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**Performance Assessment**
**Low-Level Waste**
**Trigger Value**

**Retention: Permanent**

# Software Quality Assurance Plan for GoldSim©

**Author: R. F. Swingle**

**AUGUST 30, 2006**

**WASHINGTON SAVANNAH RIVER COMPANY**
**SAVANNAH RIVER SITE**
**AIKEN, SC 29808**

PREPARED FOR THE U.S. DEPARTMENT OF ENERGY UNDER CONTRACT NUMBER DEAC09-96-SR18500

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SAVANNAH RIVER NATIONAL LABORATORY

## DISCLAIMER



**Printed in the United States of America**

**Prepared For**
**U.S. Department of Energy**

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## REVIEWS AND APPROVALS

R. F. Swingle, Author, Chemical Science and Technology — Date 9/7/06

G. A. Taylor, Chemical Science and Technology — Date 9/18/06
(Review per Manual E7, Proc 4.60)

B. T. Butcher, Level 4 Manager, Chemical Science and Technology — Date 9/9/06

S. R. Loflin, COF — Date 9/26/06

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# LIST OF ACRONYMS

| | |
|---|---|
| CA | Composite Analysis |
| CQF | Cognizant Quality Function |
| CTF | Cognizant Technical Function |
| GTG | GoldSim Technology Group LLC |
| ICRP | International Council on Radiation Protection |
| NCRP | National Council on Radiation Protection and Measurements |
| PA | Performance Assessment |

# 1.0 EXECUTIVE SUMMARY

GoldSim© is software purchased from GoldSim Technology Group LLC (GTG) to assist in developing uncertainty analyses for site radioactive disposal facility Performance Assessments (PAs) and Composite Analyses (CAs). In the future, GoldSim© may also be used to develop inventory limits for the various disposal units. This report documents the Quality Assurance steps described in PA software evaluation report.[1]

# 2.0 INTRODUCTION

GoldSim© is a highly graphical, Windows-based program for carrying out dynamic, probabilistic simulations of complex systems to support management and decision-making in engineering, science and business. The Savannah River National Laboratory (SRNL) will be using GoldSim© to model the transport of radionuclide contaminants from waste disposal facilities at SRS. Because of its Monte Carlo functionality, GoldSim will easily us allow to study this transport probabilistically, instead of just on a deterministic basis.

# 3.0 QUALITY ASSURANCE

## 3.1 FUNCTIONAL REQUIREMENTS

Functional requirements define the functions to be performed for in-house developed software and capabilities necessary for procured software to perform the simulations of interest. Functional requirements are not required to be developed by SRS for purchased software of QA "Level C" or lower. GoldSim is purchased software and is classified as QA "Level C" and as such the original functional requirements were developed by the vendor and its predecessor organization.

The original **requirements** documents used for the development stage of GoldSim© are no longer used by the vendor. Instead, these elements are maintained through the change control system (i.e., Change Requests and Problem Reports) on an item-by-item basis.[2]

## 3.2 SOFTWARE DESIGN

The software design prescribes and documents software design elements to the level of detail necessary to permit verification of logic and results. The design shall specify the theoretical basis, overall structure and breakdown of major components of the application. Typical design elements include; interfaces, mathematical model, numerical methods, control logic, data flow and structure. GoldSim is purchased software and is classified as QA "Level C" and as such the software design documentation was developed by the vendor and its predecessor organization. Design elements of use to the GoldSim user are documented in the vendor's user manual.[3] The user manual is available from the site GoldSim CTF or from the vendor's website: www.GoldSim.com.

## 3.3 IMPLEMENTATION

The implementation is the stage of software development during which software is rolled out for testing. Software is placed under configuration control. Design constraints, standards and conventions are specified in instructions for computer program use. Test cases, criteria and approvals are defined and documented.

Since GoldSim© is purchased software, this phase is conducted by the vendor using their own procedures.[2,4]

## 3.4 VERIFICATION AND VALIDATION TESTING

Verification and validation testing demonstrates that the software is functioning as intended (verification) by comparing results from the application to results produced by a second method (e.g., hand calculations). It also demonstrates the capability of the software to produce results that are consistent with field or experimental data (validation) using test cases representative of the range of conditions expected in the actual analysis. Although not required for purchased QA Level C software, GTG has developed an extensive and thorough testing program for GoldSim© that is available for review. (See reference 4 for the initial version of GoldSim© used by SRNL.)

## 3.5 USER INSTRUCTIONS

User instructions provide a description of the user's interaction with the software, input/output specifications and formats, approved operating systems, etc. An extensive set of user instructions for GoldSim© are given in the code manuals provided by the vendor (see reference 3 for the manual for the initial version of GoldSim© used by SRNL – version 9.21).

## 3.6 ACCEPTANCE TESTING

Acceptance testing confirms acceptable performance by running test cases on the installed software in the environment in which the software is to be used. The initial acceptance tests (Version 9.21) will consist of some of the same tests used by GTG for verification testing of the CT/RT modules,[4] since these are the most important portions of GoldSim© currently planned for use at SRNL. The documentation for the tests to be used as acceptance tests has been extracted from Reference 4 and is included in the Appendix.

For testing of future new versions, this same approach may be used, or a model developed in the initial process version of GoldSim© used by SRNL (Version 9.21) may be substituted.

Acceptance testing for each process version of GoldSim© used by SRNL will be documented in a separate report.

## 3.7 OPERATION AND MAINTENANCE

Operation and maintenance specifies maintenance actions necessary to correct errors, implement new requirements or adapt to changes in the operating system. This section also specifies testing to ensure that resulting code modifications have not caused unintended adverse effects.

### 3.7.1 Operation

The Manager, Environmental Analysis and Performance Modeling, approves the analysts who operate GoldSim©. These analysts will have access to the software and user's manual (see reference 3 for the manual for the initial version of GoldSim© used by SRNL – version 9.21).

### 3.7.2 Maintenance

Since GoldSim© is a purchased code, maintenance to correct software errors or to adapt changes in software requirements will be made and tested by the vendor according to its maintenance plan.[2]

## 3.8 CONFIGURATION CONTROL

Configuration control is a method established to control, uniquely identify, describe, and document the configuration of each version of a computer program. Since GoldSim© is a purchased code, configuration control in large part is the purview of the vendor.[2] However, configuration control will be initiated locally to ensure that SRNL personnel are using the version of the code approved by SRNL for use in low level waste transport modeling. The name of the software and the CTF shall be recorded in the Software Inventory Database. The date of installation, version installed, and installation notes are recorded by the CTF. Since all users will have access to a number of available versions via the vendor's website, control of the current production version in use by SRNL will be administrative. This can be accomplished by verifying that the approved version of the code was used during the design review process.

### 3.8.1 Configuration Identification

The vendor maintains its own configuration identification system.[2] This identification system will also be used by SRNL.

### 3.8.2 Changes

Any changes to the approved version of GoldSim must be approved by the manager of the Environmental Analysis and Performance Modeling Group of SRNL. Acceptance testing (§3.6) must be performed before a new version is released for use by SRNL personnel.

## 4.0 REFERENCES

[1] B. T. Butcher, PA Software Evaluation Report.

2 "GoldSim Software Configuration Management Procedures", Revision 4.0, October 2001, GoldSim Technology Group, Issaquah, WA.

[3] GoldSim User's Guide, Version 9.20, January 2006, GoldSim Technology Group, LLC, Issaquah, WA.

[4] "VERIFICATION PLAN: GOLDSIM VERSION 9.21", June 2006, GoldSim Technology Group LLC Issaquah, WA

# 5.0 APPENDIX - INITIAL ACCEPTANCE TESTS

A few of the tests from GoldSim's Verification Plan[4] will be used for the initial acceptance tests for GoldSim© at SRNL. The sections of the Verification Plan documenting the tests to be used have been copied below with some minor clarifications.

## 5.1 CT_PIPES-01 : SINGLE-POROSITY TEST PROBLEM

In this test the following components of the Pipe element are tested:

- basic advective dispersion algorithm
- effect of infill porosity
- effect of infill retardation
- effect of coating retardation
- effect of pipe fluid saturation
- effect of suspended particulates

This problem consists of the transport of a single stable solute (decay constant $l = 0.0$) by advection and dispersion in a single-porosity domain. The pipe is 40m long, with a flow rate of 1.0 $m^3$/day, the pipe's flowing area, A, equals 1.0 $m^2$ and the longitudinal dispersivity, a, is 1.0 m. Diffusion along the flow direction is neglected. The Ogata and Banks (Ogata and Banks, 1961) analytic solution is for a Dirichlet boundary condition setting the inlet concentration to 1.0 Ci/$m^3$. This is a close approximation to GoldSim's constant-flux boundary condition of 1g/day, and the difference is minor and is only apparent at very early times.

A subset of the Ogata and Banks analytic results is presented in the following table:

| **Distance along Fracture (m)** | **Time 25 days** | **Time 50 days** | **Time 75 days** |
|---|---|---|---|
| 40 | 0.0215 | 0.8679 | 0.9986 |

Test problem CT_Pipes-01 contains five pipes which should each match the above table:

1. An unretarded pipe with no infill.

2. A pipe with an infill with porosity = 0.2, density = 2600kg/$m^3$, and partition coefficient = 0.0003076923{m3/kg}. The partition coefficient produces a retardation factor of 5, which exactly cancels the effect of the porosity.

3. A pipe one tenth as long (4m), with a coating having an effective retardation of 10 (1mm of material with density = 2500kg/$m^3$ and partition coefficient = 1.8{m3/kg}). This also produces a retardation factor of 5, which exactly cancels the effect of the porosity.

4. A pipe with a saturation of 0.1, and a coating thickness of 0.0001. This gives an effective retardation factor of R=10, which counteracts the effect of the saturation.

5. A pipe one half as long (20m), with a coating and suspended solids having a combined retardation factor of R=2. (Make the amount of solute dissolved / suspended equal to the amount sorbed on the coating:

$$A(1 + C_p K_d) = P t_c \rho K_d$$

where:

| | | |
|---|---|---|
| A | = | Flowing area, $L^2$ |
| $C_p$ | = | Concentration of suspended particulates, $ML^{-3}$ |
| ρ | = | Density of the solid, $ML^{-3}$ |
| $K_d$ | = | Partition actor, $L^3M^{-1}$ |
| P | = | Perimeter, L |
| $t_c$ | = | Coating thickness, L |

Have GoldSim solve this problem three times, using the three different precision options (low, medium and high) from the model option menu. Confirm that all solutions are within acceptable accuracy (at least two significant figures correct).

## 5.2 CT_PIPES-08: DECAY-CHAIN TRANSPORT WITH MATRIX DIFFUSION

This problem models the transport of a radioactive species and its daughters in a double-porosity system comprised of parallel fractures embedded in a low-permeability, low-porosity rock matrix. The aperture of the parallel fractures, spaced at 0.1 m, is 100 μm. With this setting, the pipe area for a single 1m wide fracture, A, is $10^{-4}$ $m^2$. The pore velocity is 100 m / yr in the fractures and the longitudinal dispersivity of the fractures, $a_L$, is 10 m. The matrix porosity and tortuosity are 0.01 and 0.1, respectively. A maximum diffusion distance, d, equal to the half-spacing of the fractures (0.05 m) was used.

This analytic comparison involves the transport of the decay chain Uranium 234 → Thorium 230 → Radium 226 in a system of parallel fractures. The matrix (i.e., immobile zone) retardation factors for $U^{234}$, $Th^{230}$ and $Ra^{226}$ were assigned values equal to $1.43x10^4$, $5.00x10^4$ and $5.00x10^2$, respectively, and the decay constants equal $2.83x10^{-6}$, $9.00x10^{-6}$ and $4.33x10^{-6}$ $year^{-1}$, respectively. For simplicity, retardation on the surfaces of the fractures (i.e., pipes) was neglected. The diffusion coefficients for each of the species, $D^o$, were assigned identical values equal to $3.154x10^{-2}$ $m^2$ / year. A prescribed concentration of 1.0 mol / $m^3$ was assigned for $U^{234}$ at the fracture inlet, and 0.0 mol / $m^3$ was used as the inlet concentration for $Th^{230}$ and $Ra^{226}$.

The tabulated analytical results from Hodgkinson and Maul (1985) at 100,000 years, at selected distances along the pipe are shown below:

Analytical Solution for Verification Test CT_Pipes-08

| Distance | Concentration (mol/m3) | | |
|---|---|---|---|
| | U-234 | Th-230 | Ra-226 |
| 10 | 9.54E-01 | 1.84E-02 | 1.12E-02 |
| 50 | 6.80E-01 | 2.51E-02 | 5.79E-02 |
| 100 | 2.50E-01 | 6.39E-03 | 7.80E-02 |
| 200 | 4.27E-03 | 5.66E-05 | 7.37E-02 |
| 400 | 4.80E-09 | 0.00E+00 | 5.80E-02 |

Note: To obtain the final values for the different distances, change the value of the Length data element to each of the distances shown in the table.

## 5.3 CT_CELLS2 - ADVECTIVE CONNECTIONS FROM CELLS

These problems test simple advective connections from cells. For these problems, one or more advective connections from the cell to a sink are defined with non-zero flows. For problems in which decay is turned off, the total mass in the cell is governed by the following equation:

$$M_{is} = \sum_{c=1}^{NC_i} f_{cs}$$

where:

$M_{is}$ = rate of increase of species s in cell i [M / t];
$NC_i$ = number of mass transfer connections for cell i; and
$f_{cs}$ = influx rate of species s (into cell i) through connection c [M / t].

Note that for an advective connection from cell i, $f_{cs}$ is defined as follows:

$$f_{cs} = -(c_{ims} + \sum_{t=1}^{NPT_{im}} c_{its,\,ds} \cdot cp_{imt}) q_c$$

where:

$q_c$ = the rate of advection for connection c [L3 / t for fluid connections and M / t for solid connections];
$c_{ims}$ = the concentration of species s in medium m within cell i [M / L3 if m is a fluid; M / M if m is a solid];
$NPT_{im}$ = the number of solid media suspended in medium m within cell i;
$c_{its,ds}$ = the sorbed concentration of species s in solid medium t within cell i [M / M];
$cp_{imt}$ = the concentration of solid particulate t within fluid m in cell i [M / L3];

Note that by definition, $q_c$ cannot be a negative number.

The second term accounts for the advection of suspended solids in a fluid. Note that for solid advective connections, the second term is not applicable (i.e., $NPT_{im} = 0$).

The manner is which the concentrations (e.g., $c_{ims}$, $c_{its}$) are computed for each species in every medium in a cell was discussed above in Section 5.7.1.

### 5.3.1 CT_Cells2 -01 - Simple Fluid Advection

This problem is identical to CT_Cells1-01, except a second cell is added, with an advective connection between the two cells. The second cell contains only WATER, and the flow rate (QW) from the first cell to the second cell is 0.1 $m^3/yr$.

For a cell with only one advective connection and no decay, the governing equation is:

$$M_{is} = -c_{ims} * QW$$

Substituting for $c_{ims}$, and recalling that in this case m is WATER, the above equation becomes:

$$M_{is} = -(QW*P_{i,WATER,e})\ m_{is}$$

The solution to this equation is

$$m_{is} = m^{o}_{is} \exp-\{(QW*P_{i,WATER,e})\ t\}$$

Given the total mass in the cell as a function of time, the mass flux from the cell and the concentration in each medium can be readily computed as discussed in the previous section. The analytical solution is presented in the following table. Note that Results are not expected to match the very small exact results at time 10,000 with high precision.

| Medium | Am-241 ($g/m^3$) or (g/kg) | Am-242 ($g/m^3$) or (g/kg) | Am-243 ($g/m^3$) or (g/kg) |
|---|---|---|---|
| **WATER** | | | |
| time = 100 | 2.37E-1 | 8.37E-2 | 4.07 |
| time = 1000 | 1.06E-1 | 3.75E-2 | 1.83 |
| time = 10,000 | 3.57E-5 | 1.26E-5 | 6.14E-4 |
| **OIL** | | | |
| time = 100 | 2.37E-2 | 8.37E-3 | 4.07E-1 |
| time = 1000 | 1.06E-2 | 3.75E-3 | 1.83E-1 |
| time = 10,000 | 3.57E-6 | 1.26E-6 | 6.14E-5 |
| **SAND** | | | |
| time = 100 | 4.73E-2 | 1.67E-2 | 8.15E-1 |
| time = 1000 | 2.13E-2 | 7.51E-3 | 3.66E-1 |
| time = 10,000 | 7.13E-6 | 2.52E-6 | 1.23E-4 |
| **CLAY** | | | |
| time = 100 | 1.18 | 4.18E-1 | 2.04E+1 |
| time = 1000 | 5.32E-1 | 1.88E-1 | 9.15 |
| time = 10,000 | 1.78E-4 | 6.30E-5 | 3.07E-3 |

### 5.3.2 CT_Cells2 -07 - Advection with Multiple Connections from Different Media

This problem is identical to CT_Cells1-01, except an advective connection from the cell exists for all four media (WATER, OIL, SAND, and CLAY). The WATER flow rate is QW (0.1 $m^3/yr$), OIL flow rate is QO (0.05 $m^3/yr$ ), the SAND flow rate is QS (0.05 kg/yr) and the CLAY flow rate is QC (0.20 kg/yr). .

The governing equation is:

$$M_{is} = -c_{i,WATER,s} * QW - c_{i,OIL,s} * QO - c_{i,SAND,s} * QS - c_{i,CLAY,s} * QC$$

Substituting for the concentrations, the above equation becomes:

$$M_{is} = -(QW * P_{i,WATER,e} + QO * P_{i,OIL,e} + QS * P_{i,SAND,e} + QC * P_{i,CLAY,e})\, m_{is}$$

The solution to this equation is:

$$m_{is} = m^{o}_{is} \exp-\{(QW * P_{i,WATER,e} + QO * P_{i,OIL,e} + QS * P_{i,SAND,e} + QC * P_{i,CLAY,e})\, t\}$$

Given the total mass in the cell as a function of time, the mass flux from the cell and the concentration in each media can be readily computed as discussed in the previous section. The analytical solution is shown in the following table. Note that Results are not expected to match the very small exact results at time 10,000 with high precision.

| Medium | Am-241 ($g/m^3$) or (g/kg) | Am-242 ($g/m^3$) or (g/kg) | Am-243 ($g/m^3$) or (g/kg) |
|---|---|---|---|
| **WATER** | | | |
| **time = 100** | 9.60E-2 | 3.39E-2 | 1.65 |
| **time = 1000** | 1.28E-5 | 4.53E-6 | 2.21E-4 |
| **time = 10,000** | <1E-40 | <1E-40 | <1E-40 |
| **OIL** | | | |
| **time = 100** | 9.60E-3 | 3.39E-3 | 1.65E-1 |
| **time = 1000** | 1.28E-6 | 4.53E-7 | 2.21E-5 |
| **time = 10,000** | <1E-40 | <1E-40 | <1E-40 |
| **SAND** | | | |
| **time = 100** | 1.92E-2 | 6.78E-3 | 3.30E-1 |
| **time = 1000** | 2.57E-6 | 9.06E-7 | 4.42E-5 |
| **time = 10,000** | <1E-40 | <1E-40 | <1E-40 |
| **CLAY** | | | |
| **time = 100** | 4.80E-1 | 1.69E-1 | 8.26 |
| **time = 1000** | 6.42E-5 | 2.27E-5 | 1.10E-3 |
| **time = 10,000** | <1E-40 | <1E-40 | <1E-40 |

## 5.4 CT_CELLS3 - DIFFUSIVE CONNECTIONS FROM CELLS

These problems test simple diffusive connections from cells. For these problems, one or more diffusive connections from the cell to a sink are defined. For problems in which decay is turned off, the total mass in the cell is governed by the following equation:

$$M_{is} = \sum_{c=1}^{NC_i} f_{cs}$$

where:

- $M_{is}$ = rate of increase of species s in cell i [M / t];
- $NC_i$ = number of mass transfer connections for cell i; and
- $f_{cs}$ = influx rate of species s (into cell i) through connection c [M / t].

Note that for an advective connection from cell i, $f_{cs}$ is defined below.

Diffusive mass transfer connections can only be specified to occur through fluids. The flux $f_{cs}$ to path i is computed as follows for diffusive mass transfer connections:

$$f_{cs} = D_{cs}\left(-c_{ims} + \frac{c_{jns}}{K_{nms}}\right) + \sum_{t=1}^{NPT_{im}} PFD_{ct} \cdot D_{ct}\left(-c_{its,\,ds} \cdot cp_{imt} + c_{jts,\,ds} \cdot cp_{jnt}\right)$$

where:

- $D_{cs}$ = diffusive conductance for species s in connection c [L3 / t];
- $c_{ims}$ = the dissolved concentration of species s in medium m within cell i [M / L3];
- $c_{jns}$ = the dissolved concentration of species s in medium n within cell j [M / L3];
- $K_{nms}$ = partition coefficient between fluid medium n (in cell j) and fluid medium m (in cell i) for species s [L3 medium m / L3 medium n];
- $NPT_{im}$ = the number of particulate solid media in fluid m within cell i;
- $PFD_{ct}$ = Boolean flag (0 or 1) which indicates whether diffusion of solid t suspended in the fluid for connection c is allowed;
- $D_{ct}$ = diffusive conductance for particulate t in connection c [L3 / t];
- $c_{its,ds}$ = the sorbed concentration of species s associated with solid t within cell i [M / M];
- $cp_{imt}$ = the concentration of solid particulate t within fluid m in cell i [M / L3];
- $c_{jts,ds}$ = the sorbed concentration of species s associated with solid t within cell [M / M]; and
- $cp_{jnt}$ = the concentration of solid particulate t within fluid n in cell j [M / L3].

The first term in the equation above accounts for diffusion of dissolved species, while the second term accounts for diffusion of particulates suspended in the fluid. Note that unlike advective connections, the fluid media involved in cells i (medium m) and j (medium n) need not be identical. Note also that if j is a pathway, $c_{jns}$ and $cp_{jnt}$ are assumed to be zero.

(Hence, mass can diffuse from a cell to a pathway, but cannot diffuse from a pathway to a cell).

The diffusive conductance terms are computed as follows:

$$D_{cs} = \frac{A_c}{\frac{L_{ci}}{d_{ms} \cdot t_{Pci} \cdot n_{Pci}} + \frac{L_{cj}}{d_{ns} \cdot t_{Pcj} \cdot n_{Pcj} \cdot K_{nms}}}$$

where:

| | | |
|---|---|---|
| $A_c$ | = | the area of diffusive connection c [L2]; |
| $L_{ci}$ | = | diffusive length for connection c in cell i [L]; |
| $L_{cj}$ | = | diffusive length for connection c in cell j [L]; |
| $d_{ms}$ | = | diffusivity for species s for fluid m (in cell i) [L2/t]; |
| $d_{ns}$ | = | diffusivity for species s for the fluid n (in cell j) [L2/t]; |
| $tp_{ci}$ | = | tortuosity for the porous medium Pci defined for connection c in cell i (≤ 1); |
| $tp_{cj}$ | = | tortuosity for the porous medium Pcj defined for connection c in cell j (≤ 1); |
| $np_{ci}$ | = | porosity for the porous medium Pci defined for connection c in cell i; |
| $np_{cj}$ | = | porosity for the porous medium Pcj defined for connection c in cell j; and |
| $K_{nms}$ | = | partition coefficient between fluid media n (in cell j) and fluid media m (in cell i) for species s [L3 medium m / L3 medium n]. |

and

$$D_{ct} = \frac{A_c}{\frac{L_{ci}}{d_{mt} \cdot t_{Pci} \cdot n_{Pci}} + \frac{L_{cj}}{d_{nt} \cdot t_{Pcj} \cdot n_{Pcj}}}$$

where $A_c$, $L_{ci}$, $L_{cj}$, $t_{Pci}$, $t_{Pcj}$, $n_{Pci}$, and $n_{Pcj}$ are as defined previously, and

| | | |
|---|---|---|
| $d_{mt}$ | = | diffusivity for particulate t within the fluid m (in cell i) [L2/t]; and |
| $d_{nt}$ | = | diffusivity for particulate t within the fluid n (in cell j) [L2/t]. |

If j is a pipe, $L_{cj}$ is automatically assumed to be 0 (no diffusive resistance is present on the pipe side of the connection). The equation above does not contain a partitioning term because, as will be shown below, intermedia diffusive transport is not allowed for suspended particulates.

The partition coefficient ($K_{mns}$) present in the above equations is defined as follows:

$$K_{nms} = \frac{K_{nre}}{K_{mre}}$$

where:

$K_{mre}$ = partition coefficient between fluid medium m and reference fluid r for element e (where species s is an isotope of element e) [L3 fluid r / L3 fluid m]; and

$K_{nre}$ = partition coefficient between fluid medium n and reference fluid r for element e (where species s is an isotope of element e) [L3 fluid r / L3 fluid n].

Note that $K_{mre}$ and $K_{nre}$ are direct user inputs.

$PFD_{ct}$ is defined as follows:

IF [fluid m = fluid n]

THEN ($PFD_{ct} = 1$),

ELSE ($PFD_{ct} = 0$)

That is, diffusive transport of particulates through a fluid from cell i to receiving cell (or pipe) j is only allowed if fluid m (in cell i) is the same as fluid n (in cell or pipe j).

Particulate solid concentrations in fluids ($cp_{imt}$, $cp_{jnt}$) are specified directly by the user. Contaminant concentrations in various media ($c_{ims}$, $c_{jns}$, $c_{its}$, $c_{jts}$) are computed as described in Section 5.7.1.

### 5.4.1 CT_Cells3 -01 - Simple Diffusion

This problem is identical to CT_Cells1-01, except a second cell is added, with a diffusive connection between the two cells (WATER to WATER). Both cells contain all four media, and the diffusive connection properies are as listed below:

| | **diffusive length (m)** | **tortuosity** | **porosity** |
|---|---|---|---|
| **Cell 1** | 0.02 | 0.1 (SAND) | 0.3 (SAND) |
| **Cell 2** | 0.02 | 0.15 (CLAY) | 0.4 (CLAY) |

The diffusive area is 20 $m^2$ and the diffusivity for all species in water is 1e-3 $m^2$ / yr.

For a cell with only one diffusive connection to another cell through the same fluid, the governing equations for each species are (assuming no decay):

$$M_{1s} = D_{cs} (-c_{1,WATER,s} + c_{2,WATER,s})$$

$$M_{2s} = D_{cs} (c_{1,WATER,s} - c_{2,WATER,s})$$

Substituting for $c_{ims}$, the above equations become:

$$M_{1s} = D_{cs} (-P_{1,WATER,e}\, m_{1s} + P_{2,WATER,e}\, m_{2s})$$

$$M_{2s} = D_{cs} (P_{1,WATER,e}\, m_{1s} - P_{2,WATER,e}\, m_{2s})$$

This is a linear systems of equations. The resulting concentrations are as follows:

Cell 1

| Medium | Am-241 ($g/m^3$) | Am-242 ($g/m^3$) | Am-243 ($g/m^3$) |
|---|---|---|---|
| **WATER** | | | |
| **time = 100** | 2.54E-1 | 8.97E-2 | 4.37 |
| **time = 1000** | 2.20E-1 | 7.76E-2 | 3.79 |
| **time = 10,000** | 1.33E-1 | 4.70E-2 | 2.29 |

Sink

| Medium | Am-241 ($g/m^3$) | Am-242 ($g/m^3$) | Am-243 ($g/m^3$) |
|---|---|---|---|
| **WATER** | | | |
| **time = 100** | 4.52E-3 | 1.59E-3 | 7.77E-2 |
| **time = 1000** | 3.87E-2 | 1.37E-2 | 6.66E-1 |
| **time = 10,000** | 1.26E-1 | 4.43E-2 | 2.16 |

## 5.5 CT_CELLS4 – DECAY CALCULATIONS IN CELLS

These test problems are specifically targeted at verifying the radioactive decay algorithms in RIP. All problems in this group are run with radioactive decay. A 100 yr timestep is used for all problems unless otherwise specified

### 5.5.1 CT_Cells4-01: Radioactive Decay in a Cell

In this problem, the decay chain starting with Am-241 is examined. The problem is simply looking at decay over the first 1,000 yr. Am-241 decays to Np-237. To test split decay, two daughters are specified for Np-237, each receiving 50% of the mass. U-233a and U-233b each have identical properties. The analytical solutions for Am-241, Np-237 and U-233 are as follows (note that decay in the containers is a function of the timestep, with smaller timesteps producing more accurate results. A 2 year timestep is used in this case to exactly reproduce the analytical solution:

$$M(\text{Am-241}) = M_0(\text{Am-241})\, e^{-k_1 t}$$

$$M(\text{Np-237}) = \frac{M_0(\text{Am-241})\,\frac{AW(\text{Np-237})}{AW(\text{Am-241})}\,k_1\,A_2}{(k_2 - k_1)\,A_1}\left[e^{-k_1 t} - e^{-k_2 t}\right]$$

$$M(\text{U-233}) = \frac{A_3\,k_1\,k_2\,M_0(\text{Am-241})\frac{AW(\text{U-233})}{AW(\text{Am-241})}}{A_1} \times \left[\frac{e^{-k_1 t}}{(k_2 - k_1)(k_3 - k_1)} + \frac{e^{-k_2 t}}{(k_1 - k_2)(k_3 - k_2)} + \frac{e^{-k_3 t}}{(k_1 - k_3)(k_2 - k_3)}\right]$$

where:

| | | |
|---|---|---|
| $k_1$ | = | decay rate for Am-241 = 1.603E-03 $yr^{-1}$, |
| $k_2$ | = | decay rate for Np-237 = 3.238E-07 $yr^{-1}$, |
| $k_3$ | = | decay rate for U-233a and b = 4.372E-06 $yr^{-1}$, |
| $M_0$(Am-241) | = | Curies of Am-241 at TIME 0 = 10,000, |
| AW | = | atomic weight (amu), taken as 241, 237 and 233 respectively, |
| $A_1$ | = | specific activity of Am-241 = 3.44 Ci/g, |
| $A_2$ | = | specific activity of Np-237 = 7.06E-04 Ci/g, and |
| $A_3$ | = | specific activity of U-233 = 9.69E-03 Ci/g. |

Using t = 1,000 yr and the above constants, the results are 2,013 Ci for Am-241, 1.613 Ci for Np-237, and 4.423E-03 Ci for U-233. Since the U-233 portion is split evenly between two daughters, U-233a and U-233b each receive 2.2116E-3 Ci.

### 5.5.2 CT_Cells4-02: Radioactive Decay in a Cell with Solubility Limit

In this problem, the decay chain starting with Am-241 is examined. The problem is simply looking at decay over the first 1,000 yr. Am-241 decays to Np-237. To test split decay, two daughters are specified for Np-237, each receiving 50% of the mass. U-233a and U-233b each have identical properties. The analytical solutions for Am-241, Np-237 and U-233 are as follows (note that decay in the containers is a function of the timestep, with smaller timesteps producing more accurate results. A 2 year timestep is used in this case to exactly reproduce the analytical solution:

$$M(\text{Am-241}) = M_0(\text{Am-241})\, e^{-k_1 t}$$

$$M(\text{Np-237}) = \frac{M_0(\text{Am-241})\,\frac{AW(\text{Np-237})}{AW(\text{Am-241})}\,k_1\,A_2}{(k_2 - k_1)\,A_1}\left[e^{-k_1 t} - e^{-k_2 t}\right]$$

$$M(\text{U-233}) = \frac{A_3\,k_1\,k_2\,M_0(\text{Am-241})\frac{AW(\text{U-233})}{AW(\text{Am-241})}}{A_1} \times \left[\frac{e^{-k_1 t}}{(k_2 - k_1)(k_3 - k_1)} + \frac{e^{-k_2 t}}{(k_1 - k_2)(k_3 - k_2)} + \frac{e^{-k_3 t}}{(k_1 - k_3)(k_2 - k_3)}\right]$$

where:

| | | |
|---|---|---|
| $k_1$ | = | decay rate for Am-241 = 1.603E-03 $yr^{-1}$, |
| $k_2$ | = | decay rate for Np-237 = 3.238E-07 $yr^{-1}$, |
| $k_3$ | = | decay rate for U-233a and b = 4.372E-06 $yr^{-1}$, |
| $M_0$(Am-241) | = | Curies of Am-241 at TIME 0 = 10,000, |
| AW | = | atomic weight (amu), taken as 241, 237 and 233 respectively, |
| $A_1$ | = | specific activity of Am-241 = 3.44 Ci/g, |
| $A_2$ | = | specific activity of Np-237 = 7.06E-04 Ci/g, and |
| $A_3$ | = | specific activity of U-233 = 9.69E-03 Ci/g. |

Using t = 1,000 yr and the above constants, the results are 2,013 Ci for Am-241, 1.613 Ci for Np-237, and 4.423E-03 Ci for U-233. Since the U-233 portion is split evenly between two daughters, U-233a and U-233b each receive 2.2116E-3 Ci.

In addition to the description given above, a solubility constraint is imposed such that initially the cell is saturated. After some decay has taken place, it drops below the solubility limit.

Am-241 is given a solubility limit of 1,000 g/ $m^3$ in water. The concentration of Am-241 in the cell is in excess of this limit until sometime between 600 and 700 years.

### 5.5.3 CT_Cells4-03: Competing Decay Rates

In this problem, species A decays to species B, and species B decays to species A. This simulates an equilibrium between two species. The magnitude of the decay rates determines the ratio of species present in the cell. The stochiometry of the reaction is that A $\Leftrightarrow$ B.

To solve for the actual concentration of each species over time, the following equations can be used:

$$MA(t) = -k_f*mA(t) + k_r*(AWA / AWB)* mB(t)$$

$$MB(t) = -k_r*mB(t) + k_f*(AWB / AWA)* mA(t)$$

where:

| | | |
|---|---|---|
| $k_f$ | = | the forward reaction rate = 0.001 (1/yr); |
| $k_r$ | = | the reverse reaction rate = 0.0005 (1/yr); |
| AWA | = | the atomic weight of species A = 200 (g/mole); |
| AWB | = | the atomic weight of species B = 200 (g/mole); |
| mA(0) | = | the initial mass of species A = 0 (g); |
| mB(0) | = | the initial mass of species B = 400 (g). |

The resulting masses should be:

| Time, yr | A | B |
|---|---|---|
| 100 | 18.6 | 381.4 |
| 1,000 | 103.6 | 296.4 |
| 10,000 | 133.3 | 266.7 |

### 5.5.4 CT_Cells4-04: Stoichiometry

In this problem, species A decays to species B. The stoichiometry of the reaction is that A ⇔ 2B. There are initially 400g of A in the cell, with a decay rate of 0.001/yr.

To solve for the actual concentration of each species over time, the following equations can be used:

$$mA(t) = mA(0) \exp(-kf*t)$$

$$mB(t) = mB(0) + (b/a) * mA(0) * (1 - \exp(-kf*t))$$

The resulting masses should be:

| Time, yr | A | B |
|---|---|---|
| 100 | 361.9 | 76.1 |

| | | |
|---|---|---|
| 1,000 | 147.2 | 505.7 |
| 10,000 | 0.0182 | 800 |

## 5.6 CT_CELLS5 - TIME VARIABLE PARTITIONING AND MASS TRANSFER

In these problems, parameters controlling partitioning and mass transfer are time variable.

### 5.6.1 CT_Cells5-01 - Time Variable Partitioning Between Media in a Cell

This problem is identical to CT_Cells1-01, but at 5000 years, the partition coefficients change as follows:

| **Medium** | Partition Coefficient relative to WATER ($m^3/m^3$) for fluids; ($m^3/kg$) for solids |
|---|---|
| **WATER** | 1 |
| **OIL** | 0.2 |
| **SAND** | 0.4 |
| **CLAY** | 10 |

The resulting concentrations, before and after the change, are as follows:

| Medium | Am-241 ($g/m^3$) or (g/kg) | Am-242 ($g/m^3$) or (g/kg) | Am-243 ($g/m^3$) or (g/kg) |
|---|---|---|---|
| **WATER** | | | |
| **time = 4,900** | 2.59E-1 | 9.13E-2 | 4.45 |
| **time = 5,100** | 1.35E-1 | 4.78E-2 | 2.33 |
| **OIL** | | | |
| **time = 4,900** | 2.59E-2 | 9.13E-3 | 4.45E-1 |
| **time = 5,100** | 2.71E-2 | 9.56E-3 | 4.66E-1 |
| **SAND** | | | |
| **time = 4,900** | 5.17E-2 | 1.83E-2 | 8.90E-1 |
| **time = 5,100** | 5.41E-2 | 1.91E-2 | 9.32E-1 |
| **CLAY** | | | |
| **time = 4,900** | 1.29 | 4.57E-1 | 2.23E+1 |
| **time = 5,100** | 1.35 | 4.78E-1 | 2.33E+1 |
| | | | |

## 5.7 SOURCE TESTS

These problems test all aspects of the Sources, including associated cells linked to a source. These test problems are specifically targeted at verifying the basic source term functionality, including distributing and releasing mass to specified associated cells, sources in localized containers, and simple release from associated cells. In all cases the test problem files are set up with a single, non-decaying species. Each of 10,000 packages is assigned an inventory of 1 g.

### 5.7.1 CT_SourceBasic-01: Distribute Mass to Multiple Parallel Cells

In this problem, the mass at the source is exposed immediately and distributed evenly (in parallel) to four associated cells. Each of these cells in turn discharges to a different unassociated cell. The links between cells are all advective with very high flow rates, small cell volumes and infinite solubility cell solubility limits, insuring immediate release.

The cumulative release from the source to each of the cells should be equal to 2500g. The final mass in each of the unassociated cells should equal 2500 g.

### 5.7.2 CT_SourceBasic-02: Distribute Mass to a Single Cell

This problem is identical to CT6-1, but the mass is only distributed to the first of the four associated cells.

The cumulative release to the first cell should be 10,000g. The final mass in the first unassociated cell should be 10,000g, and 0g in the other unassociated cells.

### 5.7.3 CT_SourceBasic-05: Simple Advective Release from Associated Cells

In this problem a source discharges to a single associated cell. It tests the scaling of advective fluxes from associated cells. The source contains 10,000 packages which fail uniformly over 50 years. The cell contains 10 $m^3$ of water, which discharges at a rate of 4 $m^3/yr$. The solubility is specified as very small (such that release is linearly controlled by the advective release, which is in turn scaled by the number of failed containers). The simulation is run for 100 years. The time history of the source release rate should increase linearly with time, and become constant at 50 years.

The release rate from the source, M(t) [g/yr], at time t for an associated cell with a single media and a concentration above the saturation limit is computed as follows:

$$M(t) = Q * C_{sat} * NFail(t)$$

where:

Q = the flow rate of the advective connection [$m^3/yr$] = 4;

Csat = the saturation concentration for species A1 [$g/m^3$] = 1E-6;

NFail(t) = the rate of container failure [-]
= 10,000/50*t = 200*t for 0 <= t <= 50;
= 10,000 otherwise.

M(10) = (4 [$m^3/yr$])*(1E-10 [$g/m^3$])*(200*10) = 8.0E-7 g/yr

M(20) = (4 [$m^3/yr$])*(1E-10 [$g/m^3$])*(200*20) = 1.6E-6 g/yr

M(50) = (4 [$m^3/yr$])*(1E-10 [$g/m^3$])*(200*50) = 4.0E-6 g/yr

Note that GoldSim results may be off at the third decimal place, since when a solubility limit is reached, the solubility can be fixed at 0.999 of the solubility limit.

### 5.7.4 CT_SourceDecay-1: Decay within a Source

In this problem, the decay chain starting with Am-241 is examined. Mass is exposed and then released instantaneously from the containers at TIME = 1,000. Therefore, the problem is simply looking at decay within the source over the first 1,000 yr. Am-241 decays to Np-237. To test split decay, two daughters are specified for Np-237, each recieving 50% of the mass. U-233 and V-233 each have identical properties.

The analytical solutions for Am-241, Np-237, U-233 and V-233 are as follows:

$$M(\text{Am-241}) = M_0(\text{Am-241})\, e^{-k_1 t}$$

$$M(\text{Np-237}) = \frac{M_0(\text{Am-241})\,\frac{AW(\text{Np-237})}{AW(\text{Am-241})}\,k_1\,A_2}{(k_2 - k_1)\,A_1}\left[e^{-k_1 t} - e^{-k_2 t}\right]$$

$$M(\text{U-233}) = \frac{A_3\,k_1\,k_2\,M_0(\text{Am-241})\frac{AW(\text{U-233})}{AW(\text{Am-241})}}{A_1} \times \left[\frac{e^{-k_1 t}}{(k_2 - k_1)(k_3 - k_1)} + \frac{e^{-k_2 t}}{(k_1 - k_2)(k_3 - k_2)} + \frac{e^{-k_3 t}}{(k_1 - k_3)(k_2 - k_3)}\right]$$

where:

k1 = decay rate for Am-241 = 1.603E-03 yr-1,
k2 = decay rate for Np-237 = 3.238E-07 yr-1,
k3 = decay rate for U-233a and b = 4.372E-06 yr-1,
$M_0$(Am-241) = Curies of Am-241 at TIME 0 = 10,000,
AW = atomic weight (amu), taken as 241, 237 and 233 respectively,
A1 = specific activity of Am-241 = 3.44 Ci/g,
A2 = specific activity of Np-237 = 7.06E-04 Ci/g, and
A3 = specific activity of U-233 = 9.69E-03 Ci/g.

Note that within the source, the mass that is released during a timestep is only decayed for half of that timestep. A 10 year timestep is used in this case. Using t = 995 yr and the above constants, the results for "exposed mass" are 2,029 Ci for Am-241, 1.610 Ci for Np-237, and 2.194E-03 Ci for U-233 and V-233. The associated cell, however, decays the mass for the balance of the timestep in which it is received (990 to 1000yrs). As a result, the mass in the cell at 1000 yrs should equal the exact solution of 2,012.9 Ci for Am-241, 1.613 Ci for Np-237, and 2.212E-03 Ci for U-233 and V-233.

## 5.8 CT_PLUME

This file verifies the plume function. The test problem considers several combinations of source and aquifer geometry for a dissolved-contaminant groundwater plume. Other input parameters for the plume function are contained in the test file. GoldSim's plume function is verified by comparing results to those obtained from TPlume (Golder 1991), which uses the Domenico and Robbins (1985) solution.

The test proceeds as follows. Run the model. View the results shown in **Table CT_PLUME_FUNCTION_1** below and ensure that the results match the expected GoldSim results.

Table CT_PLUME_FUNCTION_1

| Container | Element | Expected GoldSim output at 1,000 days ($g/m^3$) | TPlume value at 1,000 days ($g/m^3$) |
|---|---|---|---|
| PointSource_ThickAquifer | XConc | 0.0154 | 0.0154 |
| PointSource_ThinAquifer | XConc | 0.0461 | 0.0477 |
| AreaSource_ThickAquifer | XConc | 0.0154 | 0.0153 |
| AreaSource_ThinAquifer | XConc | 0.0462 | 0.0478 |

Notes:

1. GoldSim differs from TPlume for the thin-aquifer case because GoldSim has a more accurate solution for thin aquifers (i.e., reflections vs. assumed vertical mixing).
2. The assumed source geometry is a point source at the groundwater table (PointSource), or a vertical rectangle with a depth equal to half the width, oriented perpendicular to the flow direction, and with the top at the groundwater table.
3. The observation point for the concentration is 50 m downgradient from the source, 25 m off the plume centerline horizontally, and 10 m below the groundwater table (i.e., x = 50m, y = 25m, and z = 10m).
4. This verification includes no decay or retardation.

Distribution

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