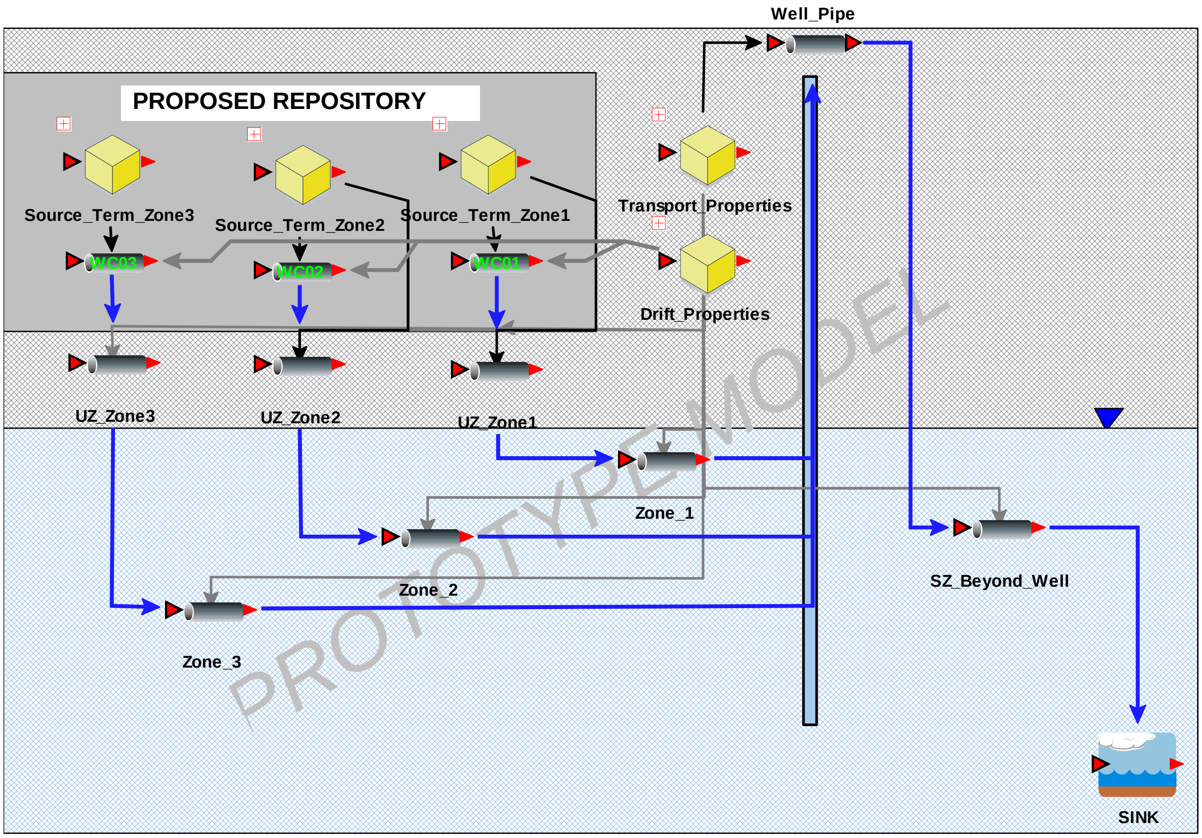


Figure 10. 1-D Pipe Model for Saturated Zone Transport

The pipe model for saturated zone transport was implemented by making use of the GoldSim Contaminant Transport Module specialized pre-defined transport elements, specifically, the pipe-pathway element. It is recommended that the analyst review the GoldSim Contaminant Transport Module User's Guide (GoldSim Technology Group, 2006) for specific details and functionality of the pipe-pathway elements used for this model. The transport module in GoldSim needs the radionuclides to be defined within the *Species* Element. The *Species* element is found in the *Materials* container at the upper level of the model structure as seen in Error! Reference source not found.. It is necessary to define the physical properties for each of the ISO species defined in the BLTMS input file. In the example shown in Figure 11, the first ISO in the BLT-MS input file, bltmsin.inp, is ^{63}Ni. Therefore the physical properties for ^{63}Ni are defined for ISO1 in the GoldSim *Species* Element. These properties include the atomic weight, decay rate and daughter products. In the example shown in Figure 11, the ISO1 (^{63}Ni) note that the "Radioactive" check box is selected, and therefore the species will be decayed in the GoldSim model during the simulation. If the ISO list in the bltmsin.inp file is changed, (e.g. number of species, order of species or species are added or removed to the list), the analyst must edit the GoldSim *Species* Element to ensure the properties are correlated and appear in the same order as in the modified bltmsin.inp file.

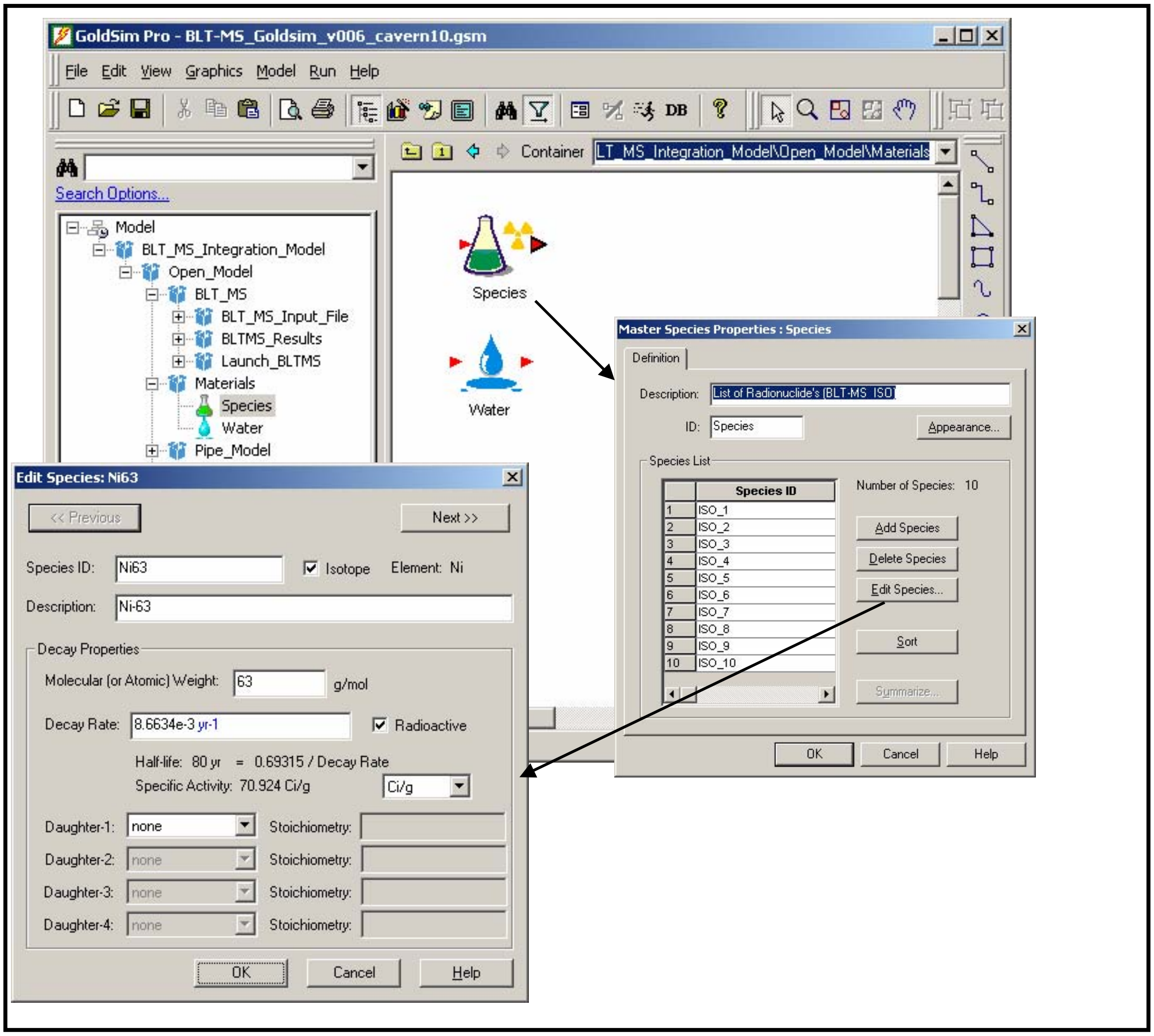


Figure 11. Editing the Species Element

The second step required for the proper functionality of the pipe pathway transport model is to place the waste container defined by Global Element Location (Data Set 20 of the BLT-MS input file) in one of the three default zones defined in the pipe model. The 1-D pipe model requires the cumulative mass releases from the waste containers defined and simulated within the BLTMS model. Since the Launch_BLTMS.DLL reads the cumulative releases from the LEACHRL*.DAT, this data is readily available to use as the source term in the pipe model. The LAUNCH_BLT.DLL is setup to automatically calculate the cumulative release for each zone; however, the analyst must place each of the containers defined in the BLTMS model in one of three source regions defined in the pipe model. The first source region, ZONE1, is the region closest to the well pathway and ZONE3 is the farthest from the well pathway (Error! Reference source not found.). The vector *NELCON_LIST* needs to be defined (Table 5). As seen in the example depicted in Figure 12, six containers are defined for Zone1. They are listed in the vector for the *Zone1_Containers* element by ***finite-element number*** associated with the location of the container. Each waste container should appear in only one of the three zones to avoid double counting of the mass release. It is important to note that BLTMS allows a maximum of 5000 containers to be defined; therefore, each of the three vectors has a maximum size of 5051.

This allows the analyst to place all of the containers in one zone or spread them out over a maximum of 50 zones. Each time a modeling case is developed, the analyst must check the *NELCON_LIST* to ensure the total number of containers are captured, finite-element number are not listed in more than one zone, and all of the locations listed are associated with containers in the bltmsin.inp file.

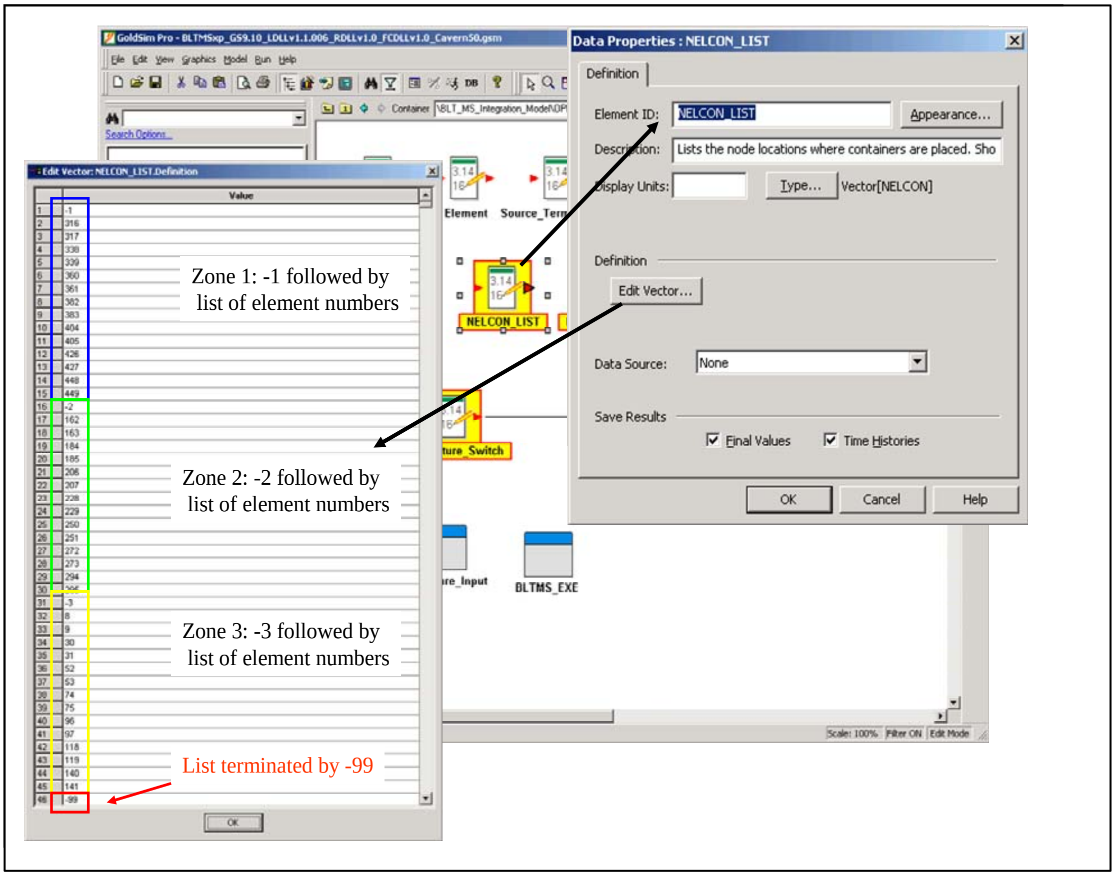


Figure 12. Editing NELCON_LIST Array Element

The last step required for the proper functionality of the pipe pathway transport model is to correlate the physical properties of the porous media (Data Set 13) defined in the BLT-MS input file with the physical transport properties used in the 1-D transport model in GoldSim. The *Transport_Properties* and the *Drift_Properties* containers shown in Error! Reference source not found. and listed in Table 7, contain the data elements used to define the properties used in the 1-D pipe pathway elements (listed in Table 6). If the the BLT-MS model is reconfigured, one must ensure the physical properties of the porous media in Data Set 13 are used in the appropriate GoldSim 1-D pipe pathway elements in the 1-D model to ensure proper correlation between the two alternative models. For instance, porous media properties like Kd values and transport properties like water flux and dispersivity are defined using parameters contained within the *UZ_Properties* and *SZ_Properties* containers. Likewise, the Drift_Properties container holds the elements that define the solid media and transport properties represented in an emplacement drift or borehole. Table 6 through Table 9 lists the 1-D model elements with a brief description for each.

Table 6. 1-D Pipe Model Containers and Elements

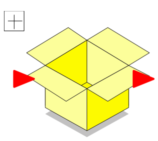
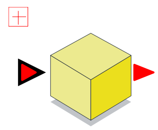
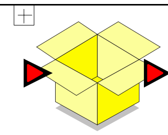
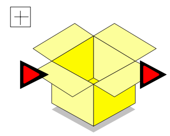
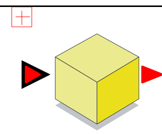
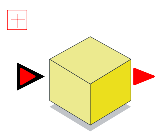
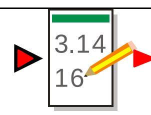
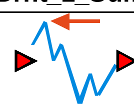
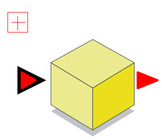
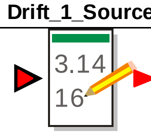
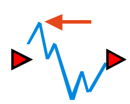
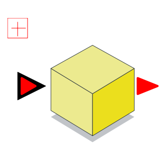
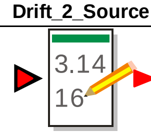
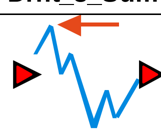
Upper Level Container	Level 2 Container	Element	Description
 Pipe_Model	 Transport_Properties	 UZ_Properties	Contains the elements used in the 1-D pipes for UZ transport properties (See Table 8)
		 SZ_Properties	Contains the elements used in the 1-D pipes for SZ transport properties (See**Error! Reference source not found.**Table 8)
	 Drift_Properties		Contains the elements used in the 1-D pipes for the drift transport properties (See Table 7)
	 Source_Term_Zone1	 Drift_1_Sum	Total cumulative mass released in Zone 1 for ISO(i) to ISO(10) from Cumr_Sum Table
		 Drift_1_Source	Total cumulative mass released in Zone 1 for ISO(i) to ISO(10)
	 Source_Term_Zone2	 Drift_2_Sum	Total cumulative mass released in Zone 2 for ISO(i) to ISO(10) from Cumr_Sum Table
		 Drift_2_Source	Total cumulative mass released in Zone 2 for ISO(i) to ISO(10
	 Source_Term_Zone3	 Drift_3_Sum	Total cumulative mass released in Zone 3 for ISO(i) to ISO(10) from Cumr_Sum Table– DO NOT EDIT
		 Drift_3_Source	Total cumulative mass released in Zone 3 for ISO(i) to ISO(10) – DO NOT EDIT

Table 6: Continued

Upper Level Container	Level 2 Container	Element	Description
Pipe_Model Cont.	**Source_Term_Zone3** Cont.	WC01	Pipe pathway for the source term release from containers in Drift 1
		WC02	Pipe pathway for the source term release from containers in Drift 2
		WC03	Pipe pathway for the source term release from containers in Drift 3
		UZ_Zone1	Unsaturated zone pipe pathway for RN releases from containers in Zone 1
		UZ_Zone2	Unsaturated zone pipe pathway for RN releases from containers in Zone 2
		UZ_Zone3	Unsaturated zone pipe pathway for RN releases from containers in Zone 3
		Zone_1	Saturated zone pipe pathway for RN releases from unsaturated Zone 1
		Zone_2	Saturated zone pipe pathway for RN releases from unsaturated Zone 2
		Zone_3	Saturated zone pipe pathway for RN releases from unsaturated Zone 3
		Well_Pipe	1-D pipe pathway element used to simulate a well intersecting the RN transport pathway through the saturated zone
		SZ_Beyond_Well	1-D pipe pathway element for saturated zone transport boundary
		SINK	Cell element used for RN sink.

Table 7. 1-D Model Drift Properties Container

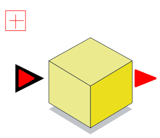
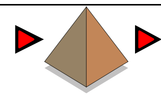
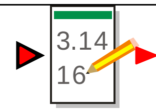
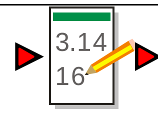
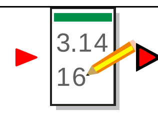
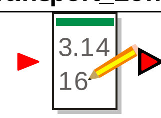
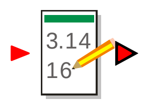
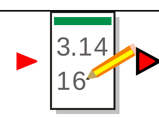
Level 2 Container	Subcontainer	Element	Description
 Drift_Properties	none	 Concrete_Matrix	Solid media added to the pipe models to represent transport through the drift and concrete over packs
		 Porosity_Cement	Porosity of the concrete used in the drifts
		 Dispersivity	Longitudinal dispersivity of pathway– The analyst must edit all zones if model configuration changes
		 Transport_Length	Pipe length that represents the distance from the waste containers through the concrete to the UZ
		 Cross_Sect_Area	Cross sectional area of pipe – The analyst must edit all zones if model configuration changes
		 Cont_Source_Length	Length of pipe over which source mass is added– The analyst must edit all zones if model configuration changes
		 Qflux	Volumetric flow rate through the waste container and emplacement drift.

Table 8. 1-D Model UZ_Properties Container Elements

Level 2 Container	Subcontainer	Element	Description
Transport_Properties	UZ_Properties	UZ_Source_Length	Length of pipe over which source mass is added– The analyst must edit all zones if model configuration changes
		UZ_Pipe_Q_Flux	Volumetric flow rate through the UZ pipe pathway.
		UZ_Pipe_Dispersivity	Longitudinal dispersivity of pathway– The analyst must edit all zones if model configuration changes
		UZ_Pipe_Transport_Length	Pipe length representing the distance from the waste containers through the concrete to the UZ
		UZ_Matrix_Porosity	Porosity of the UZ rock matrix.
		Diffusivity_UZ_Matrix	Diffusivity of the UZ rock matrix.
		UZ_Matrix	Solid media added to the pipe models to represent matrix transport through unsaturated zone
		UZ_Matrix_Bulk_Density	Bulk density of the UZ rock matrix.
		Fracture_Coating	Solid media added to the pipe models to represent fracture surfaces for fracture sorption in the unsaturated zone
		Frac_Coating_Thickness	Uncertain distribution added to the pipe models to represent fracture coating thickness for fracture sorption in the unsaturated zone
		UZ_Saturation	Value for saturation of the UZ matrix media used in the unsaturated zone pipe model.

Table 8: Continued

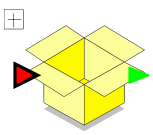
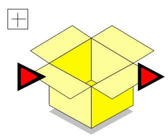
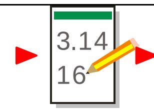
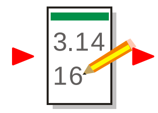
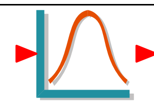
Level 2 Container	Subcontainer	Element	Description
 **Transport_Properties** Continued	 **UZ_Properties** Continued	 **Cross_Sect_Area**	Value represents the cross sectional area for each pipe used for RN transport in the unsaturated zone
		 **UZ_Pipe_Area**	Value represents the area for each pipe used for RN transport in the unsaturated zone given by =Cross_Sect_Area*UZ_Matrix_Porosity
		 **Drift_Depth**	Value represents the depth of each drift used to calculate deminsions of the pipe pathway used for RN transport in the unsaturated zone
		 **Fracture_Spacing**	Uncertain distribution used for fracture spacing necessary to for modeling fracture transport using a pipe
		 **UZ_Pipe_Perimiter**	Wetted perimeter used for the pipe model transport pathway given by: (UZ_Pipe_Area/Drift_Depth)*(Drift_Depth/Fracture_Spacing)*2

Table 9. 1-D Model SZ_Properties Container Elements

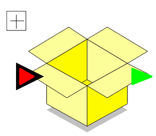
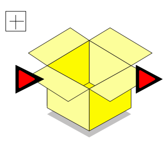
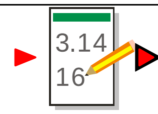
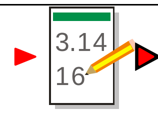
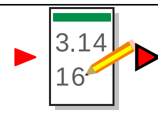
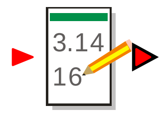
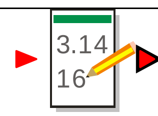
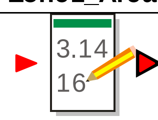
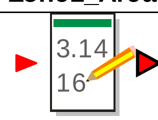
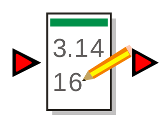
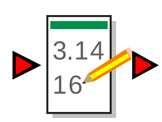
Level 2 Container	Subcontainer	Element	Description
 **Transport_Properties**	 **SZ_Properties**	 **Zone1_Transport_Length**	Zone 1 pipe length representing the RN transport distance through the SZ to the well pathway
		 **Zone2_Transport_Length**	Zone 2 pipe length representing the RN transport distance through the SZ to the well pathway
		 **Zone3_Transport_Length**	Zone 3 pipe length representing the RN transport distance through the SZ to the well pathway
		 **SZ_Source_Length**	Length of pipe over which source mass is added– The analyst must edit all zones if model configuration changes
		 **Zone1_Area**	Cross sectional area of pipe for mobile zone of zone 1 transport
		 **Zone2_Area**	Cross sectional area of pipe for mobile zone of zone 2 transport
		 **Zone3_Area**	Cross sectional area of pipe for mobile zone of zone 3 transport
		 **Zone1_Dispersivity**	SZ zone 1 longitudinal dispersivity of pathway– The analyst must edit all zones if model configuration changes
		 **Zone2_Dispersivity**	SZ zone 2 longitudinal dispersivity of pathway– The analyst must edit all zones if model configuration changes

Table 9: Continued

Level 2 Container	Subcontainer	Element	Description
Transport_Properties **continued**	SZ_Properties **continued**	Zone3_Dispersivity	SZ zone 3 longitudinal dispersivity of pathway– The analyst must edit all zones if model configuration changes
		Zone1_Qflux	Zone 1 volumetric flow rate through the SZ pipe pathway.
		Zone2_Qflux	Zone 2 volumetric flow rate through the SZ pipe pathway.
		Zone3_Qflux	Zone 3 volumetric flow rate through the SZ pipe pathway.
		Well_Pathway_Outflow	Total volumetric flux from the three SZ pipes that pass through the well pathway.
		Volume_Well_Pathway	To calculate the averge concentration from the three sources, the inflow rates from the three pipes * timestep length is used for the volume in the well pathway.
		SZ_Media_porosity	Porosity of the SZ rock matrix.
		SZ_Satruation	Value for saturation of the SZ matrix media used in the unsaturated zone pipe model.
		SZ_Media_Bulk_Density	Bulk density of the SZ rock matrix.
		SZ_Porous_Media	Solid media added to the SZ pipe pathways to represent SZ rock matrix

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4.0 DOSE MODEL

The dose model was constructed based upon ICRP-72 dose coefficients for ingestion (ICRP, 1996). The drinking water pathway was used as the dose pathway in this model. The primary radionuclides in the groundwater are given by the average concentration at the well pathway. The average concentration calculated within the Launch_BLT.DLL gives a 'vertical slice' of the concentrations from the finite element grid, e.g. representing a well intersecting the saturated zone down gradient of the proposed repository. The *NTRCEC_LIST* is used to define the vertical slice of elements to be used in the average concentration calculation. It is possible to define as many as 10 vertical slices (e.g. calculate 10 average concentration values) using any combination of elements up to the maximum number of 100 traces saved by BLTMS.exe. The average concentration values for each zone listed in *NTRCEC_LIST* are recorded in the *BLT_Concentration_Data_Table*.

The annual dose from ingestion of radionuclides in drinking water is expressed as:

Equation 1: $$Dose = EFD_{ICRP72}^{RN}\left({}^{Sv}\!/\!_{Bq}\right) \times C_{Water}^{RN}\left({}^{Bq}\!/\!_{L}\right) \times ACR\left({}^{L}\!/\!_{yr}\right)$$

, where:

EFD = effective dose conversion factor from ICRP-72 for a specific radionuclide species

C = average concentration of a radionuclide species in the well pathway

ACR = annual water consumption rate (2 L/day).

An annual consumption rate of 2 liters/day or 730 L/yr was used. The container ***\BLT_MS_Integration_Model\Open_Model\Results*** contains the elements in GoldSim used to implement the dose calculations. The analyst is not required to make any changes unless the radionuclide species changes and new dose coefficients are required.

Table 10. Dose Model Containers and Elements

Results	**Dose_Conversion_Factors**	**Dose_Coefficients**	ICRP-72 dose coefficients
		Annual_Consumption_Rate	Annual consumption rate.
	Dose	**Dose_1D_Model**	Dose from the well pathway using the 1-D pipe model results
		Dose_BLTMS_Model	Dose from the well pathway using the BLTMS model results
		Total_Dose_1D_Model	Total dose (sum of all species) calculated from the 1-D model results
		Total_Dose_BLTMS_Model	Total dose (sum of all species) calculated from the BLTMS model results

5.0 SOFTWARE

Several codes were integrated in order to facilitate a comprehensive modeling capability for the probabilistic performance assessment software package, GoldSim/BLT-MS integrated model. A list of these codes appears in Table 11. Each of the codes in the integrated software package, as well as the computer platforms available for use, have strengths and limitations that need to be accounted for in building the integrated model. A summary of these considerations is offered below.

Table 11. List of Codes used the Probabilistic Model

Preprocessors	BLTMS_WIN.EXE
	BLTMS_GRID.EXE
Executed During Model Simulation	BLTMS.EXE
	Goldsim.exe
	READ_BLTv1.1.002.DLL
	LAUNCH_BTLMSv1.1.011.DLL
	FileCapturev1.0.DLL
Postprocessors	BLTPLOT_UNCERT.EXE

In addition, the GoldSim model file,

BLTMS072006_GS9.21_LDLL1.1.0011_RDLL1.1.002FDLL1.0_Siteno7c_v1.4.1.gsm,

discussed in this manual has been designated as open-source and is freely available. It can be accessed on a Sandia National Laboratories website at the following URL: http://www.sandia.gov/icp/. Two versions of the model have been developed.

5.1 BLT-MS Preprocessors

BLTMSIN-WIN.EXE

When BLT-MS was originally developed, a DOS-based preprocessor, BLTMSIN.EXE, was also developed in order to facilitate the creation and editing of input files. This preprocessor is documented in an NRC publication (NRC, 1996a). As part of this project, a Windows-based preprocessor was developed to facilitate a modern graphical user interface for creating and editing the BLT-MS input files. This code is called BLTMSIN-WIN.EXE. The code has been designated as open-source and is freely available. It can be accessed on a Sandia National Laboratories website at the following URL: http://www.sandia.gov/icp/.

The BLTMSIN-WIN code was developed with the Lahey FORTRAN compiler. Figure 13 shows the introductory screen for BLTMSIN-WIN. Also shown in the figure is the drop-down menu for the input categories. The input categories are basically the same as those in the original BLTMSIN code, as documented in the NRC user's guide publication (NRC, 1996a). The BLTMSIN-WIN code has the same basic functionality as the original DOS-based code but with Windows features, such as radio buttons, script field input, pop-up windows, etc. The BLTMSIN-WIN code has a Help feature as well. The code is intuitive to use and any technical input issues are basically addressed by the original user's documentation (NRC, 1996a).

Figure 13. BLTMS-WIN introductory screen and input menu

BLTMS_GRID.EXE

The BLT-MS model employs a rectangular finite-element grid for the transport simulations in the far-field. The BLTMSIN and BLTMSIN-WIN input processors have a rudimentary automatic grid generating option that allows the user to specify either a uniform grid spacing setup or one that has an incrementally increasing grid spacing setup. If the user needs more specificity to create a unique grid layout, the code allows for individual node prescription. This option would be quite burdensome for a user to create if a large grid size is used. Therefore, a small DOS-based FORTRAN routine was written to help facilitate the creation of a non-uniform grid. This software package is called BLTMS_GRID.EXE. The code has been designated as open-source and is freely available. It can be accessed on a Sandia National Laboratories website at the following URL: http://www.sandia.gov/icp/.

When the user executes the BLTMS_GRID code, an output file name must first be supplied. Then the user is asked what type of format they want the grid to have: a grid with square elements, a grid with uniform height and width elements, or a grid with variable width and height elements. If the variable element option is selected, the user has the option of specifying the width and height of the elements interactively or by specifying a pre-existing input file. A Read_Me file is included that prescribes the format for the ASCII text file for the x-axis and z-axis spacing for each finite element in the model. The BLTMS_GRID code then creates the necessary data to conform to the formatting for the input file to BLT-MS. The contents of the output file need to be cut-and-pasted into the BLT-MS file using a word processor.

5.2 BLT-MS

The BLT-MS code was developed in the mid-1990s. It is a FORTRAN code that has been compiled to run under DOS or a DOS-emulator. The code's functionality relative to the process models incorporated in the code has been preserved. However, modifications to the input/output files were necessary to integrate the code with a GoldSim™ model file.

To accurately simulate the proposed sites, it was necessary to increase the size of the arrays in the code associated with these attributes to accommodate models having up to 30,000 nodes, 5000 waste containers, and 5000 time steps. Dr. Terry Sullivan, of Brookhaven National Laboratory, helped modify the code for the new requirements. Dr. Sullivan was the lead developer of the BLT-MS code when it was first developed for the NRC.

BLTMS.EXE is publicly available from the U.S. Nuclear Regulatory Commission (NRC).

5.3 GoldSim™

GoldSim™ Version 9.21 was used to develop this software package. GoldSim™ is a graphical, object oriented computer program for carrying out dynamic probabilistic simulations. GoldSim™ was developed to run probabilistic simulations using a Monte Carlo sampling technique. The code was selected for this application due to its flexibility in coupling to external codes through the use of dynamically linked libraries (DLL). GoldSim™ can be used as the integrator that samples the uncertain distributions and then launches external codes through commands executed in DLL's. See the GoldSim Users Guide (GoldSim Technology Group LLC, 2006) for a detailed description of the code's functionality.

The program runs on personal computers using 32-bit Microsoft Windows operating systems (Windows 2000 or higher is required). An Intel Pentium CPU or higher with at least 128 MB of RAM is required. GoldSim is a trademark of GoldSim Technology Group LLC. © Copyright 2006 GoldSim Technology Group LLC. All rights reserved. A copy and license for the GoldSim code can be obtained at www.goldsim.com.

5.4 Read_BLT.DLL

Read_BLT.DLL is a preprocessor for the integration of the BLT-MS (Breach, Leach, and Transport - Multiple Species) code with GoldSim™. The program is intended as a DLL for use with a GoldSim™ model file. The code is executed through a call from the GoldSim.exe during runtime. The code allocates parameters to memory to receive data from subsequent calls from goldsim.exe when the model is run. The goldsim.exe passes input values to the Read_BLT.DLL during runtime, which comprise a single array of values (Appendix C, GoldSim Users Guide, GoldSim Technology Group, 2006). The DLL parses the GoldSim array in(*) into the allocated memory and then writes a new BLTMS.EXE input file using the values passed by goldsim.exe. The BLTMS.EXE input file is named BLTMS0000#.inp, with the # being replaced by the realization number for each Monte Carlo analysis. This software is used as part of a modeling package that consists of BLTMS.EXE, GoldSim™, Read_BLT.DLL and Launch_BLTMS.DLL.

Instructions for using Read_BLT.DLL

It is necessary to define a BLTMS.exe input file before the DLL can be executed (see Section 2.2 of this document). An external DLL element must be defined within a GoldSim™ model file, which calls the Read_BLT.DLL and the read_blt subroutine. The Read_BLT.DLL requires thirty-eight inputs passed from GoldSim through the external DLL element interface. The 38 required inputs represent individual GoldSim elements (listed in Table 12). These input values are an assemblage of vectors, matrix or values that comprise a single input array passed to the READ_BLT.DLL during runtime at the beginning of each realization for a probabilistic simulation. The input array passed to the DLL must remain in the order defined in the GoldSim file and listed in the table below. The input definitions and a description are discussed in Section 2.4 of this document. In addition, five outputs are defined in the external DLL element for data values passed from the READ_BLT.DLL for use in the GoldSim model for downstream calculations. These outputs are read from the BLTMS input file and passed to the Launch_BLTMS.DLL for dynamic array allocation. The five output values are listed in Table 13. A detailed description of coupling external DLL's is contained in Chapter 10 and Appendix C of the GoldSim Users Guide (GoldSim Technology Group, 2006). the Read_BLT.DLL source code is supplied with this document in Appendix A.2 Read_BLT.DLL.

Table 12. Input Array for Read_BLT.DLL

Input	Type	Units	Description
Realization	Value	N/A	Realization number for Monte Carlo simulations.
BLT_MS_Uncertain_Param_Switch	Vector	N/A	Array that passes the DLL which parameters are treated as uncertain.
BLT_MS_Uncertain_Array_Sizes	Vector	N/A	Array that passes the DLL the maximum size of each uncertain array.
CSAT	Vector	g/cm^3	Solubility limit for contaminant iso.
prop_1_i	Vector	cm^2/s	molecular diffusion coefficient of material i.
prop_2_i	Vector	g/cm^3	bulk density of the soil of material i
prop_3_i	Vector	cm	longitudinal dispersivity (cm) of material i
prop_4_i	Vector	cm	transverse dispersivity (cm) of material i.
prop_5_i	Vector	N/A	porosity of material i.
prop1_1_k_i	Matrix	cm^3/g	distribution coefficient of material k and contaminant i.
QCBF(j,i,iso)	Vector	mass/ cm^2/ year	Specified flux value of the j^{th} data point in the i^{th} profile for contaminant, iso (mass/cm^2/year).
QNBF(j,i,iso)	Vector	mass/ cm^2/ year	Specified dispersive flux value of the j^{th} data point in the ith profile for isotope, iso.

Table 12: Continued

Input	Type	Units	Description
CDBF(j,i,iso)	Vector	mass/ cm^3	Specified concentration value of the j^{th} data point in the i^{th} profile for contaminant, iso.
THICK(J)	Vector	cm	Thickness of the J^{th} container. 55 gallon drums are typically 0.127 - 0.152 cm thick.
PITN(J)	Vector	N/A	Pitting parameter n for the J^{th} container (dimensionless). If PITN(J) = 0, a value for PITN is estimated by the code based on input parameters for clay content (CLAY), soil aeration (IAER), and the moisture content. Measured values for PITN range from 0 - 1.
PITK(J)	Vector	cm/yr	Pitting parameter k for the J^{th} container. If PITK is input as zero, a value is estimated based on the soil pH. Measured values for PITK range from 0.03 - 0.15. If soil pH is input as zero, PITK is set to 0.0737, the average for all soils.
AREA(J)	Vector	cm^2	Area of the J^{th} waste container. The area of a 55 gallon drum is 21,000 cm^2. The value is used to calculate the maximum pit depth and the area breached by pitting.
ASCALE(J)	Vector	N/A	Area scaling exponent (dimensionless) for container J. If ASCALE is input as zero, a default value of 0.2 is used.
PITS(J)	Vector	N/A	Number of penetrating pits in the container (dimensionless) for container J. The total area breached is linearly proportional to the number of pits that penetrate the container, PITS(J). The default value used by BLT-MS is 1000.
GRATE(J)	Vector	cm/s	The general corrosion rate of container J. If the input values of GRATE(J) is zero, then a default value of 3E-10 cm/s is used.
CLAY(J)	Vector	N/A	Clay fraction of the soil (0 ≤ CLAY(J) ≤ 1) around container J. If PITN is input as zero, PITN is calculated as a function of clay and moisture content as well as the degree of aeration (IAER).
SPH(J)	Vector	N/A	Soil pH. If PITK is input as zero, PITK is calculated as a function of pH. If SPH(J) is input as zero, a default value of 7.0 is used.
IAER(J)	Vector	N/A	Aeration index for the soil around container J. 1 = good, 2 = fair, 3 = poor, and 4 = very poor. Used in calculating PITN. If PITN and IAER are input as zero, PITN is set equal to 0.26, 0.39, 0.44, 0.59 for IAER = 1, 2, 3, 4 respectively. Most soils considered for low-level waste disposal will have good or fair aeration.
SFRACT(J,ISO)	Matrix	N/A	Fraction of the mass in the Jth waste form that is available for surface wash-off in the rinse release model for contaminant iso. Useful for surface contaminated waste forms such as lab trash (0 < SFRACT(J) < 1.). The user must exercise caution such that (SFRACT + PFRACT + BFRACT) = 1 for any given model realization in the probabilistic framework.

Table 12: Continued

Input	Type	Units	Description
PFRACT(J,ISO)	Matrix	N/A	Fraction of the mass in the Jth waste form that is available for diffusion controlled release for contaminant iso. Useful for cement solidified waste forms (0. < PFRACT(J) < 1.). The user must exercise caution such that (SFRACT + PFRACT + BFRACT) = 1 for any given model realization in the probabilistic framework.
BFRACT(J,ISO)	Matrix	N/A	Fraction of the mass in the Jth waste form that is available for release due to dissolution of the waste form for contaminant iso. Useful for waste forms such as activated metals or when modeling a constant release rate in time(0 < BFRACT < 1.). The user must exercise caution such that (SFRACT + PFRACT + BFRACT) = 1 for any given model realization in the probabilistic framework.
DEFF(J,ISO)	Matrix	cm^2/s	Jth waste form effective diffusion coefficient for contaminant iso. Used only if PFRACT(J,ISO) > 0.
DISOL(J,ISO)	Matrix	1/yr	Jth waste form fractional release rate (1/yr) for contaminant iso. Used only if BFRACT(J,ISO) > 0.
PARTKO(J,ISO)	Matrix	cm^3/g	Jth waste form partition coefficient for contaminant iso cm^3/g at time t = 0. Used only if SFRACT > 0.
PARTKI(J,ISO)	Matrix	cm^3/g	Jth waste form partition coefficient for contaminant iso cm^3/g at time t = 0.
PARTD(J,ISO)	Matrix	1/yr	Jth waste form partition coefficient degradation rate constant for contaminant iso. PARTD(J,ISO) must be greater than or equal to 0.
POREL(J)	Vector	cm	Radius or half-length of waste form J. Used in calculating diffusion and dissolution controlled release (PFRACT > 0).
VOLWF(J)	Vector	cm^3	Volume of waste form J. Used in calculating the height of cylindrical waste forms and initial concentrations within the waste form.
VRATIO(J)	Vector	N/A	Ratio of the volume of waste form J to the finite element in which it is located. Used in the rinse with partitioning model.
WTINIT(J,ISO)	Matrix	Ci	Initial inventory of contaminant iso in waste form J. If IACT = 0, WTINIT is input in grams. If IACT = 1, WTINIT.
VXNI_J	Value	N/A	Multiplier for all values of Darcy velocity in the X-direction.
VZNI_J	Value	N/A	Multiplier for all values of Darcy velocity in the Z-direction.
TH(IQ,J)	Value	N/A	Moisture content multiplier. Moisture content is defined at each nodal point in the finite element grid. In quadrilateral elements, there are four moisture content values associated with each element.

Table 13. Output Array from Read_BLT.DLL

Output	Type	Description
NISO	Value	Number of Isotopes defined in the BLTMS input file.
NTI	Value	Number of time steps in the simulation.
NSTPTR	Value	Number of time steps between output to the trace files.
NTRC	Value	Number of nodes with a concentration trace to the output file.
NCON	Value	Number of Containers defined in the BLTMS input file.

The program was developed and compiled using Digital™ Visual Fortran Professional Edition Version 6.0 (Digital Equipment Corporation, 1998) and runs on personal computers using 32-bit Microsoft Windows operating systems (Windows 2000 or higher is required). An Intel Pentium CPU or higher with at least 128 MB of RAM is required. The code has not been compiled or tested on any other platform. The code has been designated as open-source and is available on a Sandia National Laboratories website at the following URL: http://www.sandia.gov/icp/. Read_BLT.DLL Version 1.0 - Copyright 2005 Sandia Corporation. Under the terms of Contract DE-AC04-94AL85000 with Sandia Corporation, the U.S. Government retains certain rights in this software.

5.5 Launch_BLTMS.DLL

Launch_BLTMS.DLL is a postprocessor for the integration of the BLT-MS (Breach, Leach, and Transport - Multiple Species) code with GoldSim™. The program is intended as a DLL for use with a GoldSim™ model file. The code executes BTLMS.EXE using a standard BLT-MS input file and allocates parameters to memory for subsequent input of BLTMS.EXE output data to a GoldSim™ model file. This DLL is used for performing Monte Carlo analyses. This software is used as part of a modeling package that consists of BLTMS.EXE, GoldSim™, Read_BLT.DLL and Launch_BLTMS.DLL. The modeling package is used to run Monte Carlo analyses for performance assessment of low-level radioactive waste disposal sites.

Instructions for using Launch_BLTMS.DLL

It is necessary to define a BLTMS.exe input file before the DLL can be executed (see Section 2.2 of this document). An external DLL element must be defined within a GoldSim™ model file which calls the Launch_BLTMS.DLL and the bltms subroutine. GoldSim passes the data from nine elements as input to the Launch_BLTMS.DLL, see Table 14. The individual input arrays or values linked internally within the GoldSim model file to the external DLL element comprise the single input array passed to the Launch_BLTMS.DLL during runtime at the beginning of each realization over a probabilistic simulation. The input definitions and a description are discussed in Section 2.4 of this document. In addition, output from the DLL is listed in Table 15. These output are defined in the external DLL element array and correspond to data passed from the Launch_BLTMS.DLL to the GoldSim model file for down stream calculations. These data represent the BLTMS.EXE results from the LEACHRL*.dat and TRACEN*.dat files. Section 2.5 of this document discusses in detail the output captured by the Launch_BLTMS.DLL. A detailed description of coupling external DLL's is contained in Chapter 10 and Appendix C of the GoldSim Users Guide (GoldSim Technology Group, 2006). The DLL source code is provided in Appendix A.4.

Table 14. Input Array Elements for Launch_BLTMS.DLL

Input	Type	Description
Realization	Value	Realization number for Monte Carlo simulations.
NISO	Value	Number of isotopes in the simulation, passed to the DLL from Read_BLT.DLL output (Table 13)
NTI	Value	Number of time steps in the simulation, passed to the DLL from Read_BLT.DLL output (Table 13)
NSTPTR	Value	Number of steps between output traces in the simulation, passed to the DLL from Read_BLT.DLL output (Table 13)
NTRC	Value	Number of trace nodes in the simulation output, passed to the DLL from Read_BLT.DLL output (Table 13)
NCON	Value	Number of containers in the simulation, passed to the DLL from Read_BLT.DLL output (Table 13)
BLTMS_INPUT_OUTPUT_SWITCH	Value	Switch passed to Launch_BLT.DLL to indicate whether or not to save a copy of bltmsin.inp and bltms.out file for every realization (see Table 5)
NELCON_LIST	Vector	Vector listing element locations used for the calculation of the average concentration for one or more zones (see Table 5)
NTRCEC_LIST	Vector	Vector listing element locations used for the calculation of the cumulative mass released from waste containers defined in one or more zones (see Table 5)

Table 15. Output Array Elements from Launch_BLTMS.DLL

Output	Type	Description
TRACECN	3-D Table Definition	ISO concentration traces for specificed nodal locations from TRACECN*.DAT FILES
BAREA	3-D Table Definition	Container breached area at each source term element with a waste container.
CUMR_SUM	3-D Table Definition	Total cumulative mass released from source term for each zone (each zone defined by NELCON_LIST)

The program was developed and compiled using Digital™ Visual Fortran Professional Edition Version 6.0 (Digital Equipment Corporation, 1998) and runs on personal computers using 32-bit Microsoft Windows operating systems (Windows 2000 or higher is required). An Intel Pentium CPU or higher with at least 128 MB of RAM is required. The code has not been compiled or tested on any other platform. The code has been designated as open-source and can be accessed on a Sandia National Laboratories website at the following URL: http://www.sandia.gov/icp/. Launch_BLTMS.DLL Version 1.0 - Copyright 2005 Sandia Corporation. Under the terms of

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5.6 FileCapture.DLL

FileCapture.DLL is a runtime DLL for the use with GoldSim™ software. The program is intended as a DLL for use with the GoldSim/BLT-MS software package. The DLL is called during a GoldSim™ model simulation to copy input/output files created during the simulation to a central location on a LAN. The software is used as part of the GoldSim/BLT-MS software package that consists of GoldSim.exe and other accessory external codes linked and executed during a model simulation. The FileCapture_v1.0.DLL is used to run Monte Carlo analyses. Any input or output file can be captured when the simulation is run locally or when using the distributed processing (i.e., multi-processor run) feature in GoldSim.exe. An input file called 'FileCapture.in' is used to list the filenames and path where the user wants copy the files. FileCapture.DLL copies the files listed in 'FileCapture.in' from each node (e.g. computer used in the simuation) on the LAN to a folder called 'FCAP Files' created in the location listed in the input file. The DLL will execute once for each realization and append a number to each file copied as an identifier of the realization for which the file was generated (e.g. file.dat is copied as file_00001.dat for realization 1).

If the pre-compiled DLL is used, note that it has been compiled for Windows 2000/XP operating systems.

Instructions for using FileCapture.DLL

The DLL must first be linked to a GoldSim model file using the external DLL function within the GoldSim code. Create an External DLL element in GoldSim. Define two input values passed by GoldSim to the DLL and one output value from the DLL to GoldSim:

Input# 1) Switch (1==on) is used to execute the file copy command. It is not necessary to have the FileCapture DLL execute during a local run.

Input# 2) Realization Number. The DLL uses the realization number to tag each file it copies to the selected location.

Output #1) The output is a scalar value that is passed to GoldSim from the DLL indicating that the DLL has completed. This is necessary to ensure during Monte Carlo simulations that the GoldSim code does not begin a new realization before the DLL has finished copying the selected ouput files. When BLTMS.EXE is re-initialized, the previous output files will be deleted.

The second step is to edit the “FileCapture.in” file. The first line in the FileCapture.in file is used by the DLL to identify where to copy the files. The second line indicates how many files are to be copied. The next line begins the list the files to be copied; one per line. The basic format of the FileCapture.in file is as follows:

\\computer name\folder name\	<<***enter the path to have the files copied
3	<<***enter the number of files to be copied
input.dat	<<***list the file names, one per line
output.dat	
debug.dat	

Table 16. Input Array for FileCapture.DLL

Input	Type	Description
FileCapture_Switch	Value	A value of 1 to execute the file copy DLL, the DLL will not execute if any other value is used.
Realization	Value	Realization number for Monte Carlo simulation used to index the output files listed in the FileCapture.in file.

Table 17. Output Array for FileCapture.DLL

Output	Type	Description
Output1	Value	Value passed to GoldSim indicating that the DLL has finished copying the files.

The program was developed and compiled using Digital™ Visual Fortran Professional Edition Version 6.0 (Digital Equipment Corporation, 1998) and runs on personal computers using 32-bit Microsoft Windows operating systems (Windows 2000 or higher is required). An Intel Pentium CPU or higher with at least 128 MB of RAM is required. The code has not been compiled or tested on any other platform. The code has been designated as open-source and can be accessed on a Sandia National Laboratories website at the following URL: http://www.sandia.gov/icp/. Launch_BLTMS.DLL Version 1.0 - Copyright 2005 Sandia Corporation. Under the terms of Contract DE-AC04-94AL85000 with Sandia Corporation, the U.S. Government retains certain rights in this software.

5.7 BLTPLOT_UNCERT.EXE

A simple DOS-based FORTRAN code was written to post-process BLT-MS model results for 2-dimensional concentration data. This code is named BLTPLOT_UNCERT.EXE. The code has been designated as open-source and can be accessed on a Sandia National Laboratories website at the following URL: http://www.sandia.gov/icp/. The BLTPLOT_UNCERT code can extract information on the concentration distribution for a single model run or it can take the output from a Monte Carlo/LHS uncertainty analysis and produce an average concentration distribution from the suite of realization results. The code requires several output files from a completed BLT-MS model run. The files required as input to BLTPLOT_UNCERT are: the BLT-MS input file, the BLT-MS output file, and the concentration output file(s). In the case of a Monte Carlo/LHS run where the average 2-D concentration distribution is required, the GoldSim model will produce sequential concentration output files for each realization, and each one will have an inherent name, such as CONCENT_xxxxx, where xxxxx is the realization number. The code queries the results files and then asks the user to specify which radionuclide and what time step for which the data should be saved. The output from the BLTPLOT_UNCERT is a file containing x, z, and concentration paired data for all the finite-element nodes in the model. This data can then be plotted with 2-D plotting software, such as SURFER or TECPLOT. A Read_Me file is provided that details the requirements of the input files to the BLTPLOT_UNCERT code as well as the EXE source code in Appendix A.5.

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6. SUMMARY

The objective of this document has been to provide a guide for using the integrated software package GoldSim/BLTMS. The example problem discussed in this manual was based upon a prototype performance assessment model constructed by Sandia National Laboratories as part of a technology transfer program funded by the LLW ICP Phase I Technology Transfer Project under a Work for Others (WFO) Funds-in agreement contract between Sandia and Lockheed Martin. This work supports DOE/RW international leadership in geologic disposal of spent nuclear fuels and radioactive waste and working item IN-SNL-DD23, “Technology Transfer for Geologic Repository Science and Performance Assessment”, under the AIT/TECRO Joint Standing Committee for Civil Nuclear Cooperation. Sandia National has over 30 years experience in assessing radioactive waste disposal and at the time of this publication is providing assistance internationally in a number of areas relevant to the safety assessment of radioactive waste disposal systems.

International technology transfer efforts are often hampered by small budgets, time schedule constraints, and a lack of experienced personnel in countries with small radioactive waste disposal programs. To partially overcome these difficulties, the integrated model presents a system that utilizes a combination of commercially available codes and existing legacy codes for probabilistic safety assessment modeling that facilitates the technology transfer and maximizes limited available funding. Numerous codes developed and endorsed by the United States Nuclear Regulatory Commission and codes developed and maintained by United States Department of Energy are generally available to foreign countries after addressing import/export control and copyright requirements. From a programmatic view, it is easier to utilize existing codes than to develop new codes. From an economic perspective, it is not possible for most countries with small radioactive waste disposal programs to maintain complex software, which meets the rigors of both domestic regulatory requirements and international peer review. Therefore, re-vitalization of deterministic legacy codes, as well as an adaptation of contemporary deterministic codes, provides a credible and solid computational platform for constructing probabilistic safety assessment models.

This users guide demonstrates a successful integrated software package using the external model linkage capabilities in the GoldSim software and the techniques used to facilitate this process using legacy applications, including Breach, Leach, and Transport-Multiple Species (BLT-MS), a U.S. NRC sponsored code. The subsurface low-level waste disposal facility used in the example model file was the result of a cooperative technology transfer project between Sandia National Laboratories and the Institute of Nuclear Energy Research (INER) in Taiwan for the preliminary assessment of potential low-level waste repository sites in Taiwan. However, this integrated software package can be easily modified to model site specific conditions for assessments of other potential low-level radioactive waste repositories.

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7. REFERENCES

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2. GoldSim Technology Group LLC, 2006, Goldsim User's Guide Version 9.20, GoldSim Technology Group LLC, www.goldsim.com.

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APPENDIX A. SOURCE CODES

The source codes discussed in this document are stored on the Compact Disc (CD) distributed with this SAND report, and are also available for download at http://www.sandia.gov/icp/.

A.0 GoldSim/BLTMS Model File

BLTMS072006_GS9.21_LDLL1.1.0011_RDLL1.1.002_FDLL1.0_Siteno7c_v1.4.1.gsm
Siteno7c.dat

A.1 BLT-MS Preprocessors

BLTMS_WIN.f90

BLTMS_GRID.f90

A.2 Read_BLT.DLL

Read_BLTv1.1.002.f90

A.3 Launch_BLTMS.DLL

Launch_BLTMSv1.1.011.f90

A.4 FileCapture.DLL

FileCapturev1.0.f90
FileCapture.in
Fcap_Instructions.txt

A.5 BLTPLOT_UNCERT.EXE

BLTPLOT_UNCERT.f90
Read_Me.txt

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