USER'S GUIDE

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Integration of BLT-MS (Breach Leach and Transport-Multi Species) Code with GoldSim

INER

BLT_MS_Integration_Model

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Introduction: Sandia National Laboratories (SNL) has developed a prototype model for probabilistic performance assessment analyses of potential low-level radioactive waste (LLW) disposal sites. SNL has proposed a methodology that involves the use of the Breach, Leach, and Transport – Multiple Species (BLT-MS) code to evaluate potential releases from a disposal facility. The BLT-MS code was developed by Brookhaven National Laboratories (BNL) for the Nuclear Regulatory Commission (NRC) specifically for LLW compliance analyses. SNL has developed a probabilistic model to evaluate uncertainties through the integration of BLT-MS with GoldSim. This document is intended to provide specifications for the implementation of BLT-MS into GoldSim.

The BLT-MS code was developed in the mid-1990's. 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.

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

Conceptual Integration Structure: It is quite common in probabilistic analyses that involve the potential to address spatial variability that the physical aspects of the problem are fixed, such as the model boundaries and finite-element mesh configuration. If there is a question about the design of the finite-element mesh and the boundary conditions, then this should be evaluated in terms of potential conceptual model uncertainty and additional model configurations contemplated to address this uncertainty explicitly. Therefore, 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).

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 becomes 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, so 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. Therefore, the physical source-term configuration (e.g., elements containing containers) will be fixed/deterministic for any given probabilistic analysis, but the characteristics of each of the containers may be uncertain.

In summary, the input parameters that will remain fixed, or deterministic, 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 (because specifying different decay chains for each model realization would be burdensome);
- 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 are in these areas (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 1996)):
- CSAT(iso) = Solubility limit for contaminant iso (g/cm^3). This value can not be input with mass units of Curies.
- prop(1,i) = molecular diffusion coefficient (cm^2/s) 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 jth data point in the ith profile for contaminant, iso (mass/cm^2/year).
- QNBF(j,i,iso) = Specified dispersive flux value of the jth data point in the ith profile for isotope, iso (mass/cm^2/year).
- CDBF(j,i,iso) = Specified concentration value of the jth data point in the ith profile for contaminant, iso (mass/cm^3).
- THICK(J) = Thickness of the Jth container (cm.). 55 gallon drums are typically 0.127 - 0.152 cm thick.
- PITN(J) = Pitting parameter n for the Jth 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 Jth container (cm/yr^{n}). 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 Jth 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. Values have been measured by Logan [Logan, 1939) for wrought iron pipes buried in 47 different soils. Values ranged from 0.08 to 0.32 with a mean value of 0.15 and a standard deviation of 0.04. If ASCALE is input as zero, a default value of 0.2 is used.
- 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). Measurement of the total number of pits on Fe samples ranged from 14 - 80 pits/cm^2 [Isaacs, 1988]. Of these only a small fraction will grow large enough to penetrate the container. Based on the carbon steel pitting data obtained by Marsh [Marsh, 1985], an estimate of 0.05 penetrating pits/cm^2 has been made. For a 55 gallon drum, this implies approximately 1000 penetrating pits. The default value used by BLT-MS is 1000.
- GRATE(J) = The general corrosion rate (cm/s) of container J. Values measured in the NBS study reported by Romanoff [Romanoff,1957] for the corrosion rate of carbon steel ranged from 2.7E-11 - 6E-10 cm/s. For a wall thickness of 0.127 cm, these corrosion rates correspond to penetration in 6.7 - 150 years. If the input values of GRATE(J) is zero, then a default value of 3E-10 cm/s is used.
- CLAY(J) = Clay fraction of the soil (0 .LE. CLAY(J) .LE. 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. 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) = 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 ($0 \leq$ 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 Jth 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 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 $\leq$ 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) = Jth waste form effective diffusion coefficient for contaminant iso cm^2/s. Used only if PFRACT(J,ISO) > 0.
- DISOL(J,ISO) = Jth waste form fractional release rate (1/yr) for contaminant iso. Used only if BFRACT(J,ISO) > 0.
- PARTKO(J,ISO) = Jth waste form partition coefficient for contaminant iso cm^3/g at time t = 0. Used onl;y if SFRACT > 0.
- PARTKI(J,ISO) = Jth waste form partition coefficient for contaminant iso cm^3/g at time t = ∞.
- PARTD(J,ISO) = Jth 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 $\leq$ 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.

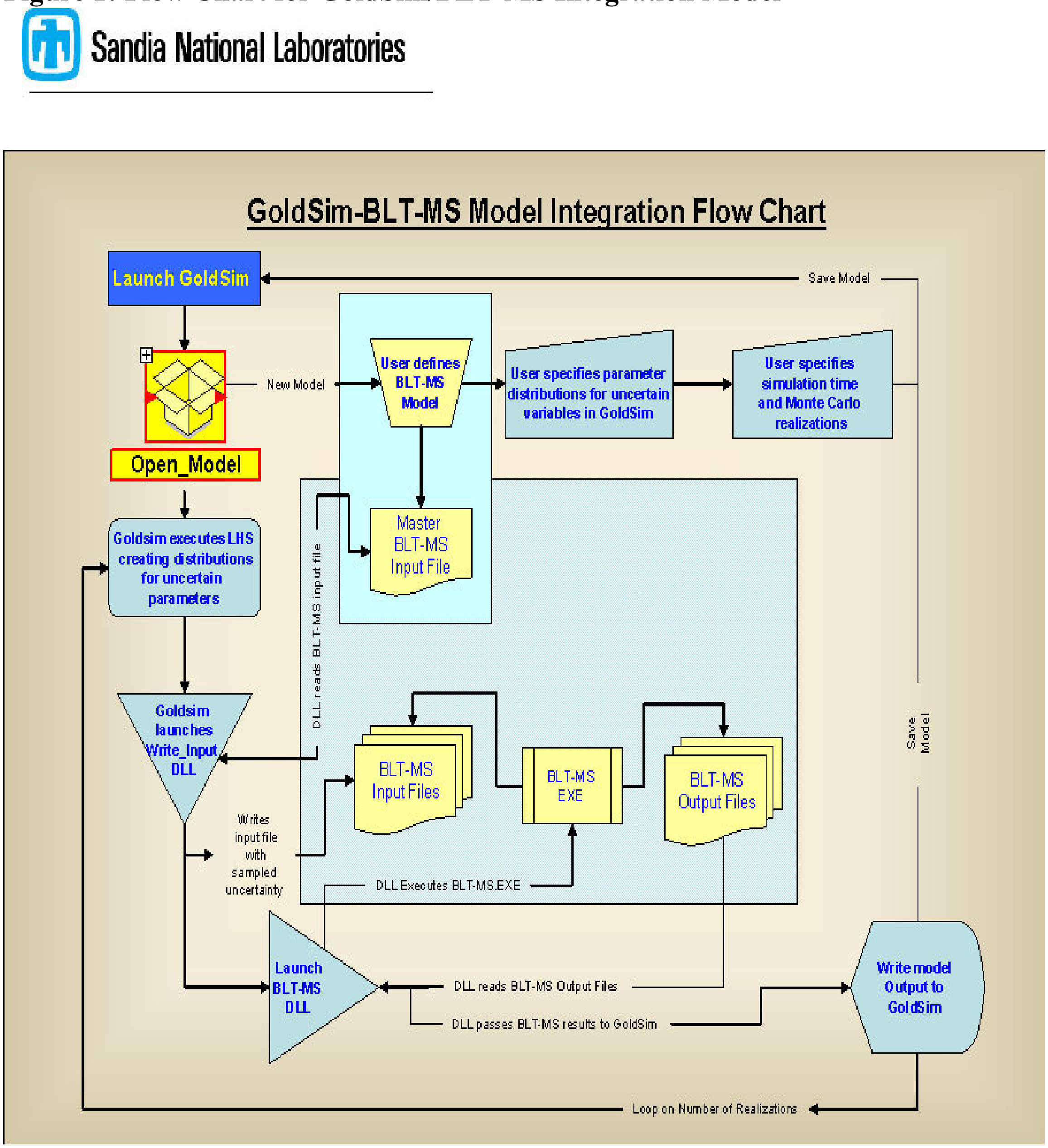
GolSim/BLT-MS Integration Model Overview: Figure 1 outlines the basic flow chart for the integration model. The basic concept starts with the generation of a BLT-MS model using the BLT-MS preprocessor. The analyst defines the problem and sets up a stand alone deterministic BLT-MS simulation. The GoldSim/BLT-MS Integration Model is designed in such a way that requires 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 distributions pre-defined within the GoldSim model. The GoldSim/BLT-MS Integration Model model executes the BLT-MS.exe over the set of input files and selected output from each realization is saved within the GoldSim/BLT-MS Integration Model. Integration of the BLT-MS code with GoldSim was accomplished though the use of two separate program modules written in FORTRAN and directly coupled to the GoldSim code. These codes are linked to GoldSim using a predefined interface and compiling the program module as dynamic linked libraries (DLL). The GoldSim code interfaces with the DLL using an external element (refernce GoldSim User's Manaual, page 451 and Appendix C).

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

1) Analyst constructs a BLT-MS Model using the BLT-MS preprocessor to generate a 'master' input file called: bltmsin.imp.
2) Analyst specifies in the GoldSim Model the uncertain distributions and selects which parameters to make uncertain. (some user specified controls are required and are detailed in the following sections)
3) Analyst specifies in the GoldSim Model the duration of the simulation and number of realizations desired.
4) Analyst Saves GoldSim/BLT-MS Integration Model.
5) Analyst Runs GoldSim/BLT-MS Integration Model.
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) Read_BLT.DLL code reads the bltmsin.inp file first (this is the file you have already generated using the preprocessor for BLT-MS) 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. The Launch_BLTMS.DLL executes BLTMS.EXE using 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.
11) Steps 7-10 are repeated until all the realizations have been executed.
12) 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 three parts: 1) Introduction to the BLT-MS Integration Model, 2) Simulation Settings for Read_BLT.DLL and Defining Uncertainty, and 3) Simulation Settings for Launch_BLTMS.DLL and model output, and 4) Simulation Settings for the Pipe-Pathway Model. This guide assumes the analyst can generate the BLT-MS model and input file using the BLT-MS preprocessor and therefore does not include instructions for these steps.

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



Introduction to the BLT-MS Integration Model:

The GoldSim/BLT-MS Integration Model utilizes a set of files necessary to execute the BLT-MS code and the GoldSim model with associated DLL's. **Table 1** lists the basic file set necessary to run the Integration Model and a brief description of each. The file set consists of the GoldSim model file (.gsm file) which is compatible with GoldSimPro Version 9.0 SP2 and above. To execute the model the analyst must have a current licensed version of GoldSimPro with the Radionuclide Transport Module enabled. In addition two 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 6.5.0, on an Intel compatible operating system. The source code for Read_BLT.DLL and Launch_BLTMS.DLL is contained in Appendix A and Appendix B of this user guide. As mentioned previously a 'master' BLTMS input file is required to execute the integrated model. The logic programmed in the GoldSim file and associated DLL's require information obtained from the bltmsin.inp file.

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

File Name	Description
BLT-MS_GoldSim_v009_9.10.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)
Read_BLT.dll	DLL accessed by GoldSim during simulation to create BLTMS input files with uncertain samples for selected parameters.
Launch_BLTMS.dll	DLL accessed by GoldSim during simulation to execute BLTMS.EXE and read 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.

Figure 2 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. As can be seen in **Figure 2** and **Table 2**, the basic structure of the integration model is broken in to two main parts:

1) BLTMS Integration
2) Pipe-Pathway Transport ACM

Each contains the logic necessary to implement their 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 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 are discussed in further detail below. For the analyst, one must ensure that the model conditions are correctly defined within the *BLT_MS_Input_File* container, before the simulation is launched.

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. You should have the Latin Hypercube Sampling

check box selected. (Run\Simulation Settings or press F2). The number of timesteps and simulation time should be the same as defined within the BLTMS input file.

2) Define physical properties for ISO's in GoldSim ***Species*** element.
3) Open the ***BLT_MS_Uncertain_Param_Switch*** element located in the ***BLT_MS_Input_File*** container. Select which parameters you want to make 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 ***Pipe_Model*** container and edit the following three arrays: ***Zone1_Containers***, ***Zone2_Containers***, and ***Zone3_Containers***, listing the element numbers that are associated with containers for each of the zones (see section below for details).
6) **Save** the Model.
7) **Run** the GoldSim Model.
8) **Save** the Model when the simulation is complete and begin analyzing the results.

In the following sections key parameters will be discussed in detail, however, each individual element contained in the GoldSim/BLT-MS Integration Model has not been discussed. It is assumed the analyst has a basic proficiency with GoldSim and the necessary understanding of the features of the GoldSim code utilized to implement this coupled model. It is encouraged that the analyst review the GoldSim User's Manaual for specific details of the model elements used in this implementation.

Figure 2: Upper Level Model Structure

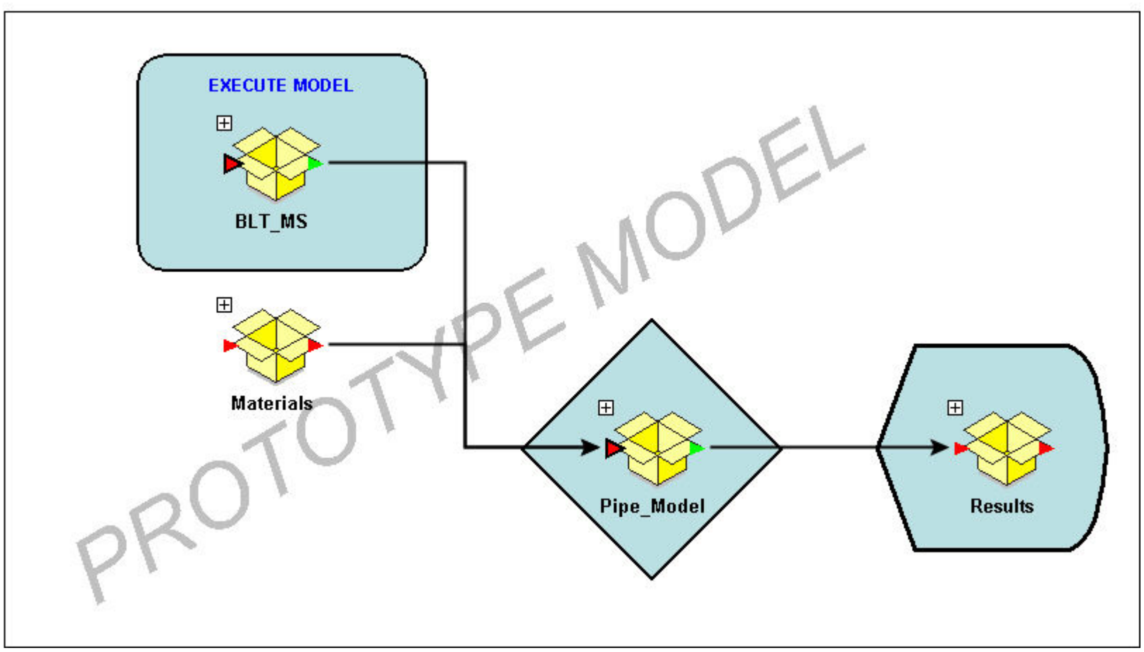


Table 2: Upper Level Hierarchy for BLTMS/GoldSim Integration Model

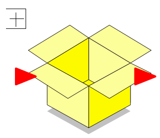
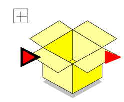
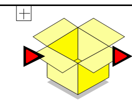
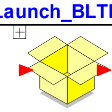
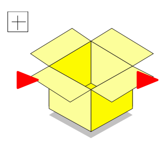
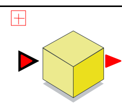
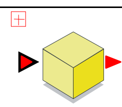
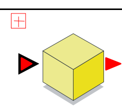
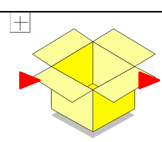
Upper Level Container	Description	Level 2 Container	Description
 BLT_MS	Contains Model Linking BLTMS.EXE with GoldSim. Allows the User to add uncertainty to the model by selecting from 36 BLTMS input parameters. Selected BLTMS output data is passed to GoldSim to record multiple realization data.	 BLT_MS_Input_File	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	None	N/A

Figure 3: Level 2 Container Structure

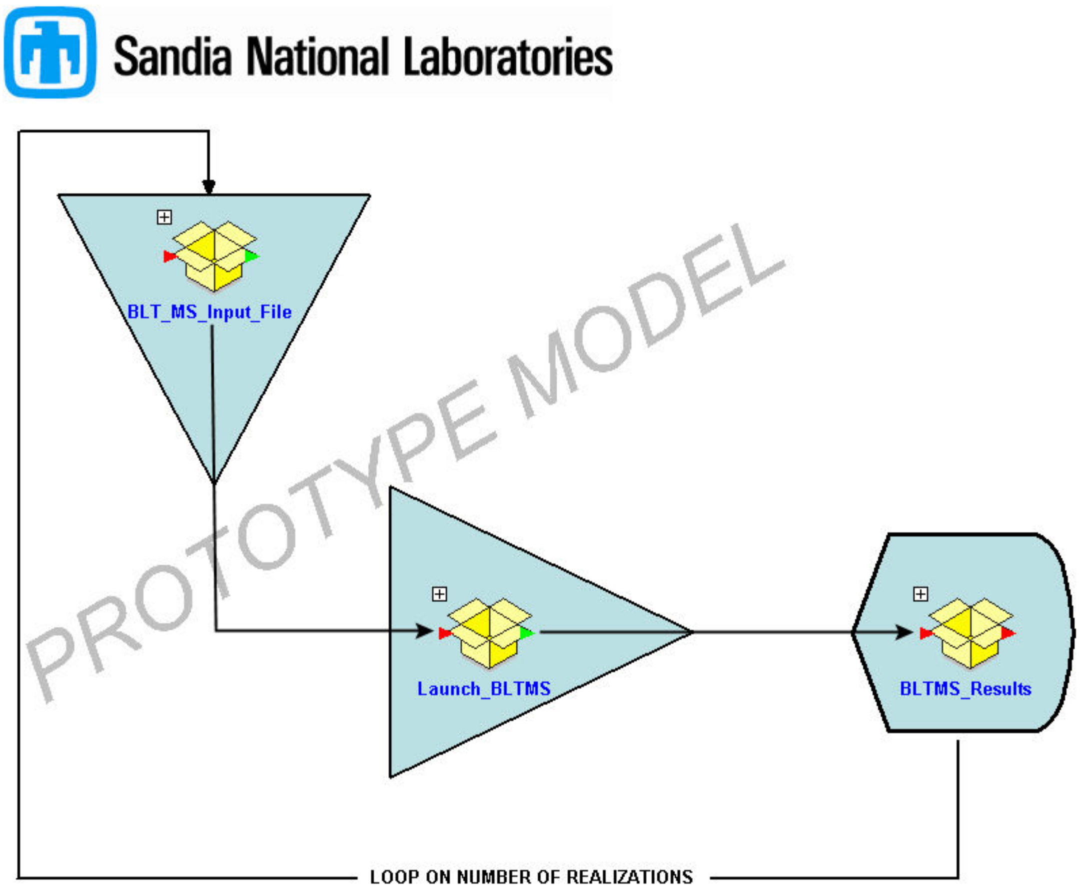


Table 3: BLTMS/GoldSim Integration Level 2 Containters

Level 2 Container	Level 3 Element	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 you want 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

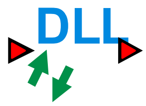
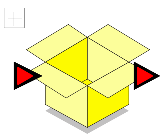
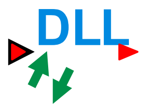
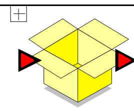
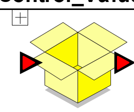
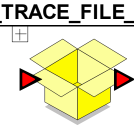
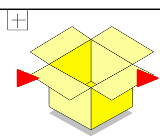
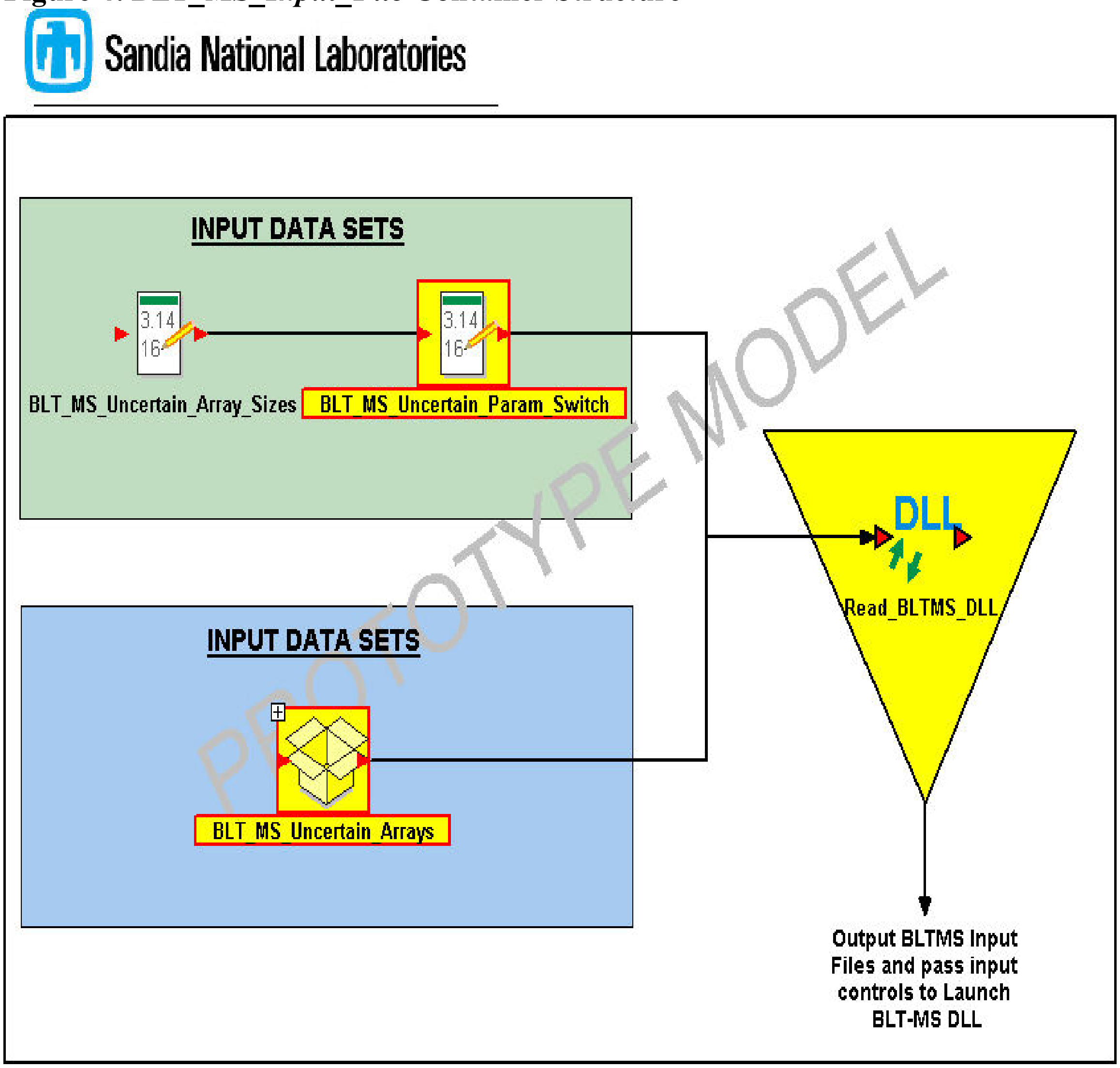
	 Read_BLTMS_DLL	DLL that writes uncertain values to the input file and passes control values to Launch_BLTMS_DLL
 Launch_BLTMS	 BLTMS	DLL that Launches BLT-MS and passes selected output data back to GoldSim.
	 Control_Values	Parameters Used to Process Output from BLTMS- DO NOT CHANGE VALUES
	 CONC_TRACE_FILE_OUTPUT	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 LEACHMS* files and passed by the DLL to GoldSim.
 BLTMS_Results	None	Contains pre-defined plots of the Concentration Traces and Selected BLTMS output.

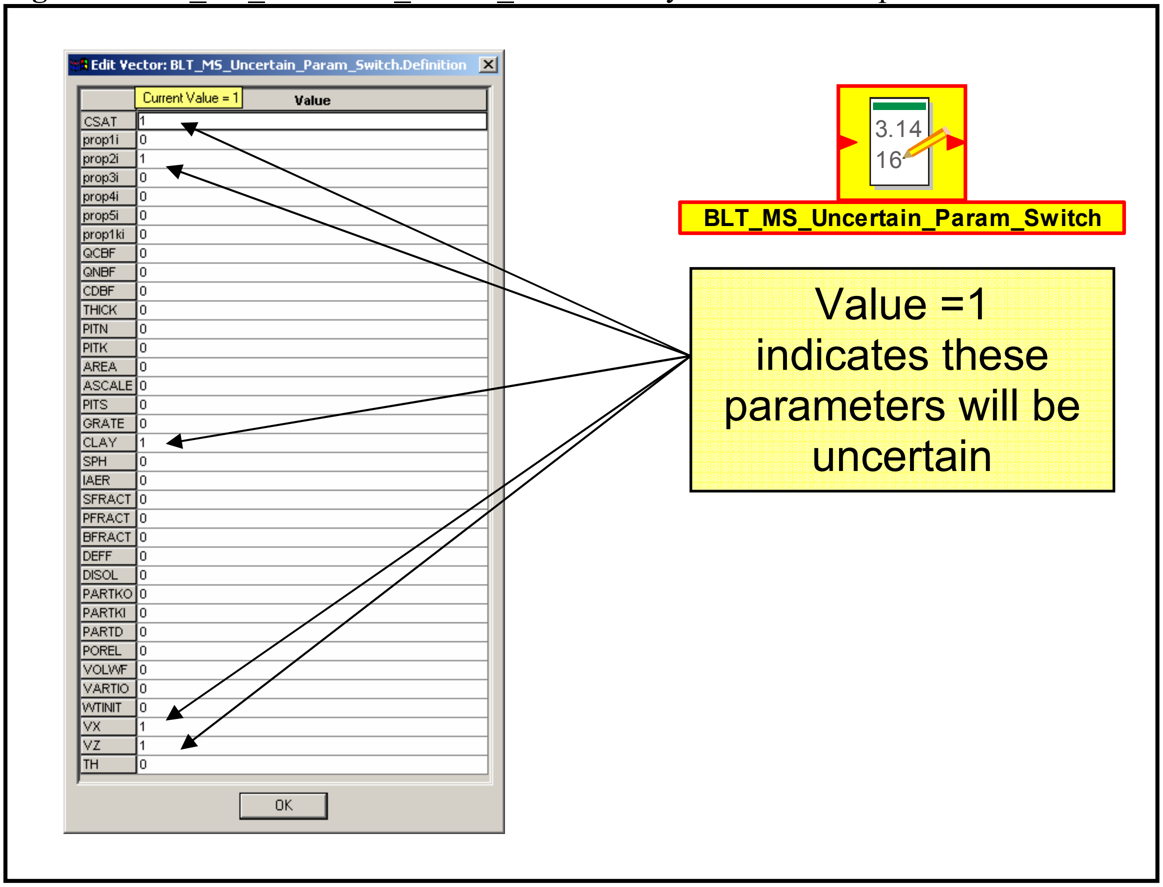
Figure 4: ***BLT_MS_Input_File*** **Container Structure**



Simulation Settings for Read_BLT.DLL and Defining Uncertainty

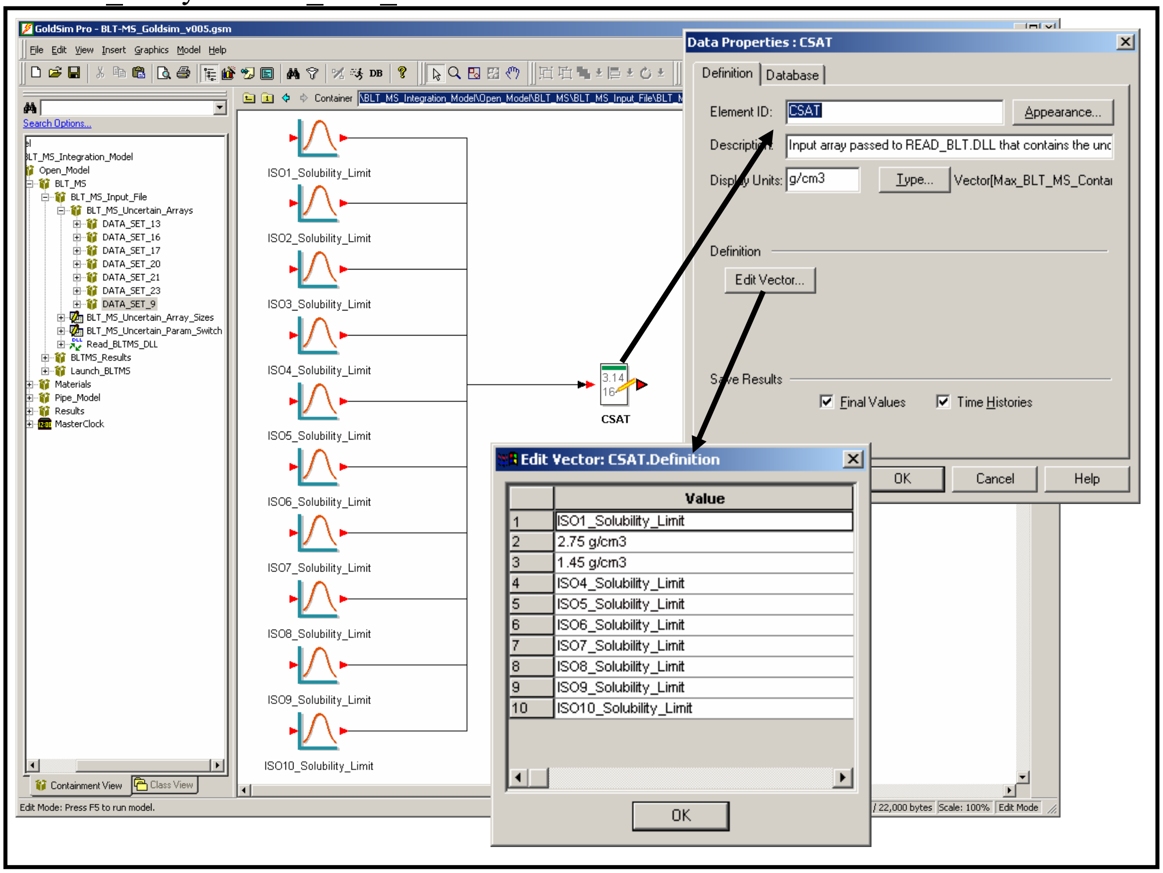
Figure 4 outlines the basic structure for *BLT_MS_Input_File* container. Within this container is the logic used to select which BLTMS parameters will be uncertain for a given model and to define the uncertain distributions with stochastic elements. The first step in this process should be to select the uncertain parameters using the *BLT_MS_Uncertain_Param_Switch* Array Element (**Table 3**). The *BLT_MS_Uncertain_Param_Switch* is a vector of 35 BLTMS parameters. 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 from GoldSim. The default value of 0 indicates that the 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. It is important to remember that each time the GoldSim/BLTMS Integration model is used that the analyst should review the *BLT_MS_Uncertain_Param_Switch* Array Element to ensure that the correct parameters are selected as uncertain.

Figure 5: *BLT_MS_Uncertain_Param_Switch* Array Element Example



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 contains the parameter data array and stochastic elements used to define the uncertainty. In our 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], **Figure 6**, reveals the input array for CSAT, labeled *CSAT*, and the stochastic elements that contain the uncertainty data for this parameter. Since, CSAT can be defined for each ISO defined in the BLTMS model, it is necessary to define up to 10 distributions, one for each ISO, as seen in **Figure 6**. If the model contains less then 10 ISO's only extra data will be ignored. However, it is important to note that if it is intended to make only some of the ISO's have uncertainty for CSAT, 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 if **Figure 6**, 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 6: *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 7**. BLTMS allows up to five material types and up to a maximum of 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 for 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 x and z directions. The uncertainty for these parameters is applied to all nodes as a multiplier term. This uncertainty represents a factor that will be applied to all locations on the defined grid. 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 the will be uncertain in the *BLT_MS_Uncertain_Param_Switch*, define the appropriate uncertainty distributions using stochastic elements or deterministic values, and link these data to the parameter input array. Play close attention to the different input array sizes for each parameter. In some cases the 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 7: *prop_2_i* and *clay_j* input arrays

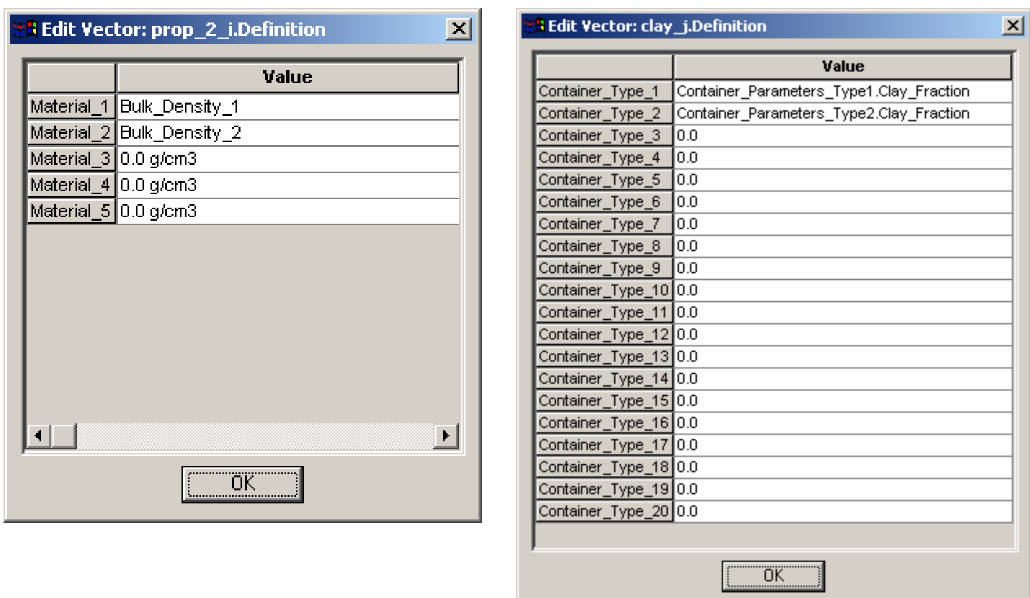
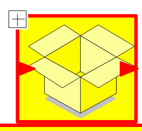
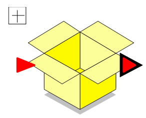
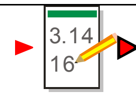
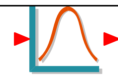
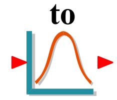
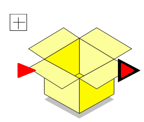
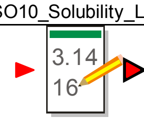
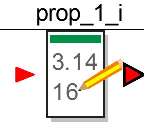
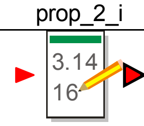
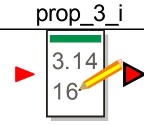
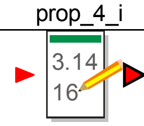
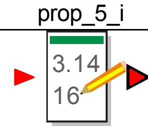
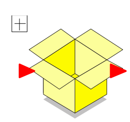
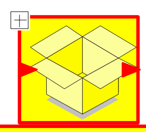
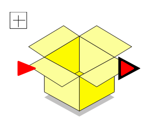
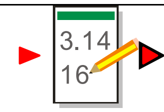
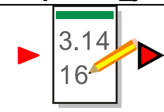
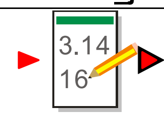
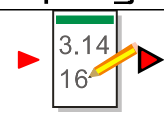
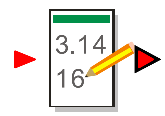
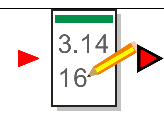
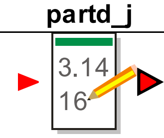
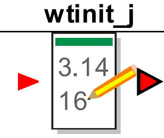
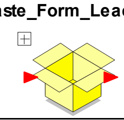


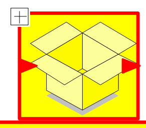
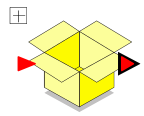
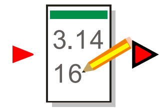
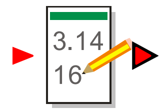
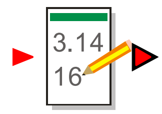
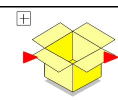
Table 4: BLT_MS Uncertain Arrays Elements used to link GoldSim to BLTMS.

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 that contains the uncertain values for solubility.
		 ISO1_Solubility_Limit **to**  ISO10_Solubility_Limit	Stochastic Elements that can be used to define distributions of uncertainty for the solubility of selected ISO 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.

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 Neuman 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

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 Waste Container 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 jth waste form that is available for surface wash off in the rinse model for contaminant ISO(i)
		disol_j	Matrix of jth waste form fractional release rates for contaminant ISO(i)
		porel_j	Array of Radius or half length of jth waste form
		volwf_j	Array of Volume of jth waste form

Level 3 Container	Container	Element	Description
 BLT_MS_Uncertain_Arrays continued	 DATA_SET_21 continued	 partk0_j	Matrix of jth waste form partition coefficient for contaminant ISO(i) at time t=0 yr
		 vartio_j	Array of Ratios for the volume of the jth waste form to the finite element in which it is located.
		 pfract_j	Matrix of mass fraction values for jth waste form that is available for diffusion controlled release for contaminant ISO(i)
		 partki_j	Matrix of jth waste form partition coefficient for contaminant ISO(i) at time t=∞ yr
		 bfract_j	Matrix of mass fraction values for jth waste form that is available for dissolution controlled release for contaminant ISO(i)
		 partd_j	Matrix of jth waste form partition coefficient degradation rate constant for contaminant ISO(i)
		 wtinit_j	Matrix of jth waste form initial inventory for contaminant ISO(i)
		 deff_j	Matrix of jth waste form effective diffusion coefficient for contaminant ISO(i)
		Waste_Form_Leaching_Uncert 	

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 paramters used to simulate a range of multipliers for vxni_j, vzni_j, and thni_j

Simulation Settings for Launch_BLTMS.DLL and model output

There are no simulation settings that the analyst needs to make for this model component area. **Figure 8** outlines the structure for the *Launch_BLTMS* container. This container contains the model logic used to execute the BLTMS.EXE and capture selected output for each realization. **Table 5**, lists the contents for each output data container. The data contained within the BLTMS output files TRACECN*.dat and LEACHMS*.dat are read by the Launch_BLTMS.DLL and the data is passed by to GoldSim for storage. The external DLL element is linked to 3-D tables used to store the data. For the concentration trace data one table is defined *BLT_Concentration_Data*. Each layer represents an ISO, with each column number representing the element location in which the concentration trace was saved. This table is linked to concentration trace output arrays used to extract the data from the table for analysis. The concentration trace output arrays in GoldSim are defined to handle the maximum number of ISO's (10) and element traces (100). Only a maximum of 100 concentration traces can be saved using BLTMS. However, in the GoldSim array there area maximum of 600 elements. The GoldSim array stores the data passed by the DLL by element number. For example, consider a given BTLMS model in which the master input file bltmsin.inp has selected element numbers 10, 62, and 442, to have the concentration data saved. The Launch_BLTMS.DLL will pass the concentration data for these elements over the time step interval selected, for all ISO's defined in the run back to GoldSim. The output arrays, defined by ISO, will be automatically populated with the concentration data output. At the end of the run, ISO_1_Concentration_Data array will have concentration data saved at array locations of 10, 62, and 442, corresponding to the saved elements in the bltmsin.inp file. For all other array locations a value of 0 is saved since no concentration data was available for these elements. For the LEACHMS*.dat output data, a set of GoldSim 3-D tables are utilized to store the extracted data. **Table 5** lists the table names with a brief description of each. Identical to the concentration data table, each layer represents an ISO, whereas each column represents an element number. The each column number in represents the element number in the bltmsin.inp file which have a waste containers at that location. Therefore there will be an element location saved for each waste container defined in the bltmsin.inp file. There are no data arrays pre-defined to extract this data except for the cumulative release data which is passed to the 1-D pipe model. Those arrays will be discussed in the following section.

Figure 8: *Launch_BLTMS* Container Structure

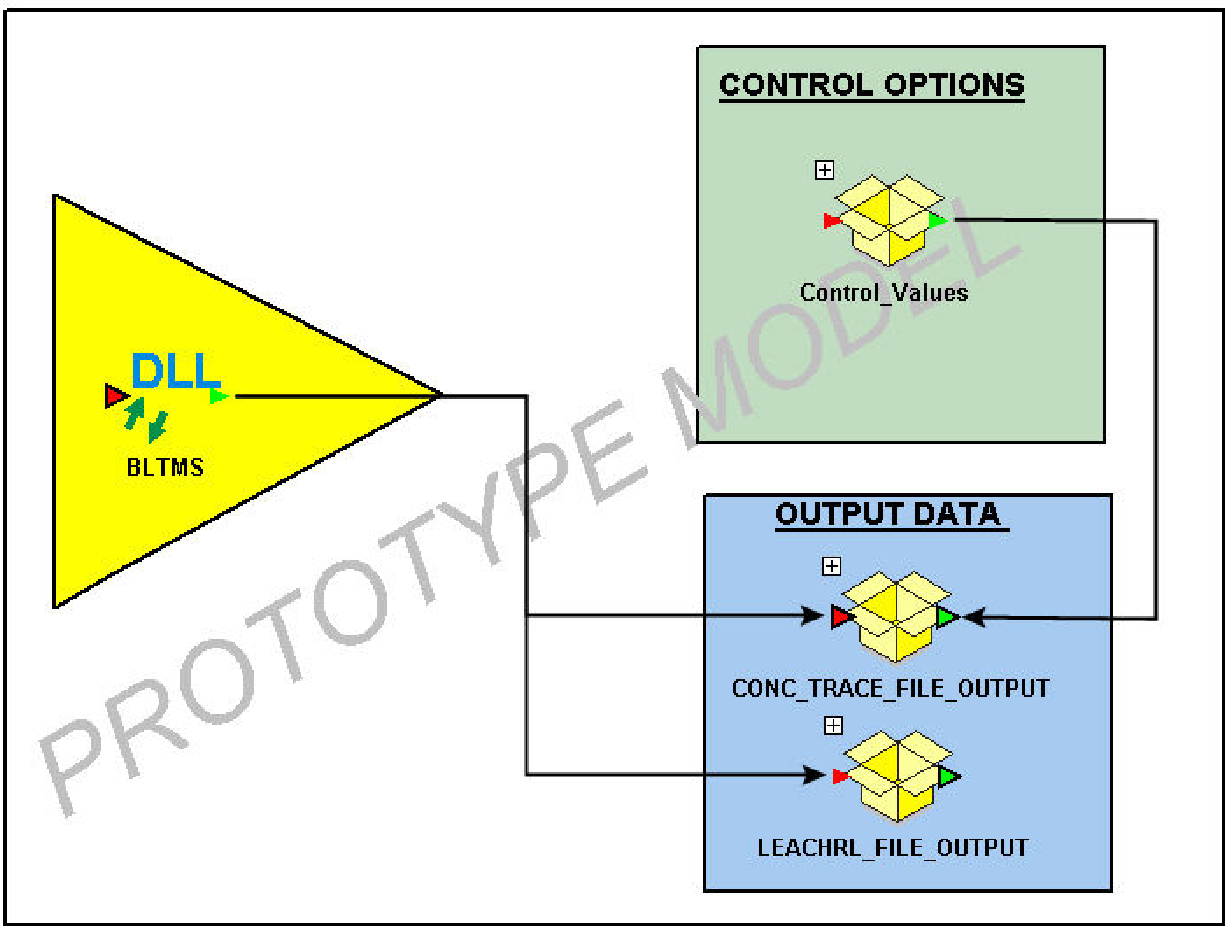
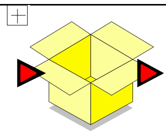
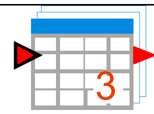
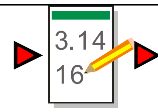
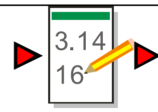
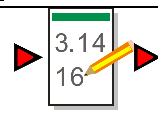
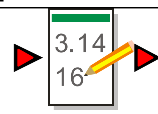
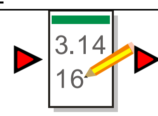
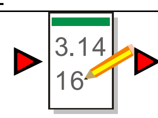
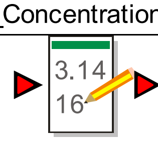
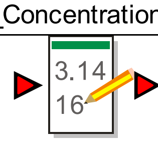
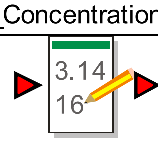
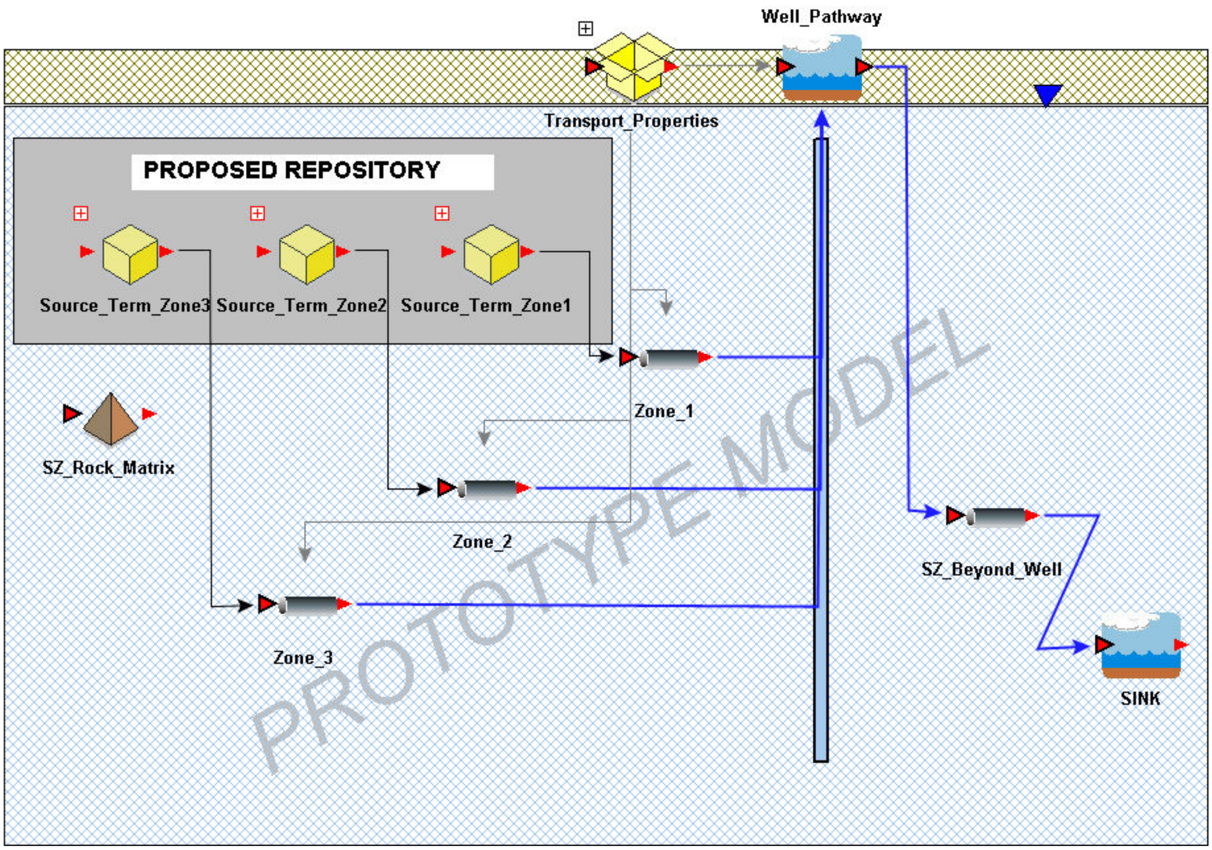


Table 5: Launch_BLTMS Output Containers

Level 3 Container	Element	Description
 CONC_TRACE_FILE_OUTPUT	 BLT_Concentration_Data	ISO concentration for specficed nodal locations from TRACECN*.DAT FILES
	 ISO_1_Concentration_Data	Array of Concentration Trace Data for All Specified Nodes for ISO1 [extracted from BLT_Concentration_Data table]
	 ISO_2_Concentration_Data	Array of Concentration Trace Data for All Specified Nodes for ISO2 [extracted from BLT_Concentration_Data table]
	 ISO_3_Concentration_Data	Array of Concentration Trace Data for All Specified Nodes for ISO3 [extracted from BLT_Concentration_Data table]
	 ISO_4_Concentration_Data	Array of Concentration Trace Data for All Specified Nodes for ISO4 [extracted from BLT_Concentration_Data table]
	 ISO_5_Concentration_Data	Array of Concentration Trace Data for All Specified Nodes for ISO5 [extracted from BLT_Concentration_Data table]
	 ISO_6_Concentration_Data	Array of Concentration Trace Data for All Specified Nodes for ISO6 [extracted from BLT_Concentration_Data table]
	 ISO_7_Concentration_Data	Array of Concentration Trace Data for All Specified Nodes for ISO7 [extracted from BLT_Concentration_Data table]
	 ISO_8_Concentration_Data	Array of Concentration Trace Data for All Specified Nodes for ISO8 [extracted from BLT_Concentration_Data table]
	 ISO_9_Concentration_Data	Array of Concentration Trace Data for All Specified Nodes for ISO9 [extracted from BLT_Concentration_Data table]

	ISO_10_Concentration_Data	Array of Concentration Trace Data for All Specified Nodes for ISO10 [extracted from BLT_Concentration_Data table]
LEACHMS_FILE_OUTPUT	**Cumr**	Total Cumulative Mass released from Source Term Elements for ISO(1) to ISO(i)
	Trinse	Cumulative mass released from source term element from the rinse model for ISO(1) to ISO(i)
	Tdif	Cumulative mass released from source term element from the diffusion model for ISO(1) to ISO(i)
	Tdis	Cumulative mass released from source term element from the degradation model for ISO(1) to ISO(i)
	Sosl	Total Mass Release Rate at each source term element for ISO(1) to ISO(i)
	Rinser	Rinse Mass Release Rate at each source term element for ISO(1) to ISO(i)
	Difr	Diffusion mass release rate at each source term element for ISO(1) to ISO(i)
	Disr	Degradation mass release rate at each source term element for ISO(1) to ISO(i)
	Barea	Container Breached Area at each source term element

Figure 9: Pipe Model ACM for Saturated Zone Transport Cavern Site

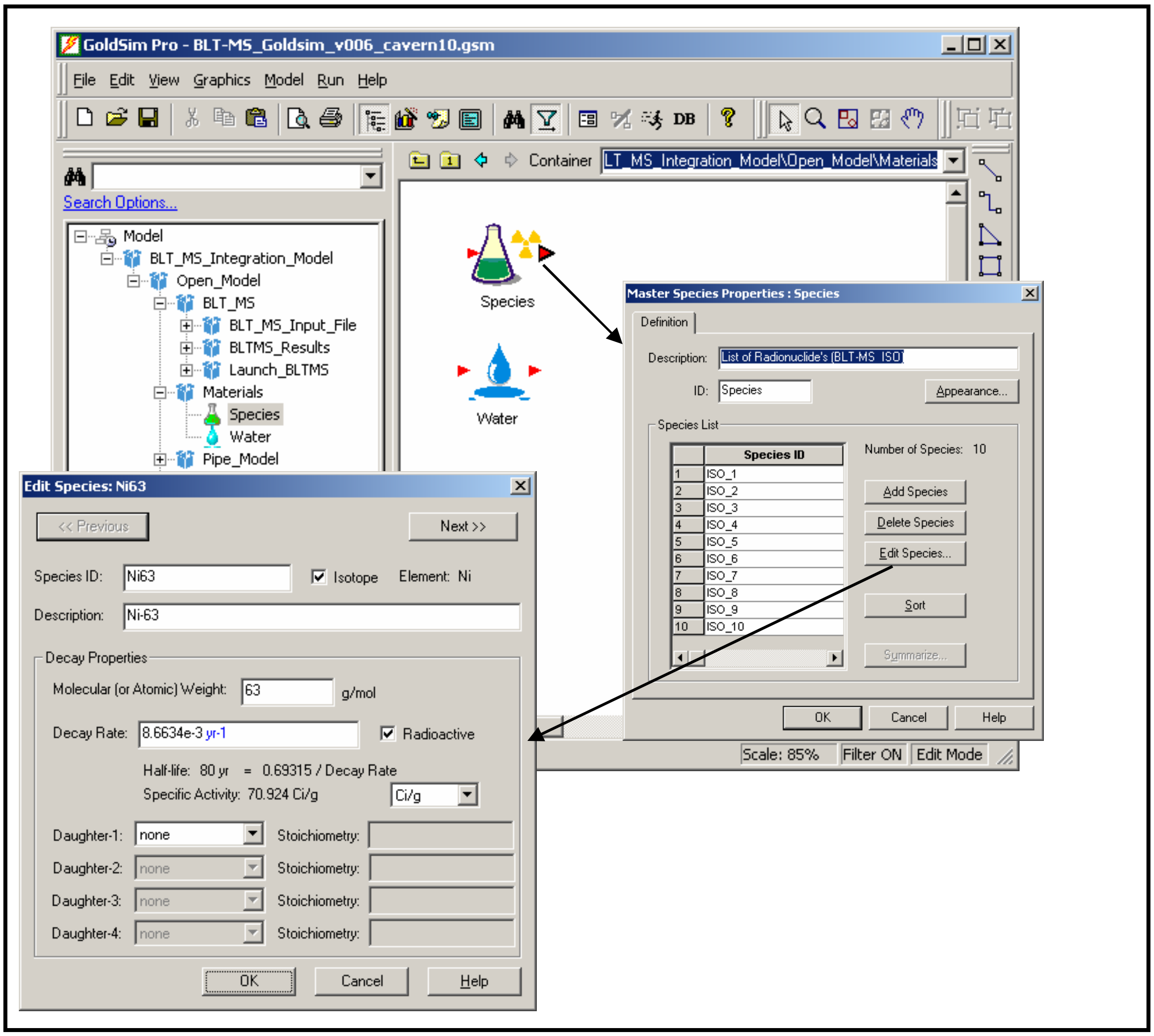


Simulation Settings for the 1-D Pipe Model

The pipe-pathway ACM is depicted in **Figure 9**. The model is setup to automatically feed the cumulative mass release from the source term containers defined in the BLT-MS model to the alternative conceptual model for SZ transport using GoldSim 1-D pipes. To steps are required for the successful invocation of the 1-D Pipe Model: 1) assign physical constants to the GoldSim Species list (found in \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.

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*** 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 **Figure 2**. 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 10**, the first ISO in bltmsin.inp is Am241, therefore the physical properties for Am241 are defined in for ISO1 in the GoldSim *Species* Element. These properties include the atomic weight, decay rate and daughter products. In the example shown in **Figure 10**, ISO1 (Am241) Radioactive check box is selected and the species will be decayed to ISO2. ISO2 (Np237) must also be defined. If the ISO list is changed in the bltmsin.inp file, either the number of species, order of species or species are added or removed, the analyst must adjust the GoldSim species list to ensure the properties are defined and appear in the same order as in bltmsin.inp file.

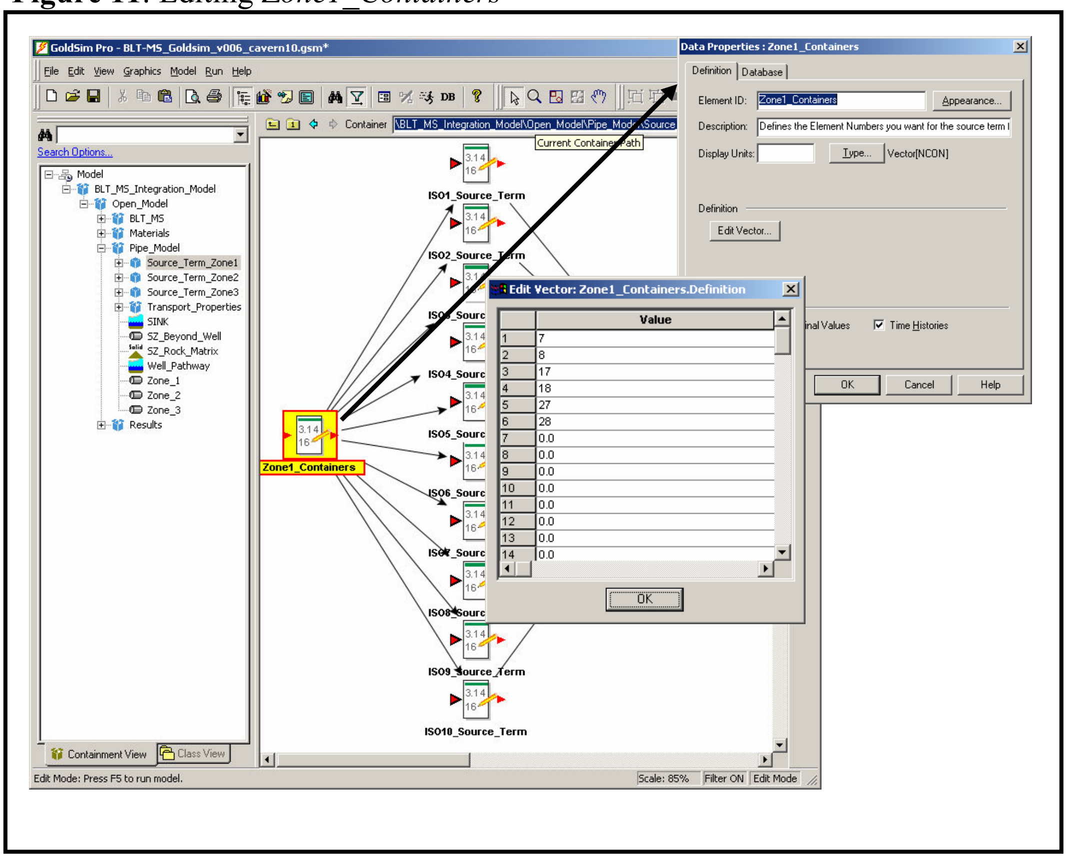
Figure 10: Editing the *Species* Element



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

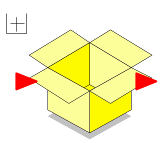
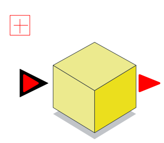
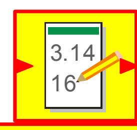
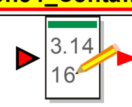
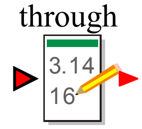
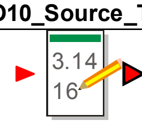
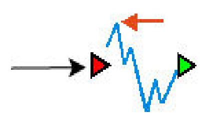
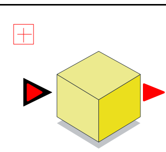
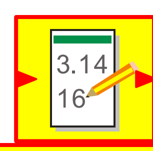
BLT-MS input file) in one of the three default zones defined in the pipe model. The 1-D pipe model requires the cumulative mass releases from the waste containers defined and simulated within the BLTMS model. Since the Launch_BLTMS.DLL reads the cumulative releases from the LEACHMS*.DAT files to GoldSim, this data is readily available to use as the source term in the pipe model. The model is setup to automatically extract the cumulative releases; 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 (**Figure 9**). Three arrays *Zone1_Containers*, *Zone2_Containers*, and *Zone3_Containers* need to be defined (**Table 5**). As seen in the example depicted in **Figure 11**, six containers are defined for Zone1. They are listed in the vector for the *Zone1_Containers* element. They are listed 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 100 containers to be defined; therefore each of the three vectors has a maximum size of 100. This allows the analyst to place all of the containers in one zone. Each time a modeling case is developed the analyst must ensure that the three arrays have been reviewed to ensure the total number of waste containers are captured over the three zones, no finite-element number has been listed in more than one zone, and all of the finite-element locations listed are associated with containers in the bltmsin.inp file.

Figure 11: Editing *Zone1_Containers*

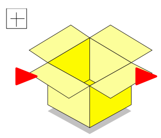
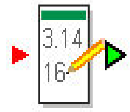
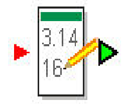
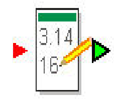
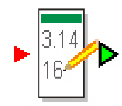
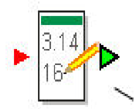
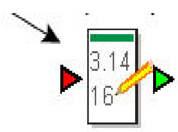
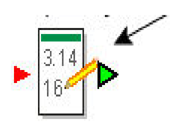
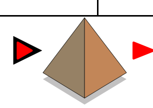


The last step required for the proper functionality of the pipe pathway transport model is to correlate the physical properties of the porous media (Data Set 13) defined in the BLT-MS input file with the physical transport properties used in the 1-D transport model in GoldSim. The *Transport_Properties* container and the *SZ_Rock_Matrix* element shown in **Figure 9**, contains the data elements used to define the properties used in the 1-D pipe pathway elements (listed in **Table 5**). If the analyst re-configures the BLT-MS model he must ensure the physical properties of the porous media in Data Set 13 are used in the GoldSim 1-D pipe pathway model to ensure proper correlation between the two alternative models. Porous media properties like Kd values are defined using the *SZ_Rock_Matrix* element, whereas transport properties like water flux and dispersivity are defined using parameters contained within the *Transport_Properties* container.

Table 5: Pipe Model Containers

<table>
<tr><th>Upper Level Container</th><th>Level 2 Container</th><th>Element</th><th>Description</th></tr>
<tr><td rowspan="5">
Pipe_Model</td><td rowspan="4">
Source_Term_Zone1</td><td>
Zone1_Containers</td><td>Array Defines the element Numbers you want for the source term for this Zone - ANALYST MUST ENTER THE ELEMENT NUMBERS</td></tr>
<tr><td>
ISO1_Source_Term
through

ISO10_Source_Term</td><td>Array of cumulative mass of ISO released over for the Source Term Elements in Zone1 – DO NOT EDIT</td></tr>
<tr><td>
Zone1_Source_Term</td><td>Total cumulative mass released in Zone 1 for ISO(i) to ISO(10) – DO NOT EDIT</td></tr>
<tr><td>
Zone1_Source_Term_Input</td><td>Total cumulative mass released in Zone 1 for ISO(i) to ISO(10) – DO NOT EDIT</td></tr>
<tr><td>
Source_Term_Zone2</td><td>
Zone2_Containers</td><td>Array Defines the element Numbers you want for the source term for this Zone - ANALYST MUST ENTER THE ELEMENT NUMBERS</td></tr>
</table>

Pipe_Model Continued		**ISO1_Source_Term** through **ISO10_Source_Term**	Array of cumulative mass of ISO released over for the Source Term Elements in Zone2– DO NOT EDIT
		Zone2_Source_Term	Total cumulative mass released in Zone 2 for ISO(i) to ISO(10) – DO NOT EDIT
		Zone2_Source_Term_Input	Total cumulative mass released in Zone 2 for ISO(i) to ISO(10) – DO NOT EDIT
	Source_Term_Zone3	**Zone3_Containers**	Array Defines the Element Numbers you want for the source term for this Zone - ANALYST MUST ENTER THE ELEMENT NUMBERS
		ISO1_Source_Term through **ISO10_Source_Term**	Array of cumulative mass of ISO released over for the Source Term Elements in Zone3– DO NOT EDIT
		Zone3_Source_Term	Total cumulative mass released in Zone 3 for ISO(i) to ISO(10) – DO NOT EDIT
		Zone3_Source_Term_Input	Total cumulative mass released in Zone 3 for ISO(i) to ISO(10) – DO NOT EDIT
	Transport_Properties	Zone1_Transport_Length	Distance from Zone 1 to well pathway – Analyst Must Edit All Zones if Model Configuration Changes

 **Pipe_Model** Continued		 Zone1_Area	Cross Sectional Area of pipe for mobile zone of zone 1 transport– Analyst Must Edit All Zones if Model Configuration Changes
		 Zone1_Perimeter	Wetted perimeter of pathway– Analyst Must Edit All Zones if Model Configuration Changes
		 Zone1_Dispersivity	Longitudinal Dispersivity of pathway– Analyst Must Edit All Zones if Model Configuration Changes
		 Zone1_Source_Length	Length of pipe over which source mass is added– Analyst Must Edit All Zones if Model Configuration Changes
		 Zone1_Qflux	Flow Rate for Zone1– Analyst Must Edit All Zones if Model Configuration Changes
		 Volume_Well_Pathway	To calculate the averge conc. from the three sources, the inflow rates from the three pipes * timestep length is used for the volume – DO NOT NEED TO EDIT
		 Well_Pathway_Outflow	To calculate the averge conc. from the three sources, the inflow rates from the three pipes * timestep length is used for the volume – DO NOT NEED TO EDIT
	 **SZ_Rock_Matrix**		Data Set 13: Porous Media Properties – Kd's, porosity, bulk density and tortuosity

Simulation Settings for the Dose Model

The dose model was constructed based upon ICRP-72 dose coefficients for ingestion. The drinking water pathway was used as the dose pathway in this model. The primary radionuclides in the groundwater was given by the average concentration at the well pathway. The annual dose from ingestion of radionuclides in drinking water is expressed as:

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

The 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 6: Dose Calculation 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 1-D pipe 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 1-D Model Results