Institute of Nuclear Energy Research

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FRAMES and MEPAS Training

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Agenda

- **Day 1**
  - Introduction to FRAMES and MEPAS
  - Constituent Database
  - Source Term
  - Vadose Zone Transport
  - Case Study Example
- **Day 2**
  - Aquifer Transport
  - Exposure Models (Exposure Pathways, Receptor Intake, Health Effects)
  - Sensitivity/Uncertainty Model
  - Adding Additional Modules

Hands-on examples will be provided in each lesson

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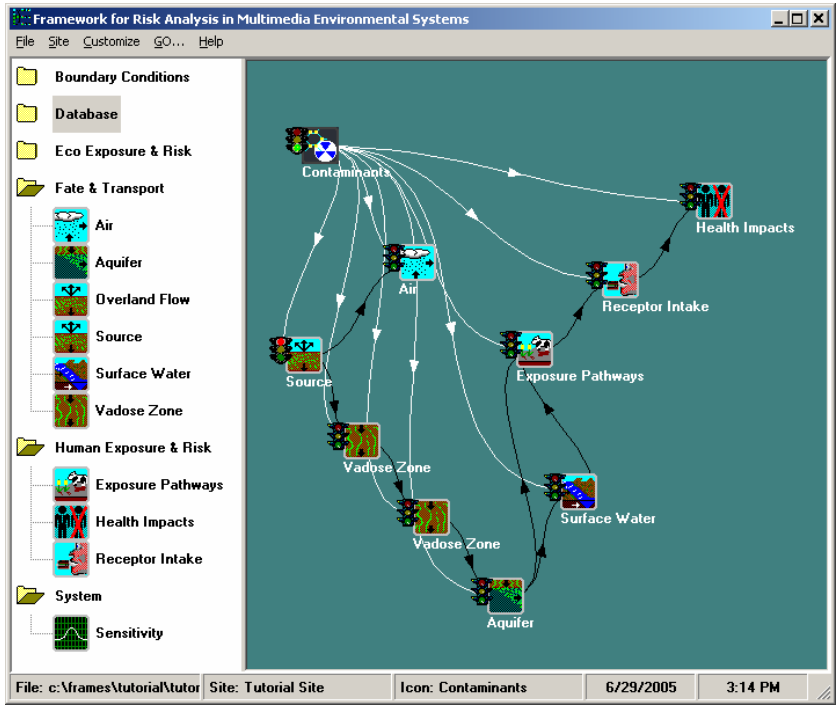
Introduction to FRAMES and MEPAS

Overview of FRAMES

- Framework tool developed by PNNL that links various models under one integrated system using pre-defined data-file specifications
- Defines conceptual site model using “drag-and-drop” module icons in a Windows-based interface
- Conducts sensitivity and uncertainty analyses on any model integrated into FRAMES
- Provides user with graphical and text viewers for analyses of intermediate and final results



http://mepas.pnl.gov/FRAMESV1/

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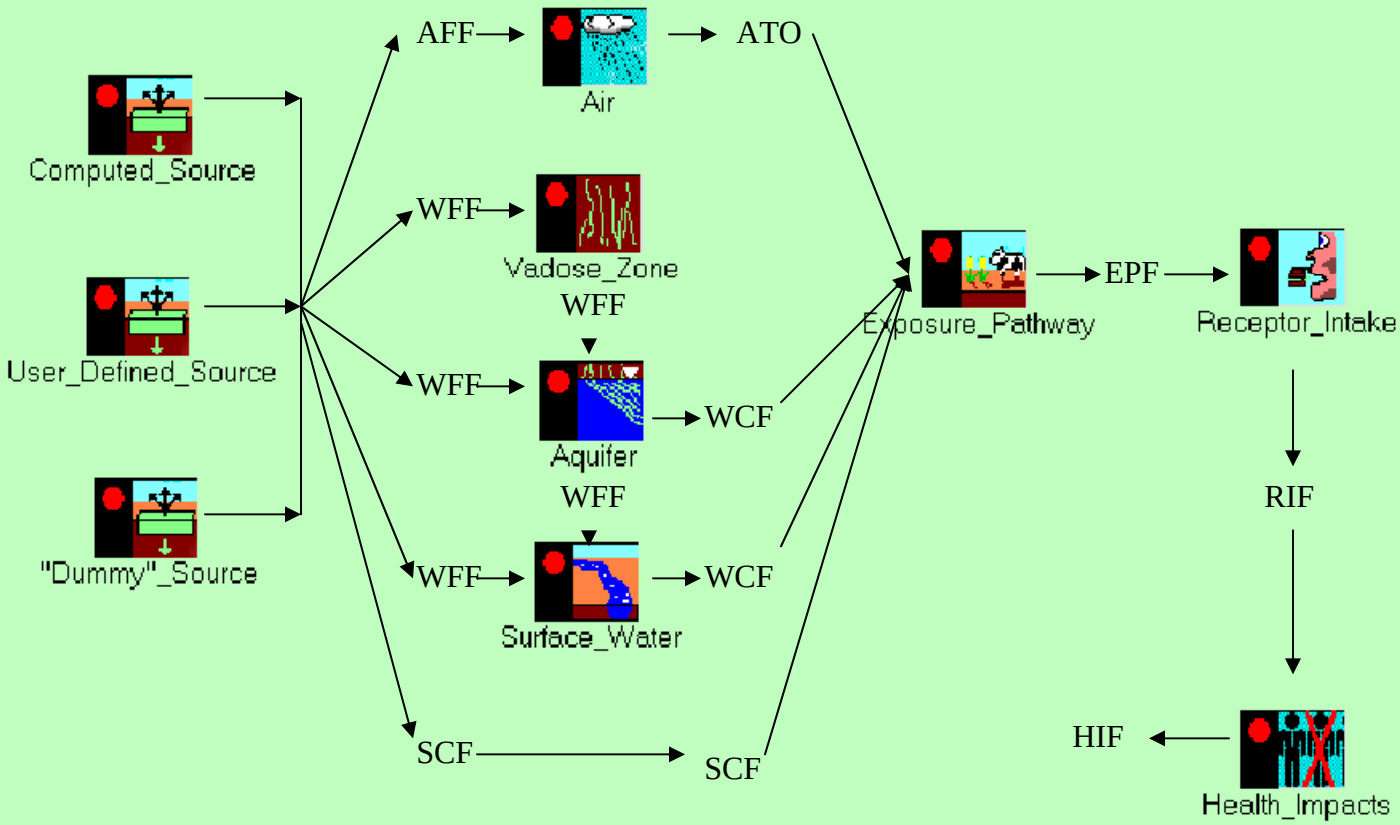
Multimedia Framework

File Scenario Customize GO... Help

- Database
  - Contaminant
- Model
  - Air
  - Aquifer
  - Exposure Pathways
  - Health Impacts
  - Overland Flow
  - Receptor Intake
  - Source
  - Surface Water
  - Vadose Zone
- Sensitivity
  - Sensitivity
- Viewer
  - Viewer

Data Transfer Between Modules

AFF -- Air Flux File
ATO-- Air Concentration File
EPF -- Exposure Pathway File
HIF -- Health Impacts File
RIF -- Receptor Intake File
SCF -- Source Concentration File
WCF-- Water Concentration File
WFF-- Water Flux File



FRAMES File Types

- GID -- Global Input Data
- SCF -- Source Concentration File
- AFF -- Air Flux File
- WFF -- Water Flux File
- WCF -- Water Concentration File
- ATO -- Air Concentration File
- EPF -- Exposure Pathway File
- RIF -- Receptor Intake File
- HIF -- Health Impacts File
- SUF -- Sensitivity/Uncertainty File

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Overview of MEPAS

- **Suite of environmental models developed by PNNL to evaluate contaminant transport**
  - **Source-term release**
  - **Aqueous transport (vadose-zone, aquifer, rivers)**
  - **Atmospheric transport**
  - **Exposure (pathways, receptor intake, health impacts)**
  - **http://mepas.pnl.gov/earth/mepasmain.html**
- **Individual models integrated in FRAMES**

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History

MEPAS

- DOE recognizes the need (1984)
- MEPAS V1.0 Released (1987)
- MEPAS V2.0 Released (1989)
- MEPAS V3.0 Released (1994)
- MEPAS V3.1 Released (1995)
- MEPAS V3.2 Released (1996)
- MEPAS V4.0 Released (1998)
- MEPAS V4.1 Released (1999)
- MEPAS V4.1.1 Released (2000)

FRAMES

- Initial concept (1994)
- Initial funding (1997)
- FRAMES V1.0 Released (1998)
- FRAMES V1.2 Released (2000)
- FRAMES V1.3 Released (2002)
- FRAMES V1.5 Released (2005)

Support from U.S. DOE, EPA, DoD, NRC

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Software Comparison

	HELP[1]	FRAMES/MEPAS	PRESTO[2]
Infiltration through Covers			
Water infiltration through multi-layer cover	✓		
Water infiltration through single-layer cover	✓	✓	✓
Consideration of environmental factors	✓	✓	✓
Transport Pathways			
Radionuclide transport		✓	✓
Chemical transport		✓	
Aqueous transport		✓	✓
Atmospheric transport		✓	✓
Exposure Models			
Multiple exposure pathways		✓	✓
Health impacts		✓	✓
Other Features			
Probabilistic modeling		✓	

[1]http://el.erdc.usace.army.mil/products.cfm?Topic=model&Type=landfill
[2]www.epa.gov/radiation/assessment/presto.html

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FRAMES/MEPAS Quality Assurance

- **Validation and benchmarking documentation**
  - http://mepas.pnl.gov/FRAMESV1/referenc.html
- **Software configuration management**
  - http://mepas.pnl.gov/FRAMESV1/qaqc.html
  - http://mepas.pnl.gov/Wiki/page.jsp?website=FWikiWiki&path=QAQCDoc
- **Contact**
  - Gariann Gelston, Pacific Northwest National Laboratory, (509) 372-6060, gariann.gelston@pnl.gov

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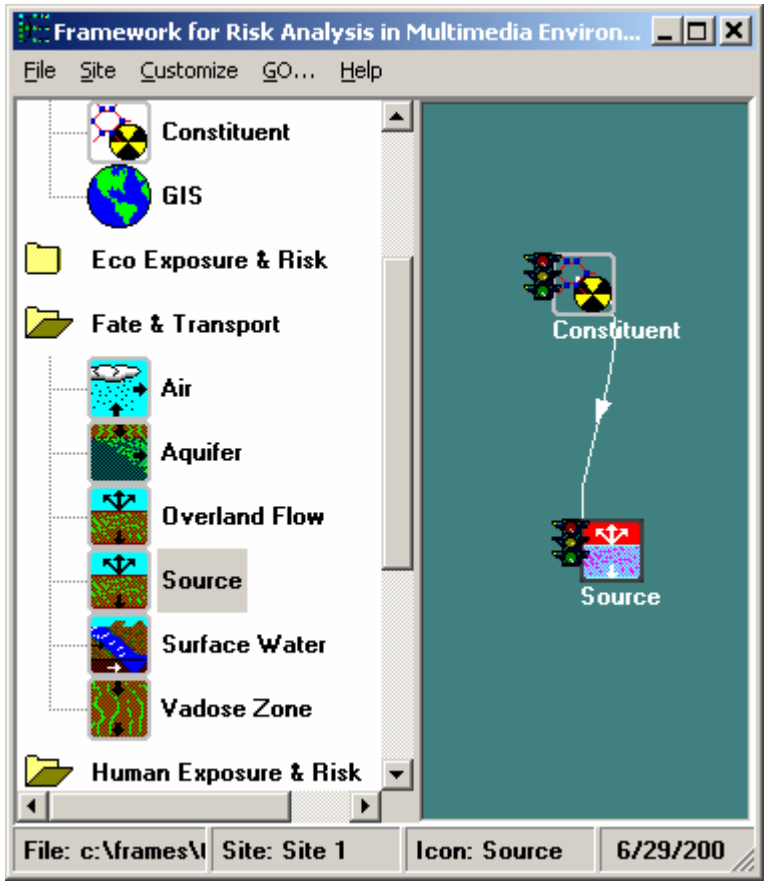
FRAMES Fundamentals

Agenda

- Create or open GID (Global Input Data) file
- Double click icons to insert modules into model
- Arrange icons with left mouse button
- Use shift key and left mouse button to connect icons/models
- Right click on icons to choose model and enter input data
  - note color-coded status
    - Red: model selected, need input data
    - Yellow: input data entered, model not run
    - Green: model completed



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Constituent Database

Constituent Database Features

- Contains numerous radionuclides and chemicals
- Can select multiple constituents
- Many properties are listed and referenced for constituents
- Use on-line help (F1) to see definitions of property fields
- Can use constituent database as a stand-alone program
  - Start → Programs → FRAMES → FRAMES Constituent Database

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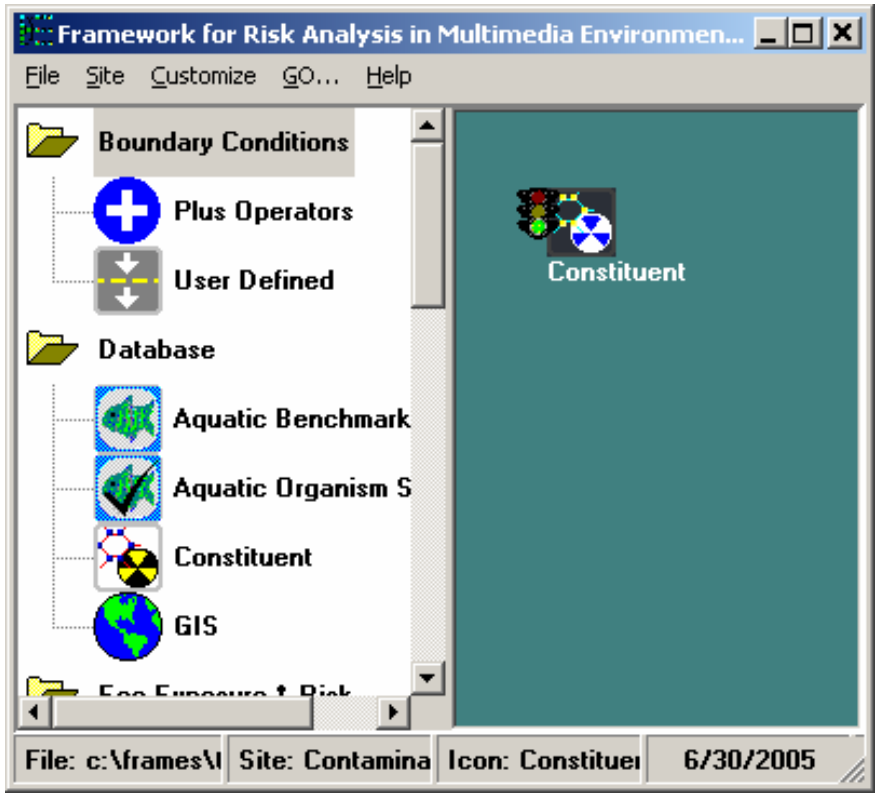
Constituent Database Implementation

- All models must contain a contaminant (constituent) database
- Double-click the 'Constituent' icon to place it in the main window
- Right-click icon, select General Info, and select model
- Right-click, select User Input, and select constituents from database
- Save changes and exit



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Constituent Database Exercise

Agenda

- **Select the following constituents from the database**
  - **H-3**
  - **C-14**
  - **Ni-59**
  - **Co-60**
  - **Ni-63**
  - **Sr-90**
  - **Nb-94**
  - **Tc-99**
  - **I-129**
  - **Cs-137**
  - **Am-241**

See ‘contam.gid’ in directory ‘Training_files’ for solution

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Source-Term Release Model

Source-Term Models

- **Source-term models calculate time-varying changes in inventory and constituent mass-flux releases to the following transport pathways:**
  - **Air transport module**
  - **Vadose zone transport module**
  - **Saturated zone transport module**
  - **Surface Water transport module**
  - **Exposure pathway module**

- **MEPAS has three source-term models**
  - **Source in Soil**
  - **Source in Standing Surface Water**
  - **Source in an Aquifer**

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Assumptions

- Source is a “well-mixed reactor”
- Mass loss occurs from decay, leaching, wind suspension, water erosion of soil, overland flow of contaminated water, and volatilization
- Degradation/decay is first-order
- Leaching controlled by solubility or aqueous/sorbed equilibrium (K_d)
- Volatilization theories based on EPA-recommended models
- Computed contaminant fluxes based on user-provided inventories or concentrations

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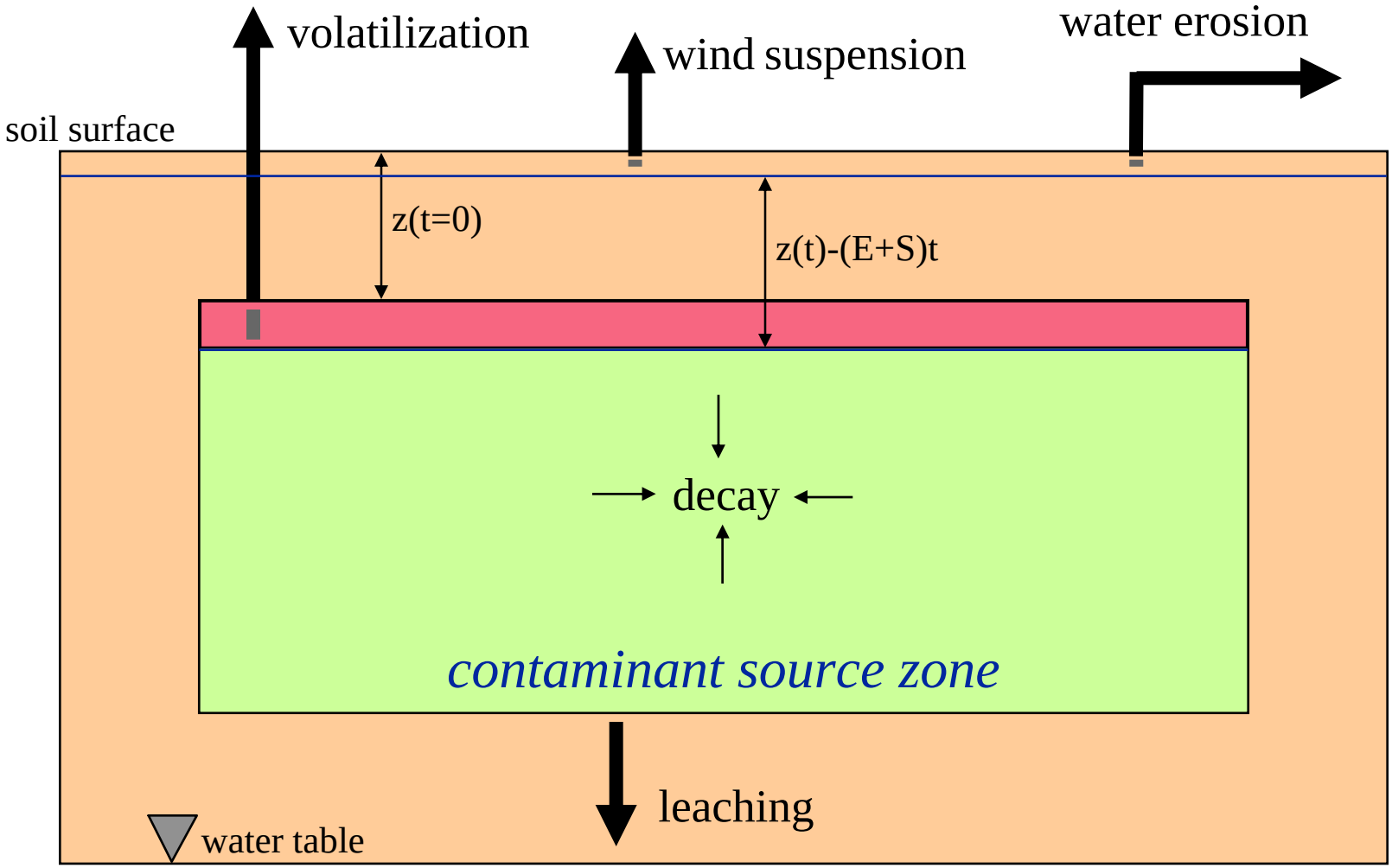
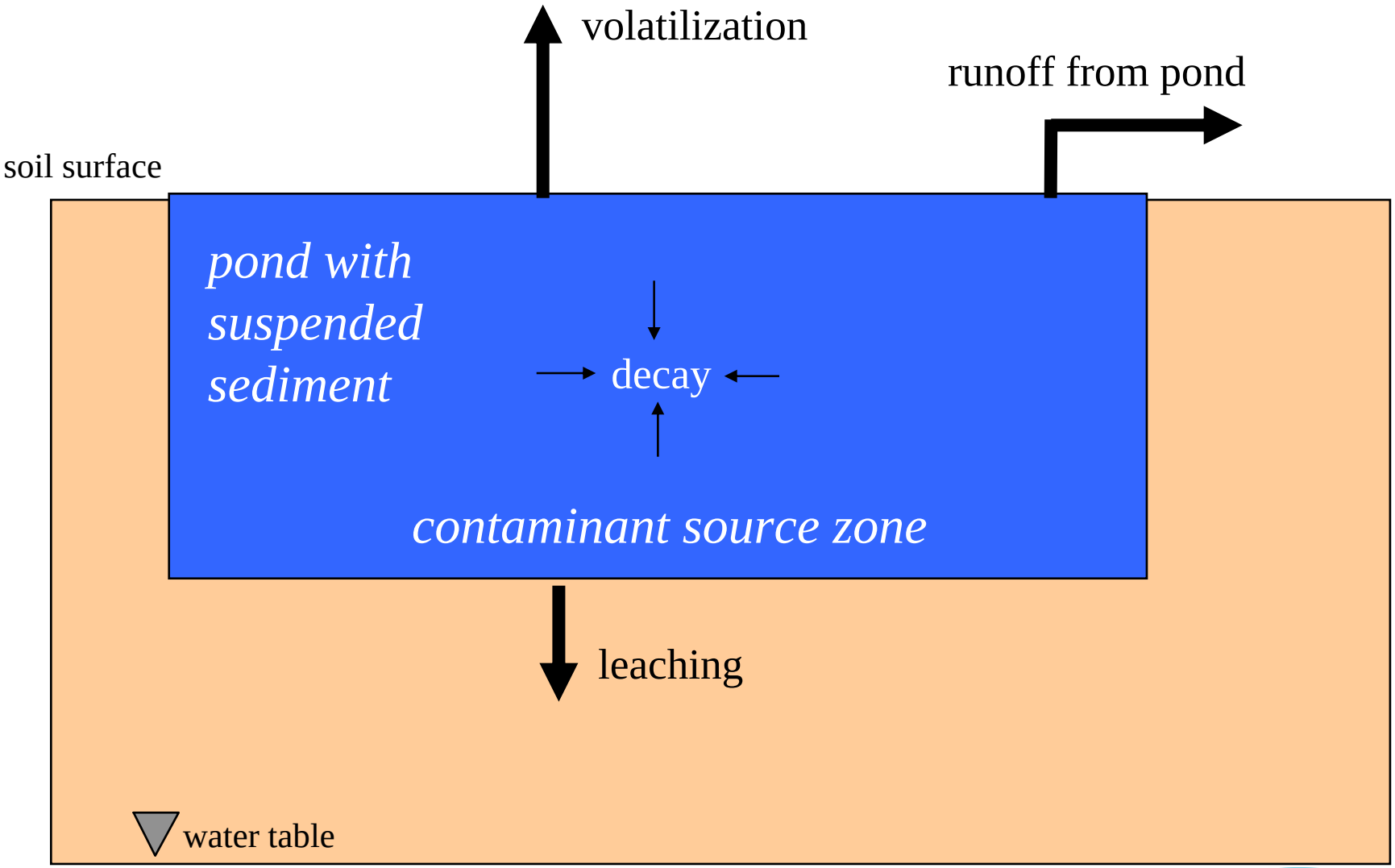
Contaminated Vadose Zone

"Source in Soil" Loss Routes



Contaminated Pond

"Source in Standing Surface Water" Loss Routes



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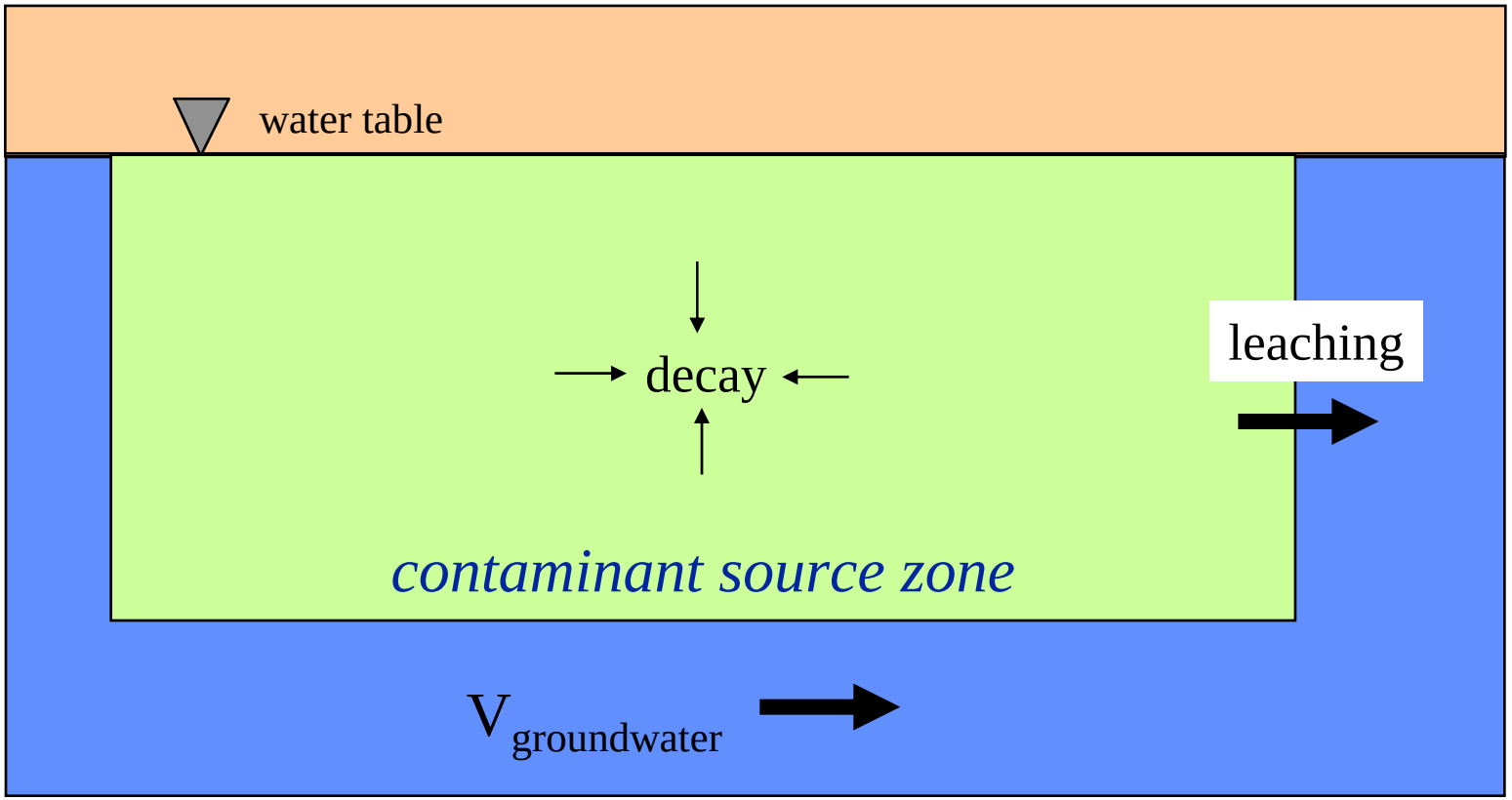
Contaminated Aquifer

"Source in Aquifer" Loss Routes



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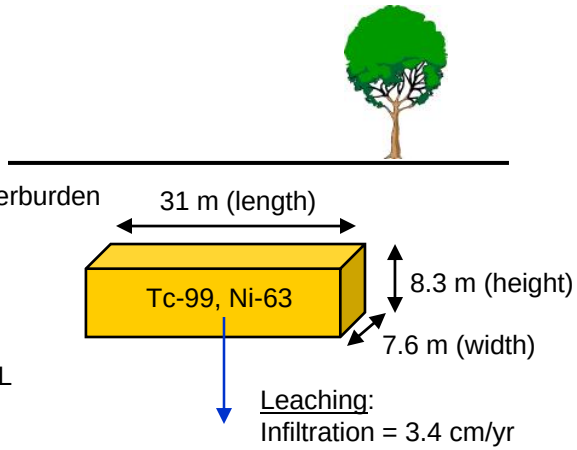
Source Exercise

- **Source Model:**
  - **Source in soil**
- **Options:**
  - **Only consider leaching and decay**
    - **Assume known infiltration through waste, but note computed pathway option for cover**
  - **1000-year simulation**
    - **Residual mass fraction for simulation = 0.01**
- **After running the model, right-click Source icon and view WFF and SCF graphical files**
- **See 'source.gid' for model solution**
- **See 'source.xls' for results and validation**

Assume no clean overburden

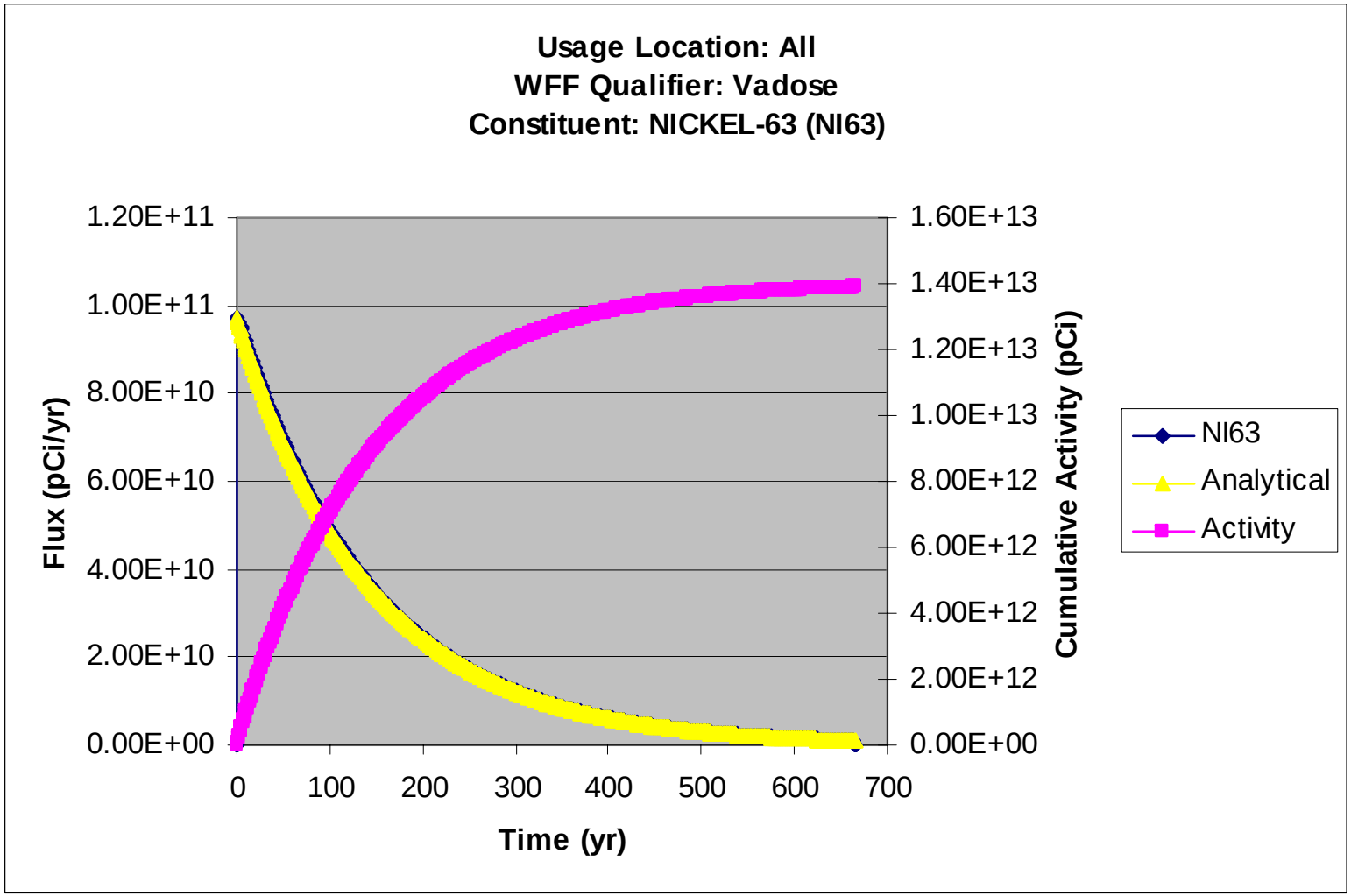


Tc-99:
Inventory = 16 Ci
Half-life = 2.12e5 yr
Solubility = 5e-3 mg/L
Kd = 0.5 mL/g

Ni-63:
Inventory = 13,000 Ci
Half-life = 100 yr
Solubility = 6.3 mg/L
Kd = 230 mL/g

Soil Properties:
Bulk density = 2385 kg/m^3
Total porosity = 0.1
Moisture content = 0.095
Average air temperature = 20C

Source Exercise Results



Vadose-Zone Transport Model

Vadose-Zone Module

- **<u>Vadose Zone Module</u> - simulates the movement of solutes through *partially saturated porous media***
- **Transport Mechanisms (for all groundwater models)**
  - **<u>Advection</u> - the transport of solutes due to the bulk movement of water**
  - **<u>Hydrodynamic Dispersion</u> - the combined effect of molecular diffusion and mechanical dispersion**
  - **<u>Degradation/Decay (i.e., persistence)</u> - removal of solute mass due to chemical transformations or radiological decay**
  - **<u>Retardation (i.e., mobility)</u> - reduction of the rate of solute movement due to adsorption/desorption on the surface of soil particles**

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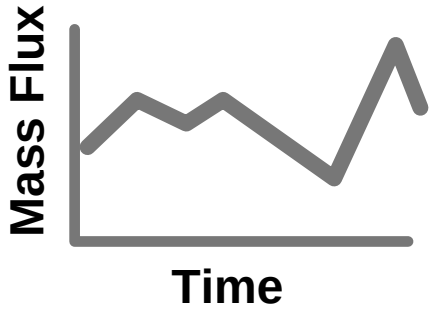
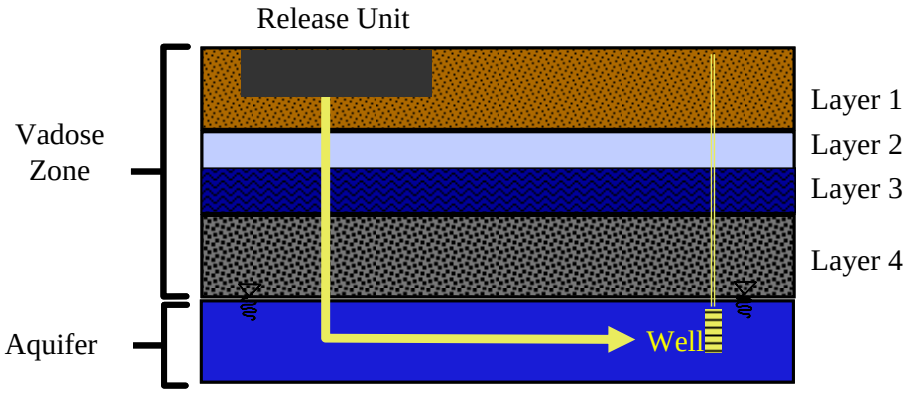
Vadose-Zone Module Features

- One-dimensional advection in a steady, uniform flow field
- One-dimensional hydrodynamic dispersion along the flow direction (i.e., longitudinal or x-direction)
- First order degradation/decay
- Adsorption/desorption is assumed to be linear and instantaneous, so retardation is described by a constant representing the ratio between the dissolved and sorbed concentrations (Kd)

Vadose-Zone Module Features (cont.)

- Decay products travel at the same rate as their parent
- Semi-analytical solution allows transient mass flux as input
- Heterogeneity can be simulated by subdividing the vadose zone into homogenous layers, and running the vadose zone module separately for each layer





Vadose-Zone Module Output

- **Volumetric water flux and time-varying, solute mass flux exiting the vadose zone layer (Water Flux File)**
- **A listing file showing**
  - **1) the input data actually read in by the model itself**
  - **2) intermediate calculation results (e.g., retardation factors, moisture content, dispersion coefficients, etc.)**
  - **3) a table of peak solute mass fluxes and the time of the peak (WLS file)**

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Vadose-Zone Module Output (cont.)

- **User can compute aqueous concentration exiting the layer by dividing the output contaminant flux by the water flux (both contained in the Water Flux File (WFF):**

$$\text{Concentration (mass/volume)} = \frac{\text{Contaminant Flux (mass/time)}}{\text{Water Flux (volume/time)}}$$

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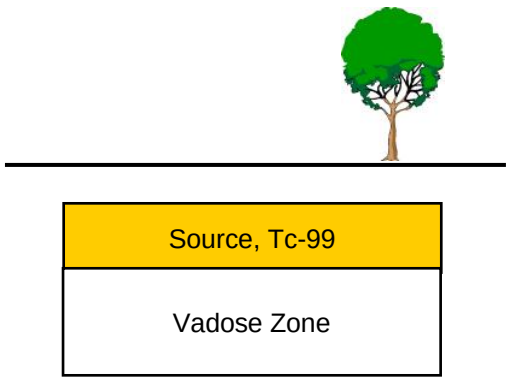
Vadose-Zone Exercise

- **Same source-term model as before ('source.gid')**
  - **Only consider Tc-99**
- **Add Vadose Zone module**
  - **Use parameter values as shown**
- **After running the model, right-click Vadose-Zone icon and view WFF graphical file**
- **See 'vadose.gid' for model solution**
- **See 'vadose.xls' for results and validation**

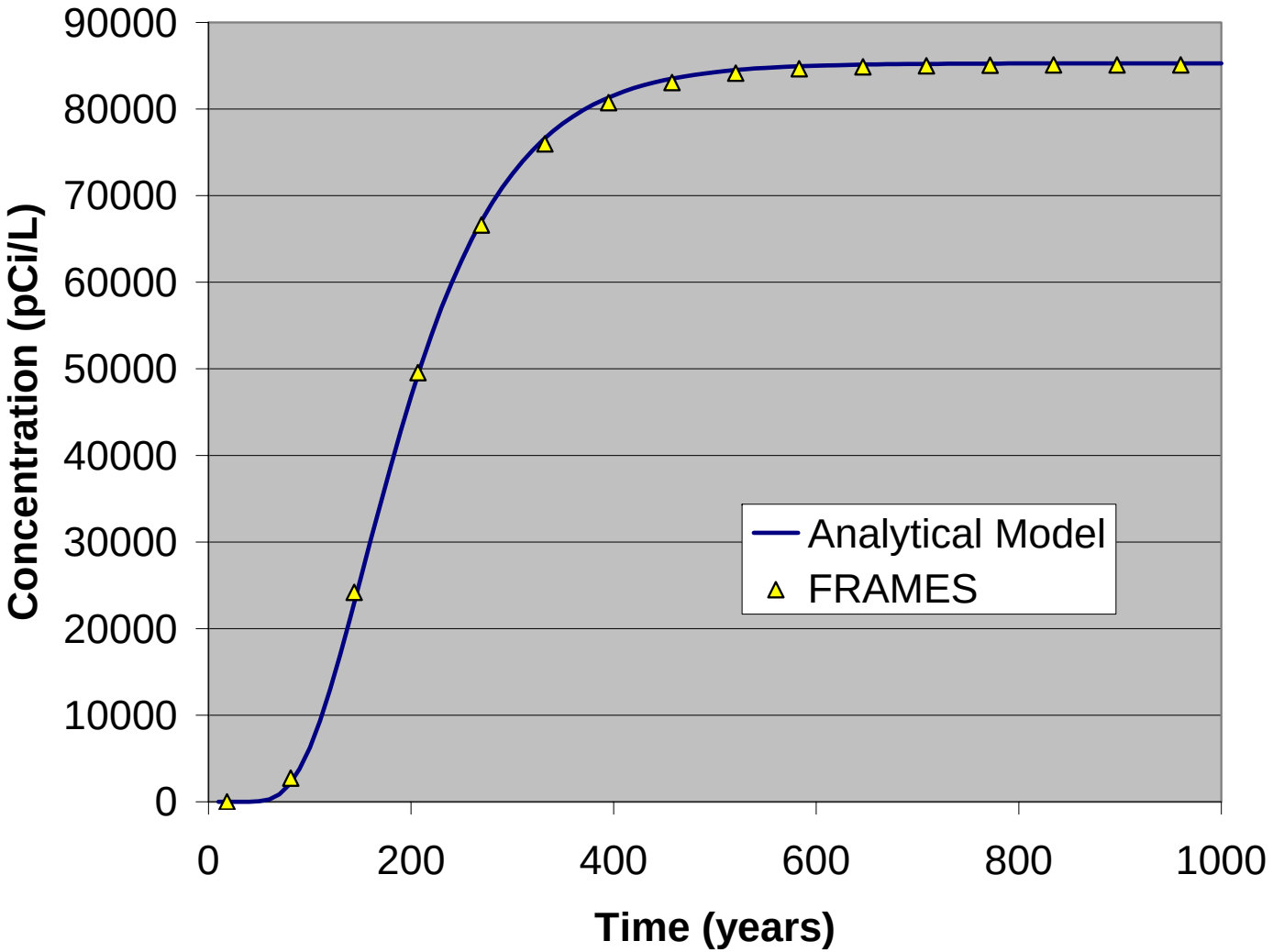


Tc-99:
Inventory = 16 Ci
Half-life = 2.12e5 yr
Solubility = 5e-3 mg/L
Kd = 0.5 mL/g
Specific activity = 0.017 Ci/g

Vadose-Zone Properties:
Composition: Sandy clay
pH = 7
Total porosity = 0.1
Field capacity = 0.02
Ksat = 1e-7 m/s
Thickness = 5 m
Longitudinal dispersivity = 0.5 m
Bulk density = 2385 kg/m^3

Vadose-Zone Exercise Results

Agenda



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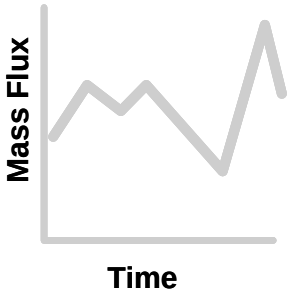
Aquifer Transport Model

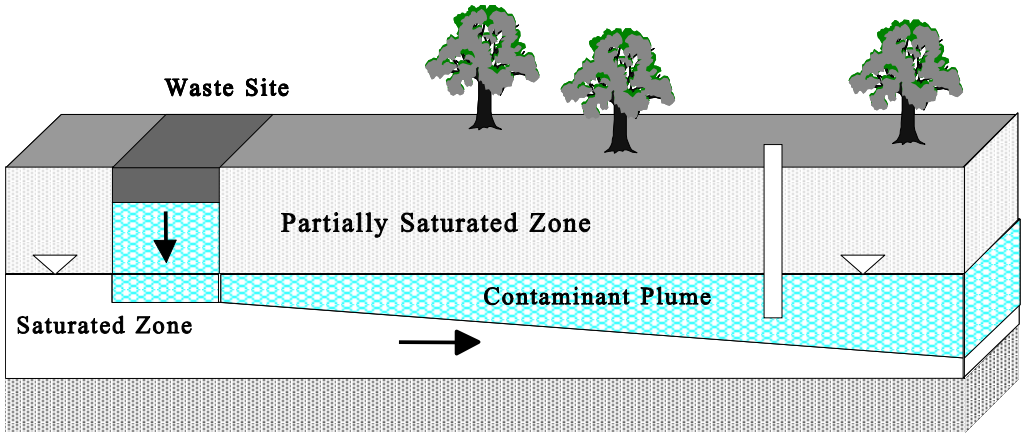
Aquifer Module Features

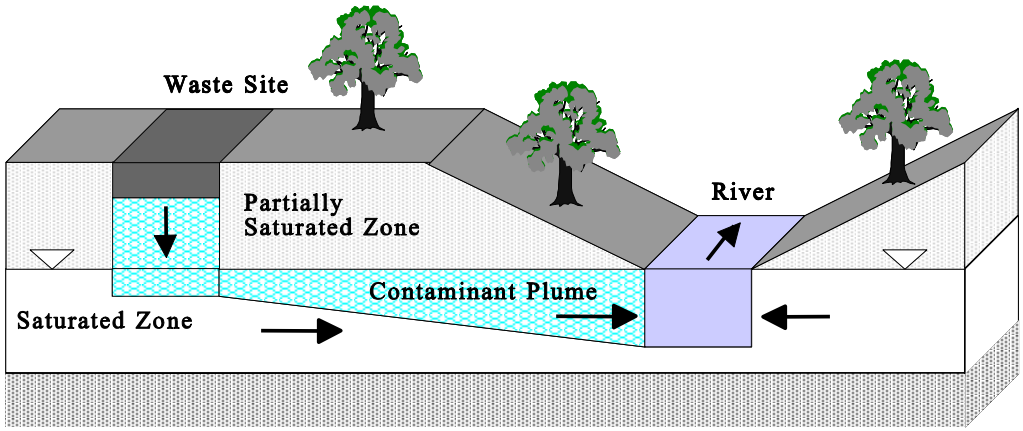
- One-dimensional advection in a steady, uniform flow field
- Three-dimensional hydrodynamic dispersion [longitudinal (x-direction), lateral (y-direction) and vertical (z-direction)]
- First order degradation/decay
- Adsorption/desorption is assumed to be linear and instantaneous, so retardation is described by a constant representing the ratio between the dissolved and sorbed concentrations (Kd)
- Decay products travel at the same rate as their parent
- Semi-analytical solution allows transient mass flux as input



Aquifer Module Output

- **Time-varying, solute concentrations (aqueous) at a specific point (i.e., an x,y,z location) when the aquifer module is connected to an exposure module (Water Concentration File)**
- **Volumetric water flux and time-varying solute mass flux exiting the aquifer when aquifer module is connected to surface water module (Water Flux File)**





Aquifer Module Output (Cont.)

- A listing file showing
  - 1) the input data actually read in by the model itself
  - 2) intermediate calculation results (e.g., retardation factors, dispersion coefficients, decay constants, etc.)
  - 3) a table of peak solute mass fluxes or concentrations and the time of the peak (WLS file)

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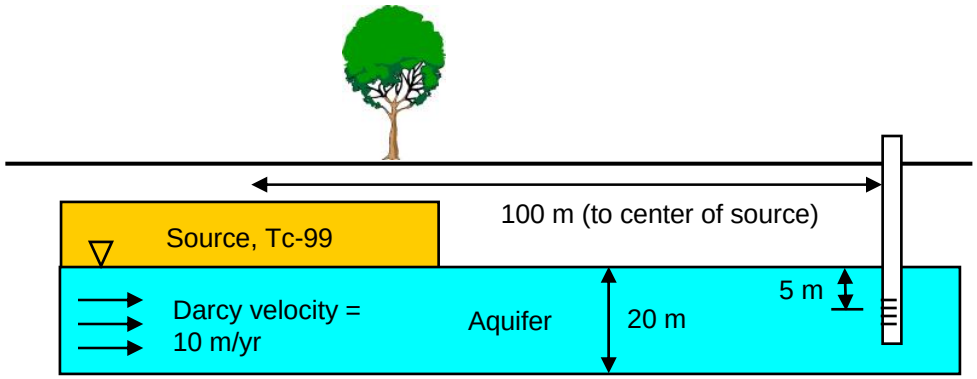
Aquifer Exercise #1

- **Same source-term model as before**
  - **Only consider Tc-99**
- **Add Aquifer module using parameters as shown**
- **See 'aquifer.gid' for model solution**
- **After running the model, right-click the aquifer icon and view WCF graphical file**
- **Vary parameters (e.g., longitudinal distance, distance to plume centerline, etc. to see the effect on the concentration**



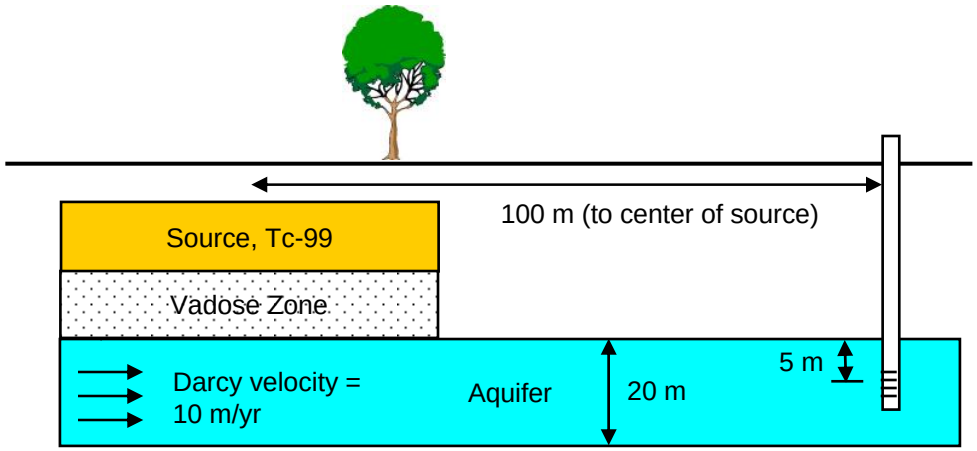
Tc-99:
Inventory = 16 Ci
Half-life = 2.12e5 yr
Solubility = 5e-3 mg/L
Kd = 0.5 mL/g
Specific activity = 0.017 Ci/g

Aquifer Properties:
Composition: Sandy clay
pH = 7
Percent of constituent entering aquifer = 100%
Total porosity = 0.1
Effective porosity = 0.1
Bulk density = 2385 kg/m3
Dispersivities: Allow FRAMES to estimate
Distance to plume centerline = 0 m

Exposure Pathways:
Need to add Exposure Pathways module and connect it to aquifer icon and constituent database, but it does not need to be populated at this point. This allows for specification of concentration location.

Aquifer Exercise #2

- **Repeat Exercise #1 using a vadose zone between the source and the aquifer**
  - **start with 'vadose.gid'**
- **Add Aquifer module using parameters as shown**
- **After running the model, right-click the aquifer icon and view WCF graphical file**
- **See 'aquifer2.gid' for model solution**



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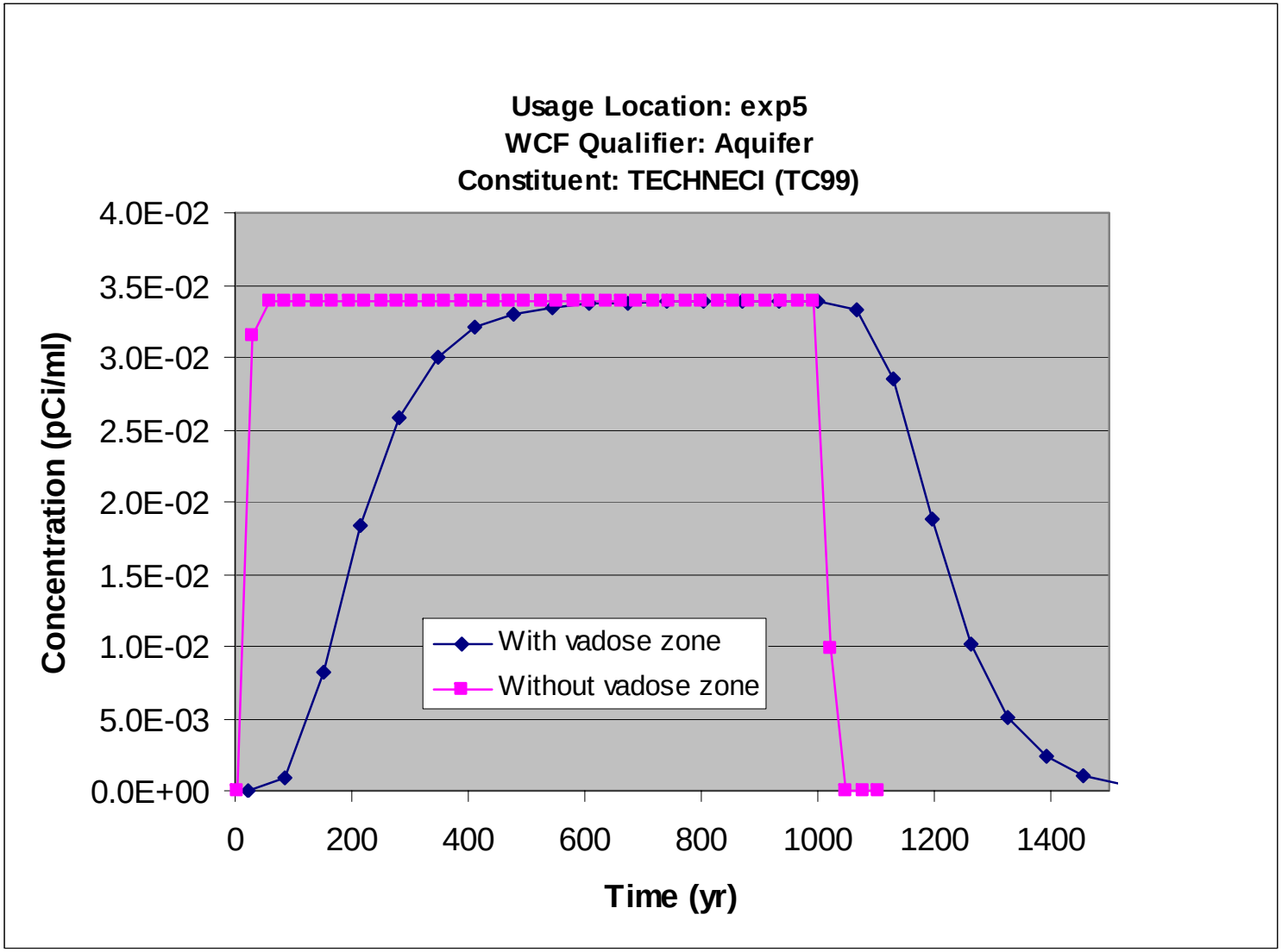
Dispersivities: Allow FRAMES to estimate
Distance to plume centerline = 0 m

Aquifer Exercise Results



Exposure Models

Exposure Pathways Model

Receptor Intake Model

Health Impacts Model

Exposure Models

- Converts constituent concentration (e.g., from WCF file) to average daily dose for exposed individuals
- Average daily dose is then used to estimate health impact
  - Lifetime risk of cancer incidence
  - Cancer fatality
- Exposure models contained in three modules
  - Exposure Pathways Model (constituent concentration)
  - Receptor Intake Model (intake)
  - Health Impacts Model (dose/risk)

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Exposure Pathways Module

- Calculates constituent concentrations for each exposure pathway (.epf file)
- For groundwater-transport pathway, exposure pathways include
  - Ingestion
    - Drinking water, vegetables, meat, milk
  - Dermal absorption
    - Shower water contact
  - Inhalation
    - Air while showering
- See MEPAS formulation for formulations and addition pathways

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Receptor Intake Module

- Uses constituent concentration (from .epf file) and calculates the intake of the constituent by the exposed individual based on input parameters
  - Individual's weight
  - Consumption rate
    - Water
    - Vegetables
    - Meat
    - Milk
  - Frequency and duration of shower
  - Exposure duration
- Output is the constituent intake for various pathways (.rif file)
  - Units of Bq for radiounuclides

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Health Impacts Module

- **Uses constituent intake (from .rif file) and calculates risk or dose**
  - **Lifetime cancer incidence**
  - **Cancer fatality**
  - **Cumulative dose during exposure period**

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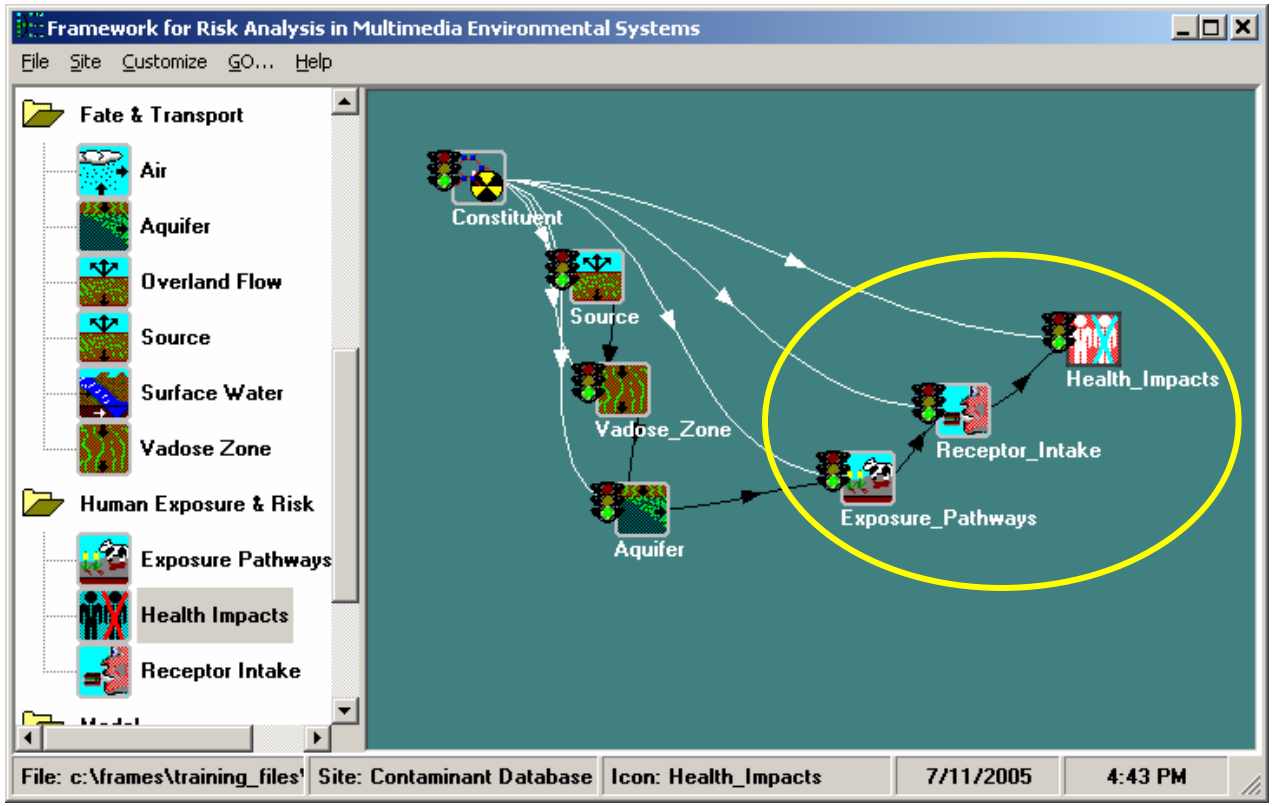
Exposure Exercise

- Using ‘aquifer2.gid,’ add the Exposure Pathways, Receptor Intake, and Health Impacts Modules
- Use the following screen images to populate the input parameters for each module
- See ‘exposure.gid’ for solution



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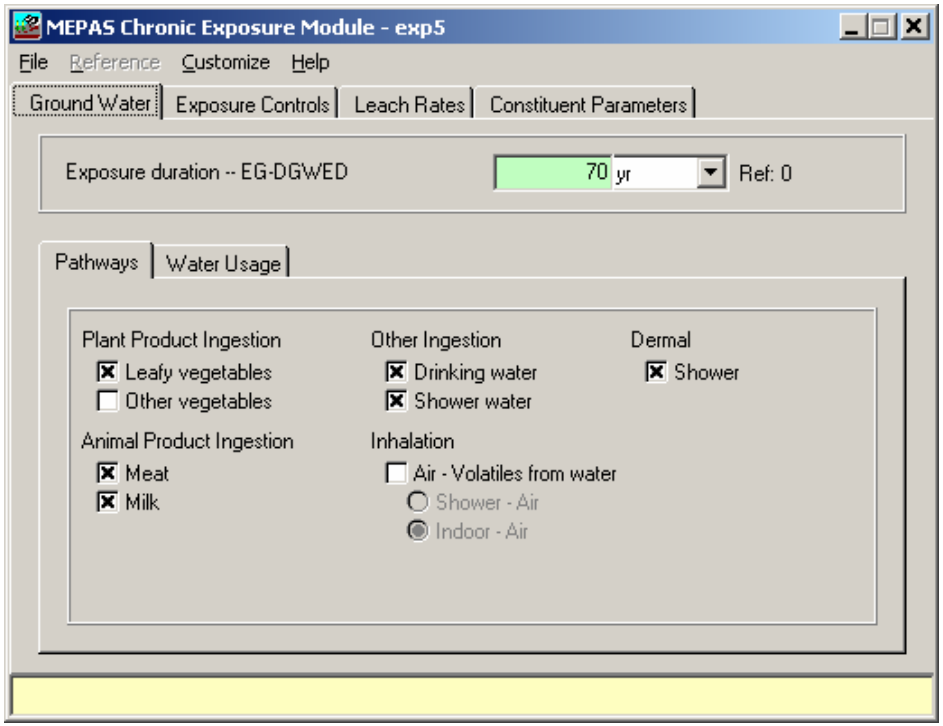
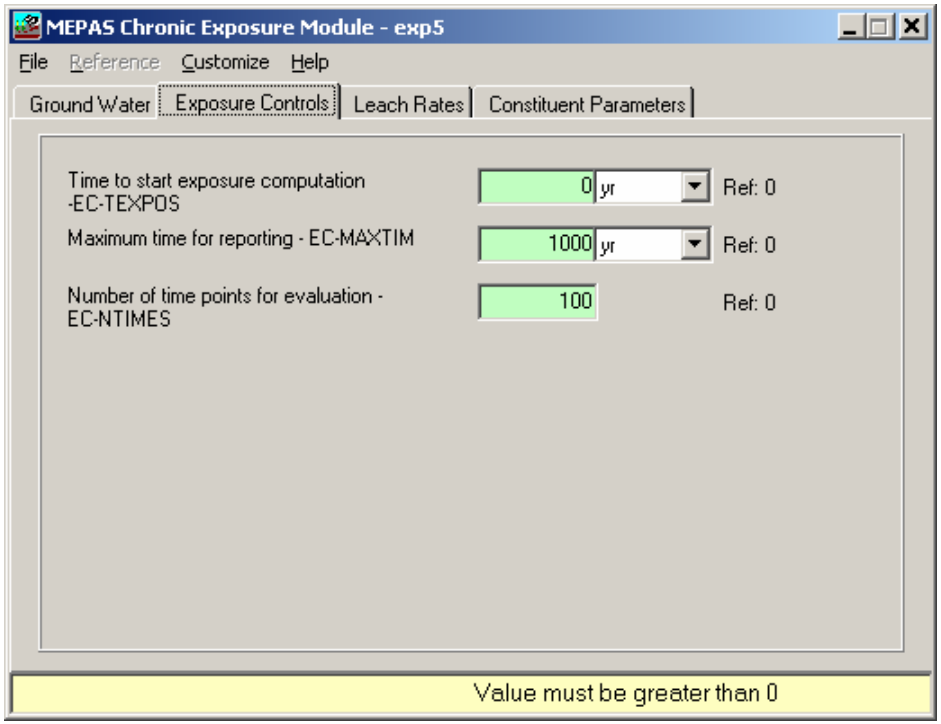
Exposure Pathways Exercise

Input Parameters

Ground Water Tab



Exposure Controls Tab



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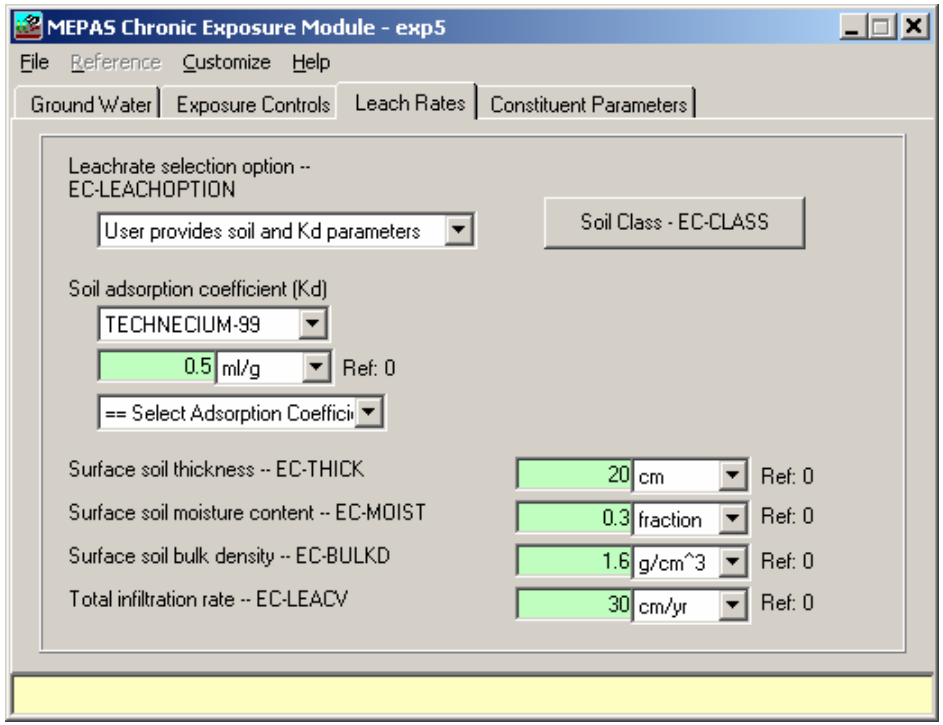
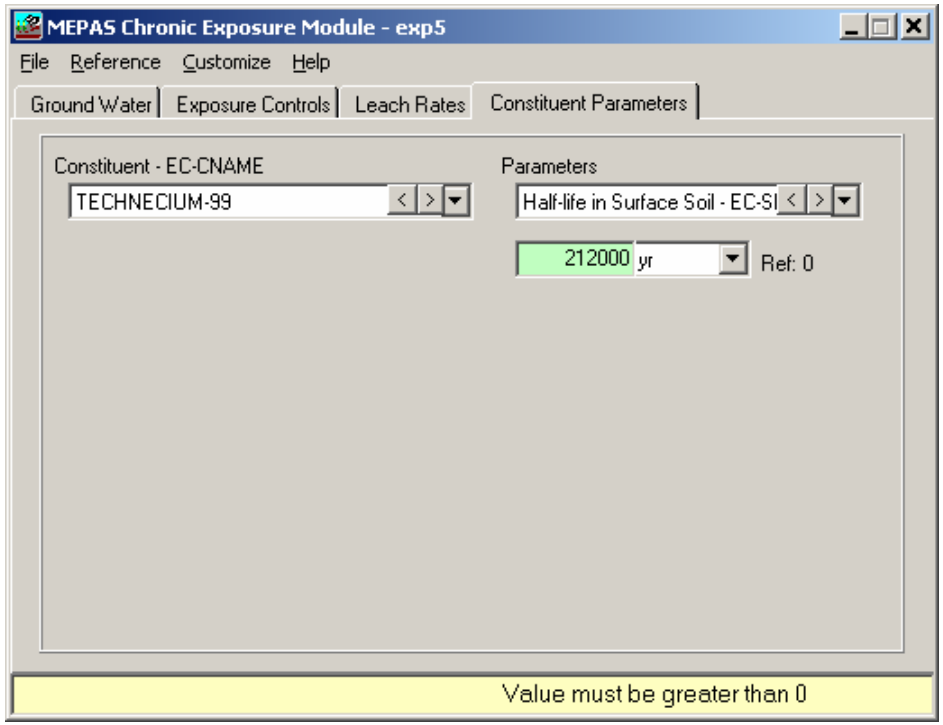
Exposure Pathways Exercise

Input Parameters (cont.)

Leach Rates Tab



Constituent Parameters Tab



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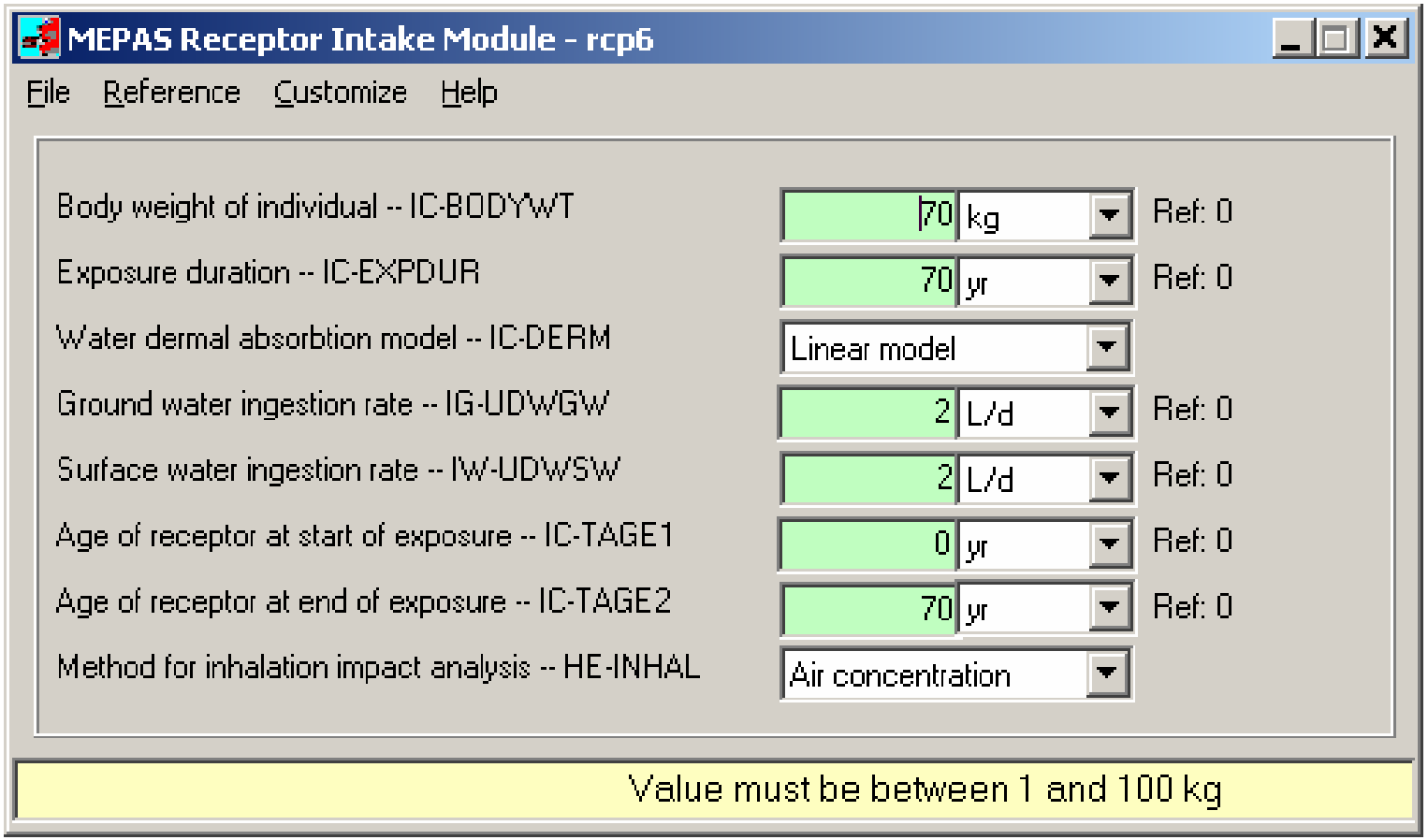
Receptor Intake Exercise

Input Parameters



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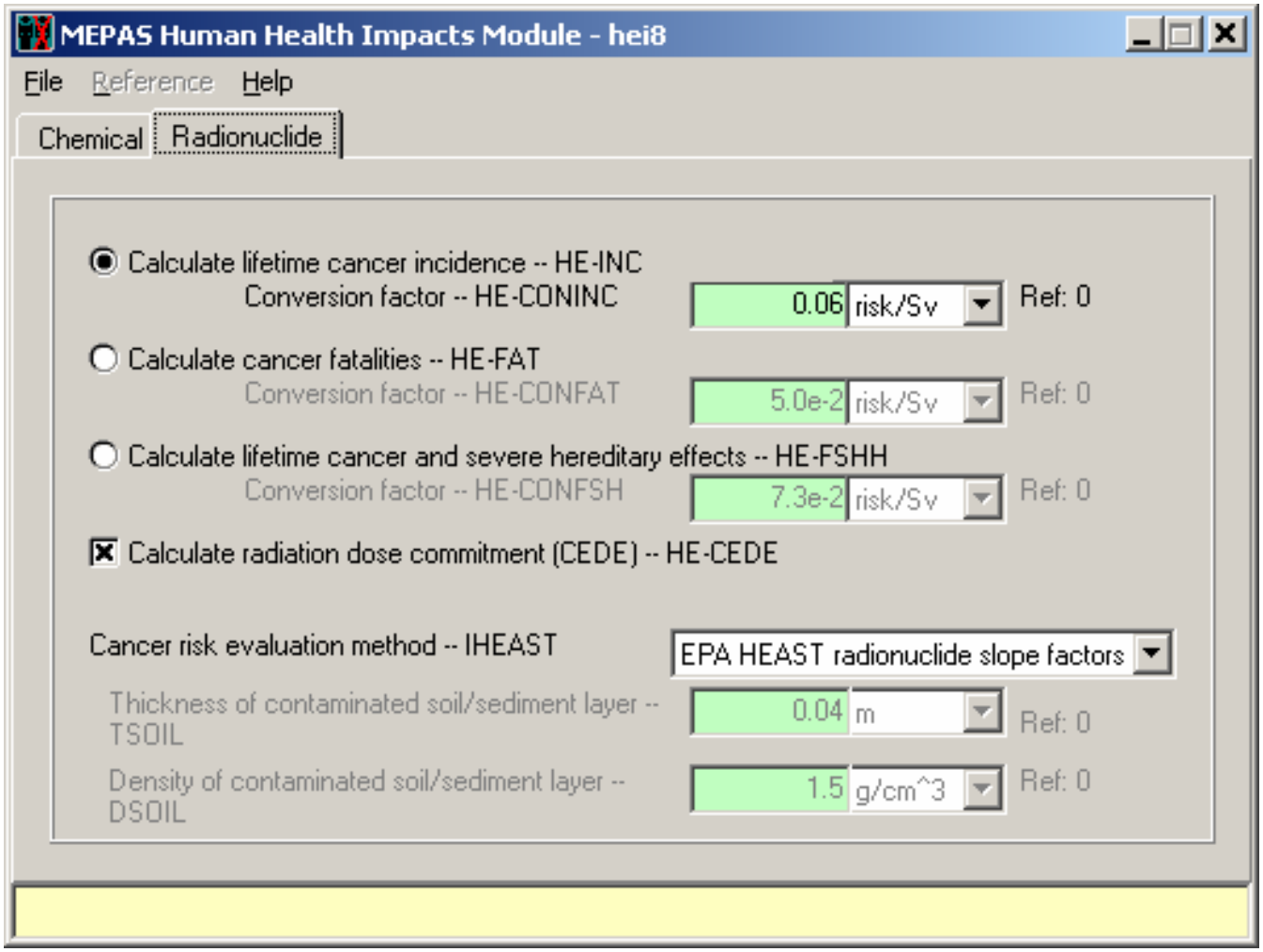
Health Impacts Exercise

Input Parameters



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Output from Exposure Modules

- **Right-click on exposure modules and view graphical files**
  - **EPF file from Exposure Pathways**
  - **RIF file from Receptor Intake**
  - **HIF file from Health Impacts**
- **To calculate annual dose (e.g., mSv/year), divide cumulative dose from HIF file by exposure duration in years (i.e., 70 years in our example)**

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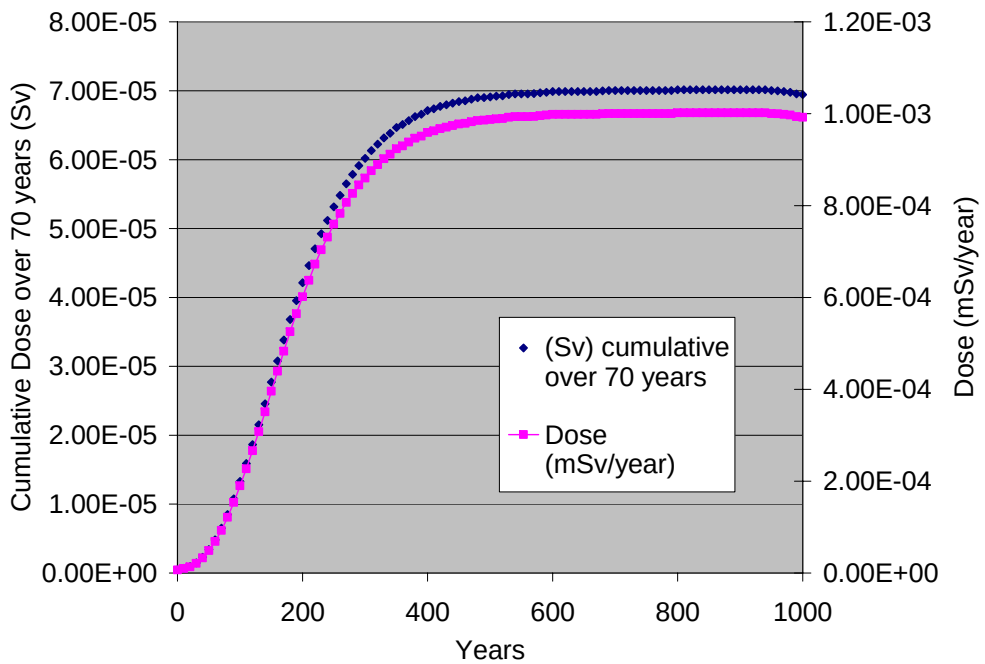
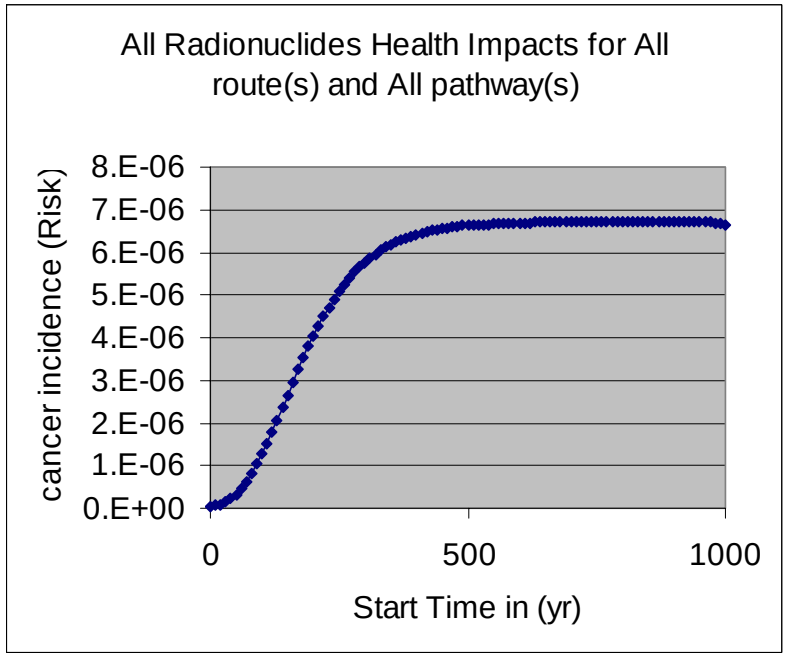
Exposure Exercise Results

Agenda

See ‘exposure.xls’ for results





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Sensitivity/Uncertainty Model

Overview

- The Sensitivity/Uncertainty module randomly samples input variables from parameter distributions and performs a Monte Carlo analysis
- Provides probabilistic analysis and statistical distributions of performance metrics to quantify uncertainty
- Can use results to determine sensitivity of performance metrics to various input parameters

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Features

- Latin-Hypercube Sampling Technique
- Multiple Parameter Distributions
  - Uniform, log uniform, normal, log normal
- Up to 70 Variables at one time
- Up to 500 iterations
- Monte Carlo: One Module or Multiple Modules in Sequence
- Cross Correlations
- Equations (Cross Correlation of Unity): Explicit Relationships
- Combination of Cross Correlation and Equation

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Using the Sensitivity Module

- Set up deterministic FRAMES analysis first, entering a value for each parameter required
- Run deterministic model to ensure no errors (all green lights)
- Add sensitivity module to main screen
  - Connect all modules that contain stochastic parameters to the sensitivity module
  - Right click sensitivity module and choose ‘General Info’
  - Select available model, click OK
  - Right click sensitivity module and choose ‘User Input’

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User Input for Sensitivity Module

- **Select variables of interest under 'Variables' tab**
  - **Highlight variable and add 'Alias' (8 characters, no symbols)**
- **Under 'Parameters' tab, specify distributions, correlations, and/or equations for each parameter**
- **Under 'Outputs' tab, select seed value, number of realizations, and output variables (metrics) to be preserved from each realization**
  - **Highlight variable and add 'Alias' (8 characters, no symbols)**

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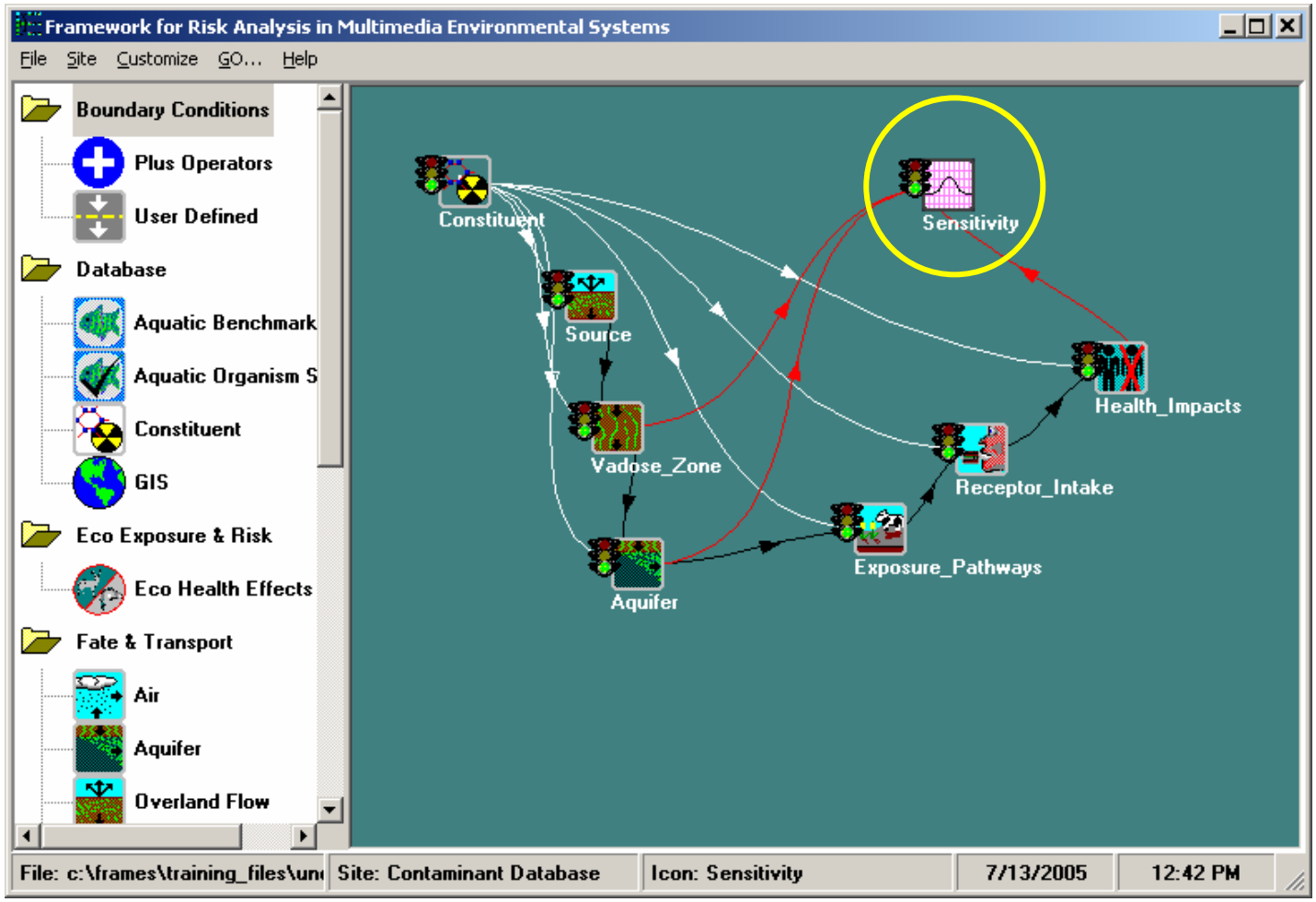
Sensitivity Exercise

- Add the sensitivity module to the existing ‘exposure.gid’ file as shown
- Save file as ‘uncert.gid’



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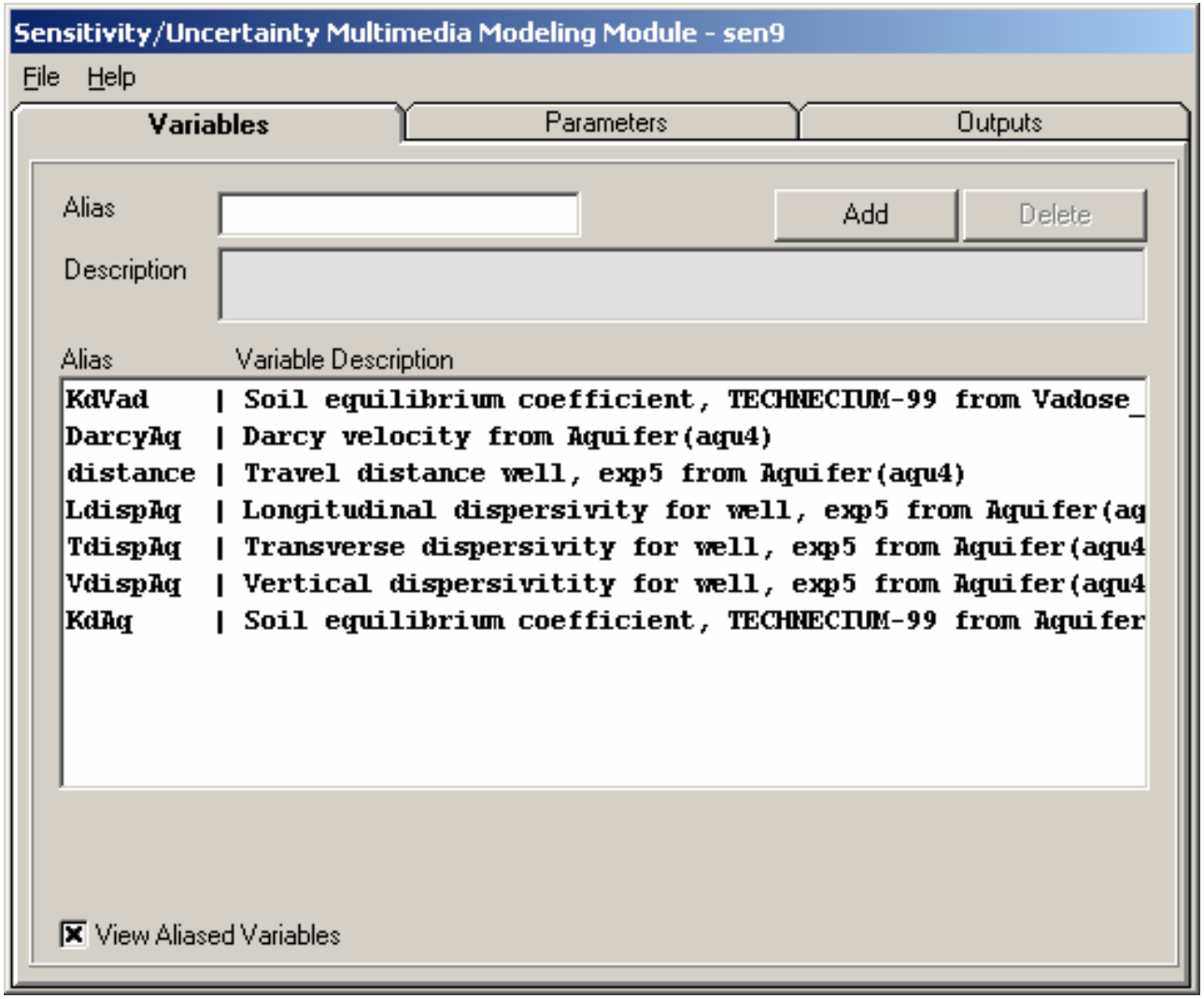
Sensitivity Exercise (cont.)

- **Select the variables as shown for stochastic analysis**
- **Assign the aliases as shown**



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Sensitivity Exercise (cont.)

- **Assign the following distributions or equations to each of the stochastic parameters**
  - **KdVad (ml/g): Log-uniform, Min = 0.01, Max = 1**
  - **DarcyAq (m/yr): Uniform, Min = 1, Max = 20**
  - **distance (m): Log-uniform, Min = 16, Max = 1000**
  - **LdispAq (m): Equation: distance*0.1**
  - **TdispAq (m): Equation: distance*0.1**
  - **VdispAq (m): Equation: distance*0.01**
  - **KdAq (ml/g): Log-uniform, Min = 0.01, Max = 1**
- **Assign the following correlations**
  - **KdVad and KdAq are positively correlated at 0.9**

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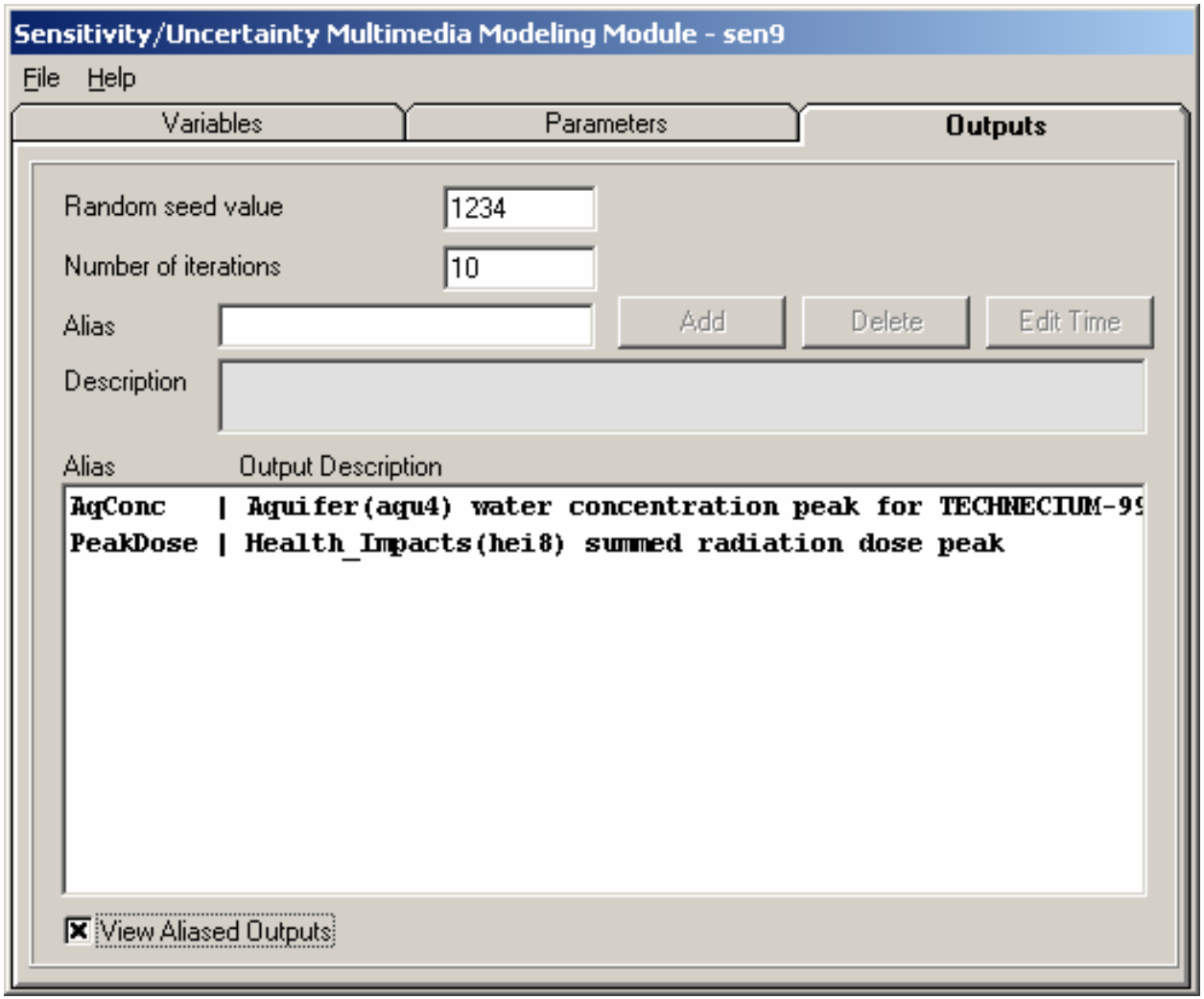
Sensitivity Exercise (cont.)

- Assign the seed value and number of iterations as shown
- Select the output variables and assign Aliases as shown
- Save and Exit
- Run the sensitivity module
- Open the ‘uncert.suf’ file in Excel



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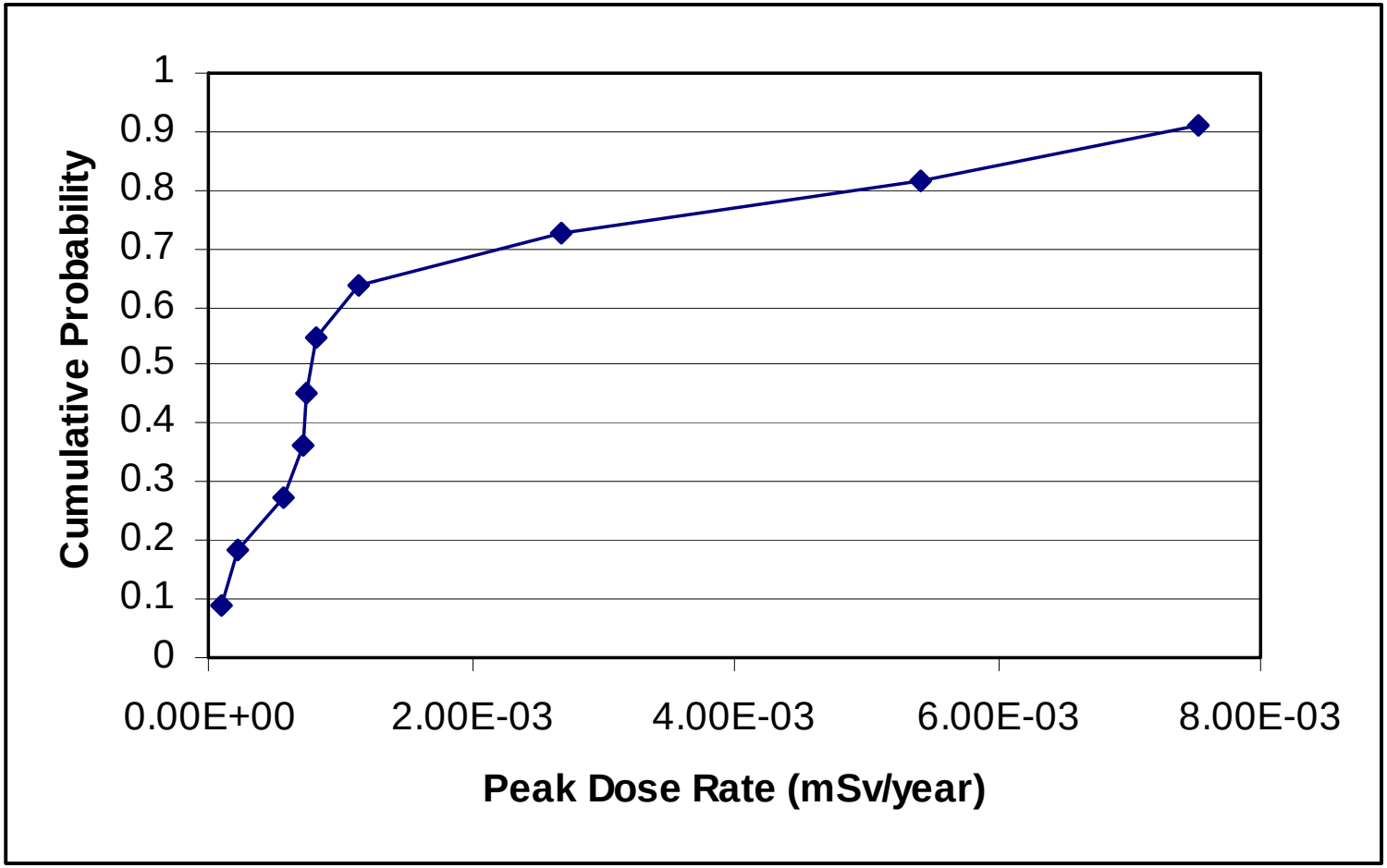
Sensitivity Exercise Results

Cumulative Probability Distribution of Peak Dose

See 'uncert.xls' for processed results



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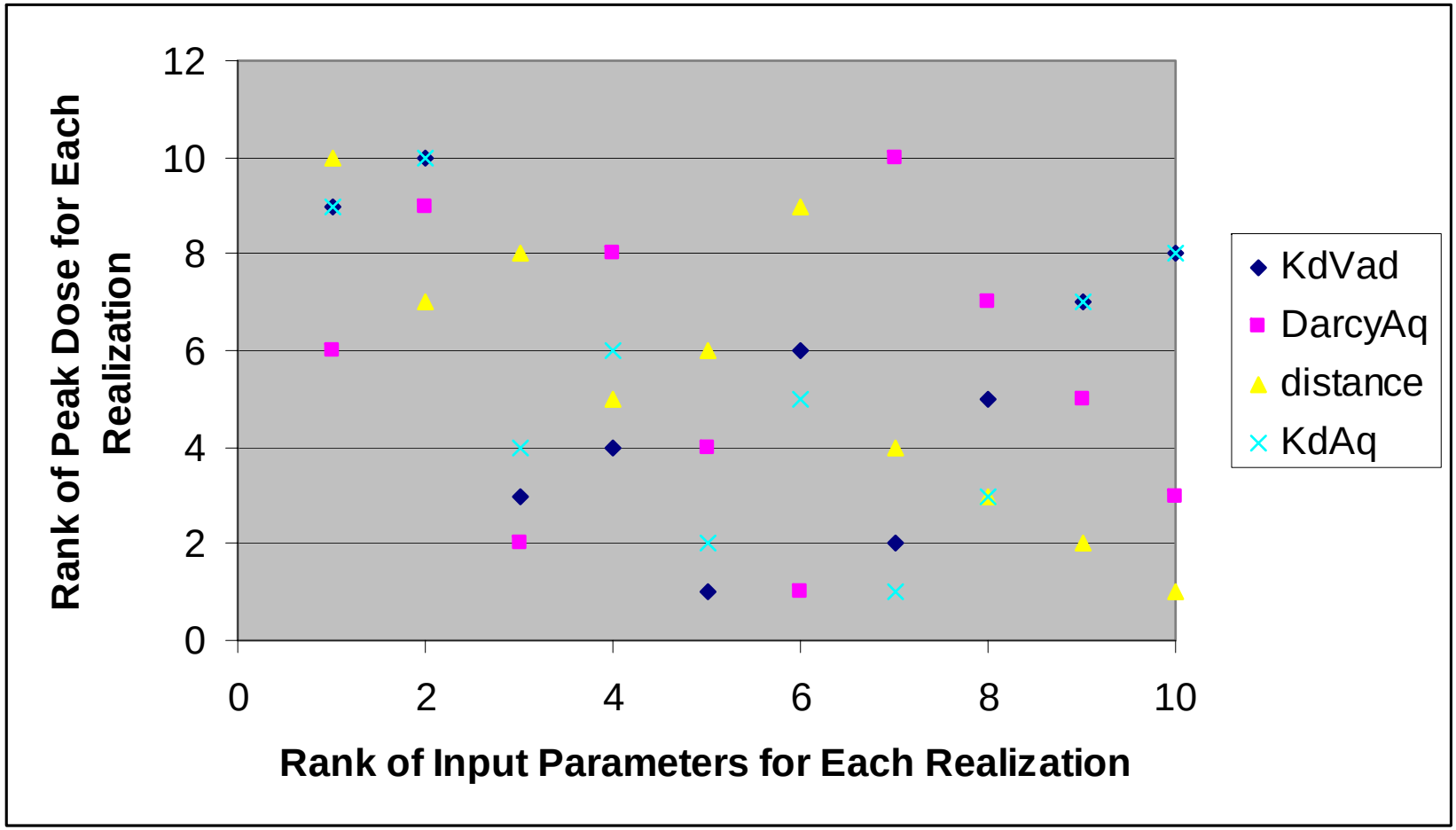
Sensitivity Exercise Results

Plot of Peak Dose vs. Input Parameter Value for Each Realization (Ranked)

See 'uncert.xls' for processed results



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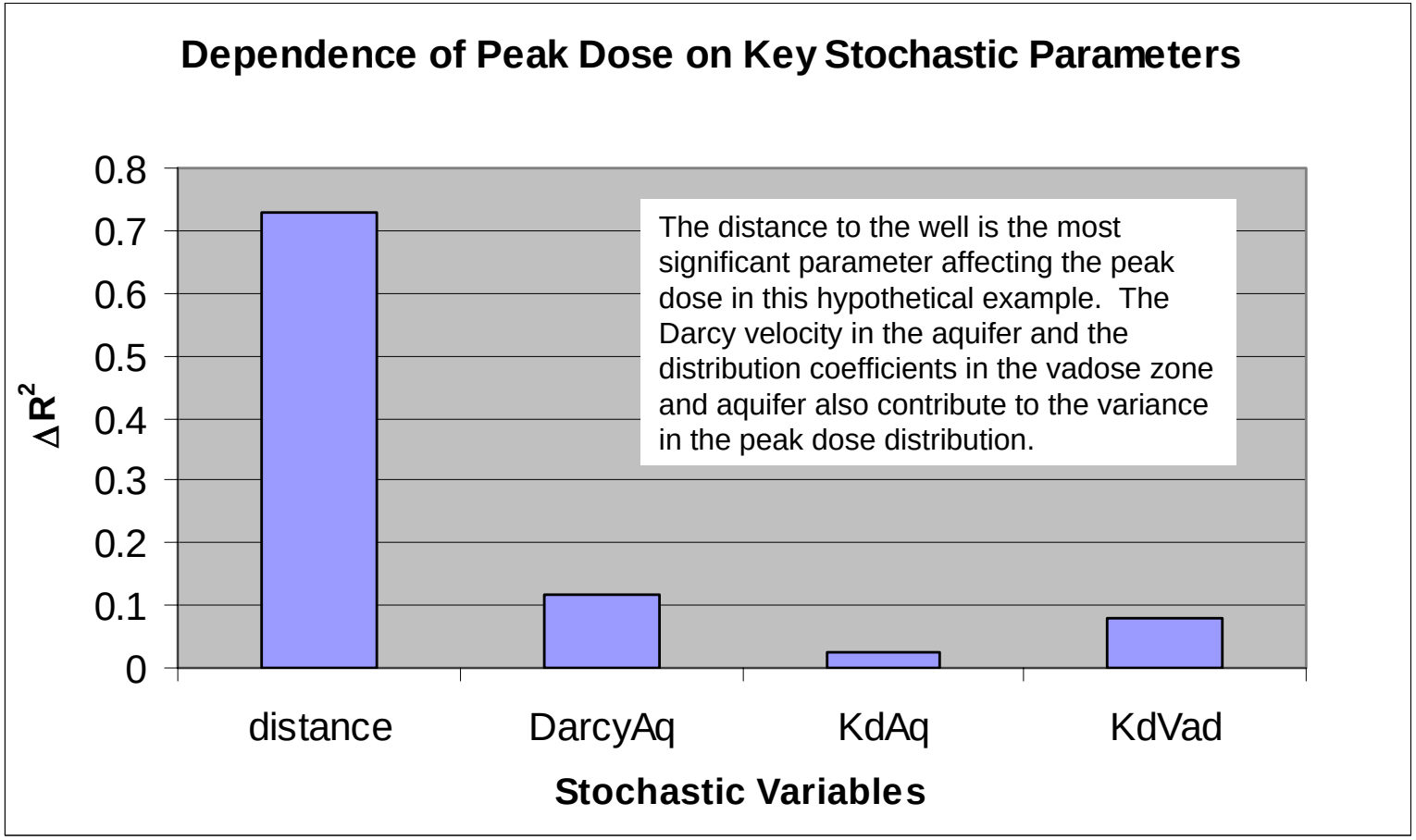
Sensitivity Exercise Results

Stepwise Linear Rank Regression

See 'uncert.xls' for processed results



The distance to the well is the most significant parameter affecting the peak dose in this hypothetical example. The Darcy velocity in the aquifer and the distribution coefficients in the vadose zone and aquifer also contribute to the variance in the peak dose distribution.

Adding Additional Modules

Linking Other Models to FRAMES

- Other computer codes can be linked to the FRAMES code for execution within the FRAMES model
- Linkage requires parameter and model output information to be passed between FRAMES and the other computer code (sub-program)
- Information must match the input/output specifications for FRAMES
- Executable file for other computer code is called sequentially for multiple realizations in the FRAMES code

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Linkage Structure and File Types

- The .DES file contains information on the sub-program being called and a list of parameters being passed between the sub-program and FRAMES
- A pre-processor program writes input files for the sub-program
- A post-processor program writes output from the sub-program into a file that is properly formatted for the FRAMES code
- A DOS batch file sequentially calls the pre-processor, the sub-program, and the post-processor

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Example Linkage: RAECOM

Agenda

- **The RAECOM computer code was linked to FRAMES for performance assessment of uranium mill tailings disposal***
- **RAECOM (Rogers et al., 1984**) simulates one-dimensional ^{222}Rn diffusion through a multi-layered landfill cover and calculates flux at the top of the cover (limited to 20 pCi/m^2/s by U.S. regulations)**
- **RAECOM was coupled to the Sensitivity module in FRAMES to perform probabilistic analyses with parameter uncertainty**

*Ho, C.K., B.W. Arnold, J.R. Cochran, and R.Y. Taira, 2002, *Development of a Risk-Based Probabilistic Performance-Assessment Method for Long-Term Cover Systems – 2nd Edition*, SAND2002-3131, Sandia National Laboratories, Albuquerque, NM.

** Rogers, V.C., K.K. Nielson, and D.R. Kalkwarf, 1984, Radon attenuation handbook for uranium mill tailings cover design, NUREG/CR-3533, U.S. Nuclear Regulatory Commission,Washington, D.C.

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