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Code-to-Code Benchmarking of the PORFLOW and GoldSim Contaminant Transport Models using a Simple 1-D Domain - 11191

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ABSTRACT

An investigation was conducted to compare and evaluate contaminant transport results of two model codes, GoldSim and PORFLOW, using a simple 1-D string of elements in each code. Model domains were constructed to be identical with respect to cell numbers and dimensions, matrix material, flow boundary and saturation conditions. One of the codes, GoldSim, does not simulate advective movement of water; therefore the water flux term was specified as a boundary condition. In the other code, PORFLOW, a steady-state flow field was computed and contaminant transport was simulated within that flow-field. The comparisons were made solely in terms of the ability of each code to perform contaminant transport. The purpose of the investigation was to establish a basis for, and to validate follow-on work that was conducted in which a 1-D GoldSim model developed by abstracting information from PORFLOW 2-D and 3-D unsaturated and saturated zone models and then benchmarked to produce equivalent contaminant transport results. Although prior validation and verification work has been conducted for both PORFLOW and GoldSim [2, 4, 5] a direct comparison of results from both codes, when evaluating the same model domain, was conducted to confirm this work and justify the benchmarking exercises that compared 1-D to multi-dimensional models.

A handful of contaminants were selected for the code-to-code comparison simulations, including a non-sorbing tracer and several long- and short-lived radionuclides exhibiting both non-sorbing to strongly-sorbing characteristics with respect to the matrix material, including several requiring the simulation of in-growth of daughter radionuclides. The same diffusion and partitioning coefficients associated with each contaminant and the half-lives associated with each radionuclide were incorporated into each model. A string of 10-elements, having identical spatial dimensions and properties, were constructed within each code. GoldSim's basic contaminant transport elements, Mixing cells, were utilized in this construction. Sand was established as the matrix material and was assigned identical properties (e.g. bulk density, porosity, saturated hydraulic conductivity) in both codes. Boundary conditions applied included an influx of water at the rate of 40 cm/yr at one end of the string and no-flow lateral flow boundaries. A unit quantity of each contaminant was introduced at the influx boundaries and the rate of outflux at the opposite end of the 10-element string was recorded to make the comparisons. Saturated conditions were assumed in this evaluation. Under these carefully controlled conditions the two codes produced essentially identical results, demonstrating that both codes appear to be accurately implementing the contaminant transport mechanisms. The conclusion is that a satisfactory basis was established to justify the exercise in which 1-D GoldSim model was benchmarked against the 2-D unsaturated zone and 3-D saturated zone PORFLOW models used at the Savannah River Site (SRS).

INTRODUCTION

The two modeling codes utilized in this study are PORFLOW version 5.97 [1] and GoldSim version 10.11 [3]. PORFLOW is a commercially available computer code developed by ACRi, Inc, and acquired by the Savannah River National Laboratory (SRNL) for use in simulating ground water flow and contaminant transport in the vadose zone and underlying aquifers. The PORFLOW software package is a comprehensive mathematical model for simulation of multi-phase fluid flow, heat transfer and mass transport in variably saturated porous and fractured media. The porous medium may be anisotropic and heterogeneous and may contain discrete fractures or boreholes with the porous matrix. The main features of PORFLOW that are relevant to Performance Assessment (PA) modeling at SRNL include variably saturated flow and transport of parent and progeny radionuclides. Testing a relevant sample of problems in PORFLOW and comparing the outcome of the simulations to analytical solutions or other commercial codes has been conducted and is documented in [2].

The second modeling code, GoldSim, is a highly graphical, object-oriented computer program for carrying out dynamic, probabilistic simulations. GoldSim can represent uncertainty in processes, parameters and future events. The GoldSim Radionuclide Transport (RT) Module is a program extension to the GoldSim simulation framework that allow the user to dynamically model radionuclide transport within complex engineered and/or natural environmental systems. Although not required for purchased QA Level C software, the GoldSim Technology Group (GTG) has developed an extensive and thorough testing program for GoldSim that is available for review [4]. Verification and validation testing demonstrates that the software is functioning as intended 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 using test cases representative of the range of conditions expected in the actual analysis. Acceptance testing conducted at SRNL [5] verified that the same results were obtained for test problems defined and tested by GTG [4].

The Savannah River National Laboratory has developed a “hybrid” approach to Performance Assessment (PA) modeling, using these two codes, which has been used for a number of PAs. [6] The hybrid approach uses a multi-dimensional modeling platform, PORFLOW version 5.97 [1], to develop deterministic flow fields and to perform contaminant transport simulations. The GoldSim [3] modeling platform is used to perform the Sensitivity and Uncertainty analyses that are also a part of PA investigations. A key difference in the development of the deterministic flow field models (PORFLOW) and the Sensitivity and Uncertainty models (GoldSim) is in dimensionality, where the flow field models are 2-D for the unsaturated zone (UZ) and 3-D for the saturated zone (SZ) while the equivalent Sensitivity and Uncertainty models are 1-D or pseudo-2-D. Because these codes are performing complementary tasks, it is incumbent upon them that for the deterministic cases they produce very similar results. To demonstrate the comparability of deterministic results from both models, a benchmarking exercise was conducted.

Prior to performing this benchmarking study, however, an investigation was conducted to demonstrate that the two codes, PORFLOW and GoldSim, implement the processes of radioactive decay, contaminant transport retardation via the partitioning coefficient (or K_d) concept, and implementation of solubility limits accurately and consistent from one code to the other. This code-to-code comparison is the subject of this investigation and its purpose is to validate the follow-on benchmarking of deterministic results by demonstrating that the codes produce comparable results. The follow-on benchmarking work was accomplished through

abstracting information from PORFLOW 2-D and 3-D unsaturated and saturated zone models so as to form the basis of input to the 1-D equivalent contaminant transport model in GoldSim.

In performing the code-to-code comparison, a simple, 1-D, transport model was established and implemented within both codes. The implementations were identical with respect to noding, material properties, boundary and initial conditions, and temporal discretization (time steps). One of the codes, GoldSim, does not simulate advection of water therefore the water flux term was specified as a boundary condition. In the other code, PORFLOW, a steady-state flow field was computed and contaminant transport was simulated within that flow-field. The comparisons were made solely in terms of the ability of each code to perform contaminant transport.

A handful of contaminants were selected for the code-to-code comparison simulations, including a non-sorbing tracer and several long- and short-lived radionuclides exhibiting both non-sorbing to strongly-sorbing characteristics with respect to the matrix material, including several requiring the simulation of in-growth of daughter radionuclides. The same diffusion and partitioning coefficients associated with each contaminant and the half-lives associated with each radionuclide were incorporated into each model. Following the comparison, a case study illustrating a potential pitfall, when solubility constraints are factored into the analysis, is presented.

MODEL DEVELOPMENT AND DESCRIPTION

The simple Base Case model was a column of 10 computational elements populated with sand. An illustration of this model domain is presented in Figure 1. The dimensions of individual computational cells were established at 1m x 1m x 1cm. The overall length of the 10-cell column was therefore 10m. The lateral boundaries of the domain were established as Neumann boundaries, with flux = 0 (no-flow boundaries), and one end of the column assigned a Dirichlet boundary condition with a specified influx of 40 cm/yr. Under these boundary conditions, the water flux exiting the domain through the bottom end is equal to the specified flux at the influx end. A group of contaminants species were introduced at the influx end and the contaminant mass fluxes at the exit end of the column were evaluated. The contaminant species included a tracer (non-radioactive, non-retarded), ^{14}C, ^{3}H, ^{99}Tc, ^{233}U and ^{234}U. PORFLOW simulations evaluated each species individually, allowing in-growth of daughter radionuclides, although the code has the capability to simulate all of the radionuclides simultaneously. GoldSim simulations evaluated all species in a single simulation and also accommodated in-growth of daughter radionuclides. Saturated conditions were established in both codes.

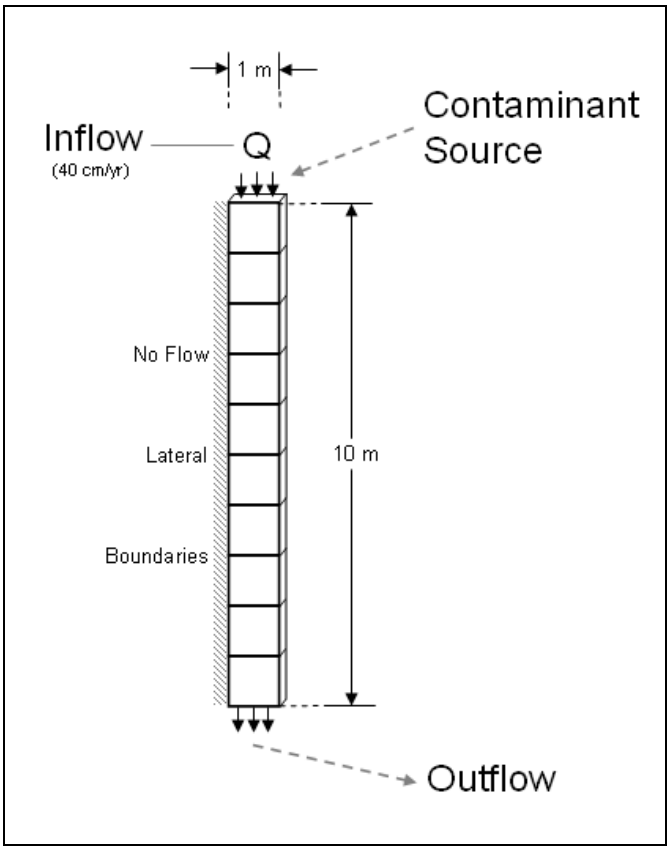


Figure 1. Conceptual model implemented within PORFLOW and GoldSim

Materials present within the computational elements included sand and water. The sand was defined as having a porosity of 0.39, a particle density of 2.66 g/cm^3 (or bulk density = 1.62 g/cm^3), and diffusivity of 167.25 cm^2/yr. Advective and diffusive transport of contaminants was enabled within both codes. A summary of the radionuclides simulated, their half-lives, K_d's and relevant progeny are presented in Table I.

BASE CASE TRANSPORT ANALYSIS

Transport simulations were conducted for a nominal period of 0-1000 years. In the case of the mobile contaminants, tracer, ^{14}C, ^{3}H, ^{14}H, and ^{99}Tc, the peak concentration fluxes occur at time periods less than 20-years, hence PORFLOW simulations were conducted from 0-200 years with time-steps established at 0.1 years. The less-mobile parent radionuclides, ^{233}U and ^{234}U, were simulated for the full period of 0-1000 years, also with time-steps set to 0.1 years. Within GoldSim, time-steps were established at 0.1 years for the period 0-80 years then increasing the time-steps to 0.5 years for the time-period of 80-1000 years.

A unit quantity (1 mole) of each contaminant was introduced at the influx boundaries and the rate of outflux at the opposite end of the 10-element string was recorded to make the comparisons. Saturated conditions were assumed in this evaluation.

Table I . Contaminant species evaluated and relevant transport properties

	Half Life (yrs)	K_d in Sand (ml/g)	Progeny
Tracer	n/a	0	
^{14}C	5.73E+03	0	
^{3}H	1.23E+01	0	
^{99}Tc	2.11E+05	0.1	
^{233}U	1.59E+05	200	^{229}Th
^{234}U	2.46E+05	200	$^{230}Th \rightarrow ^{226}Ra \rightarrow ^{210}Pb$
^{229}Th	7.34E+03	900	
^{230}Th	7.55E+04	900	$^{226}Ra \rightarrow ^{210}Pb$
^{226}Ra	1.6E+03	5	^{210}Pb
^{210}Pb	2.22E+01	2000	

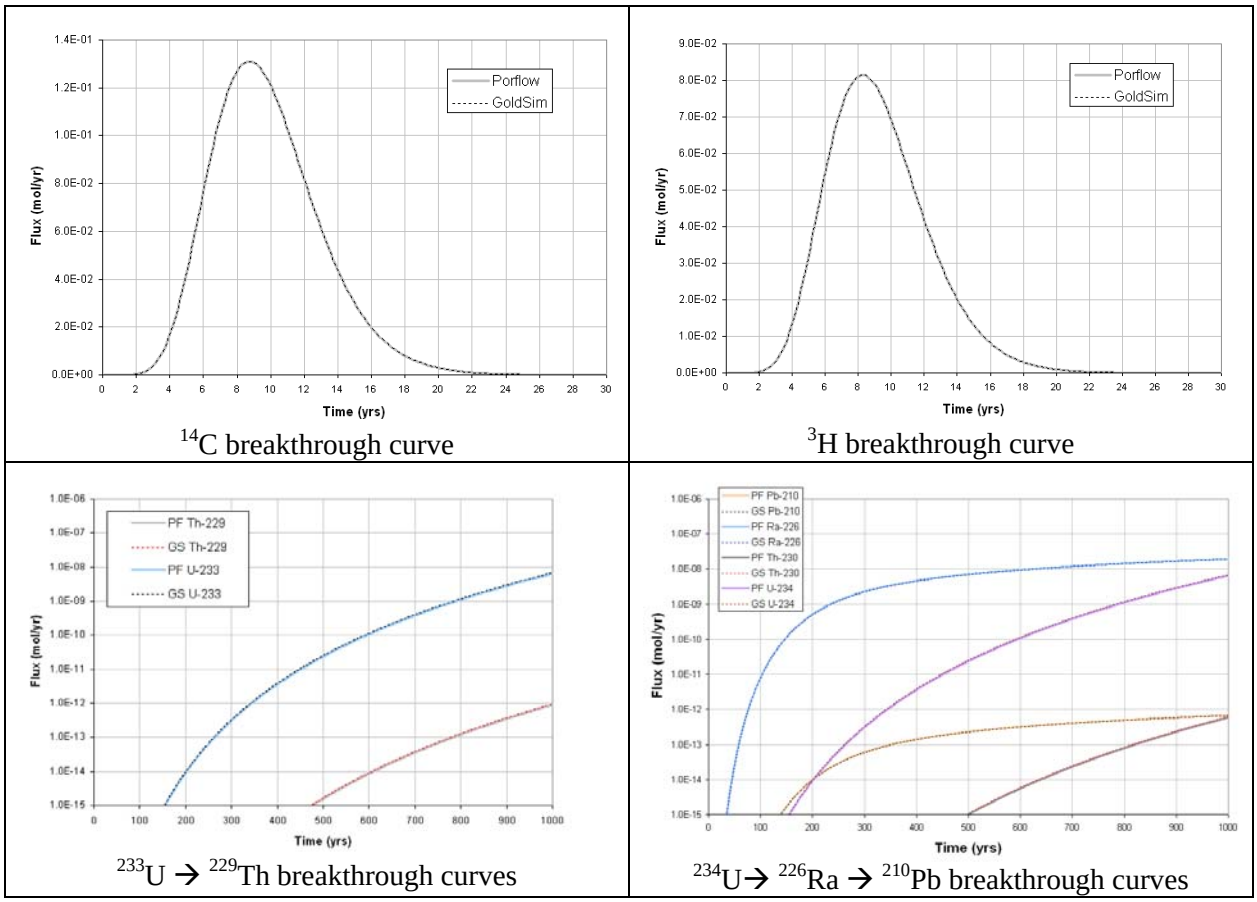
Note: Radionuclide species listed in gray text were progeny of the parent species. Their presence in the simulation was due strictly to in-growth.

The results from both model codes were directed into an Excel file where graphs could be created to illustrate the breakthrough concentration profile for each contaminant and where the results from both codes could easily combined into a single graph. The results for selected radionuclides are shown in Figure 1. Note that the breakthrough concentration curves for two mobile contaminant species, ^{14}C and ^{3}H are depicted, along with the two less-mobile parent species, ^{233}U and ^{234}U. For ^{233}U and ^{234}U, the daughter species are also illustrated. On each of the sub-graphs, the breakthrough concentration profiles are illustrated for output from both transport codes. Strictly speaking, the transport calculations presented here apply to fully saturated conditions however identical results are also obtained when unsaturated conditions have also been evaluated. The striking feature of these results is how closely the curves track, all within the width of the lines used to illustrate the results.

SOLUBILITY CONSTRAINED TRANSPORT ENVIRONMENT

Beyond the Base Case comparison, in which the ability to implement radioactive decay and contaminant transport in accordance with the K_d concept, a comparison was made of the ability of each code, PORFLOW and GoldSim, to impose a solubility limit. Again, the Base Case model domain, material properties and other assumptions were retained, with the only change being the imposition of the solubility limit. An arbitrary concentration limit for ^{99}Tc of 1200 mg/L was selected and an arbitrarily high source term of 1.0E+06 moles of ^{99}Tc were introduced into the model to ensure that dissolved concentrations would exceed the imposed concentration limit.

The simulation results from both codes produced identical breakthrough curves, approaching the solubility limit at approximately 27 years. The graph indicating results from both GoldSim and PORFLOW is presented in Figure 2. The concentration breakthrough curves for both codes, PORFLOW and GoldSim, gradually increase over the first ~20 years of the simulation until they approach the concentration limit at approximately 25 years. The concentration curves track extremely close to one another and such adherence indicates that both codes correctly implement solubility constraints.



^{14}C breakthrough curve

^{3}H breakthrough curve

$^{233}U \rightarrow {}^{229}Th$ breakthrough curves

$^{234}U \rightarrow {}^{226}Ra \rightarrow {}^{210}Pb$ breakthrough curves

Figure 2. Concentration curves for parent radionuclides ^{14}C, ^{3}H, ^{233}U and ^{234}U

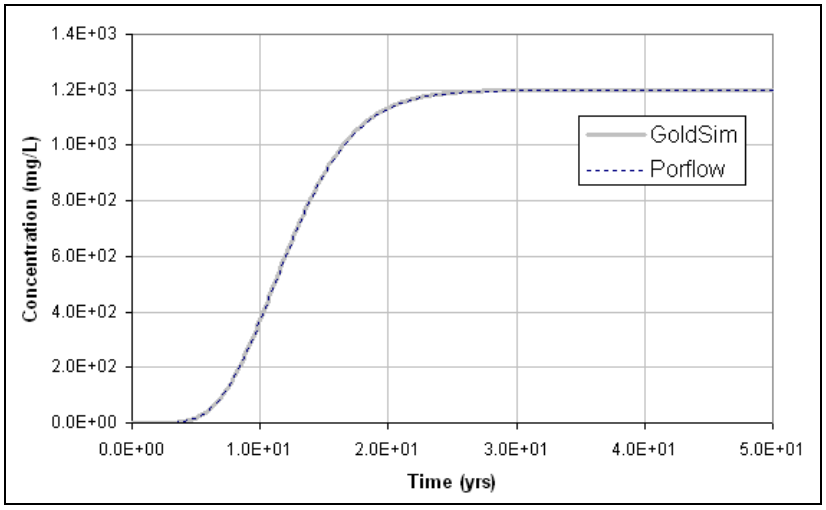


Figure 3. Imposition of a solubility constraint for ^{99}Tc and resulting concentrations

POTENTIAL PITFALL IN SOLUBILITY CONSTRAINED ENVIRONMENTS

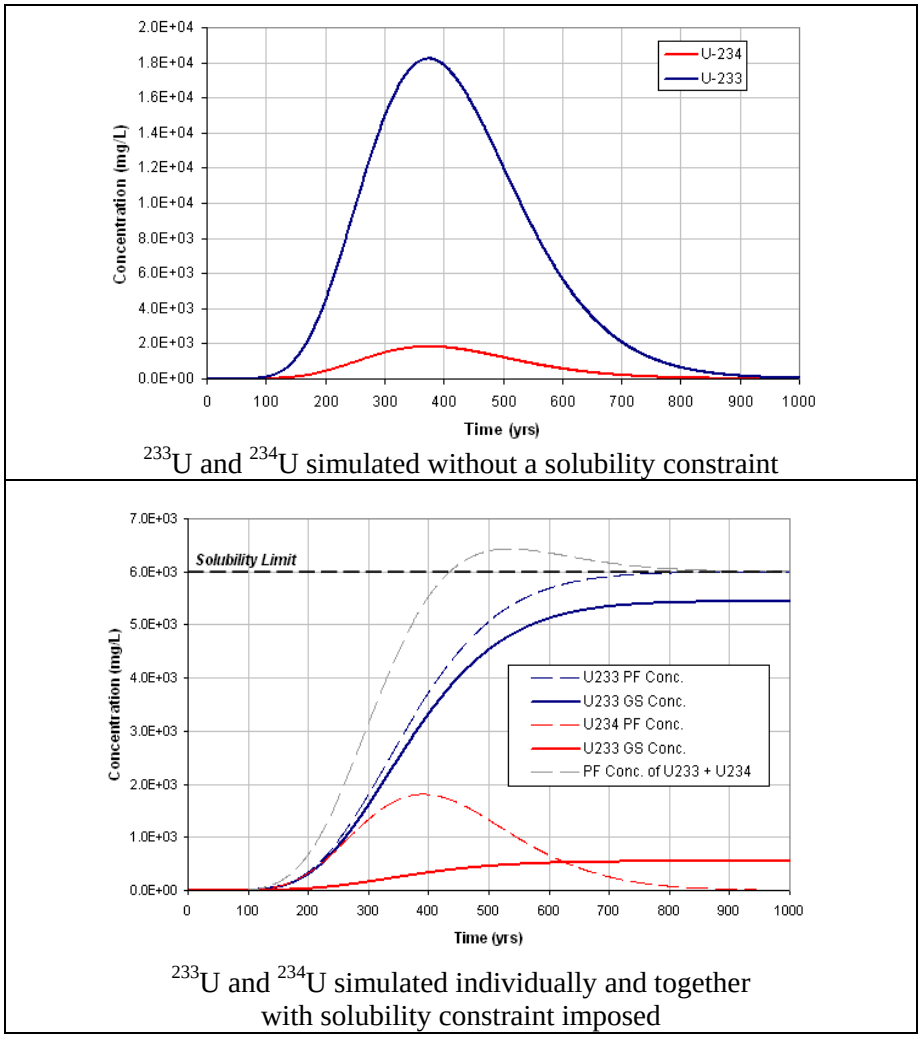
A potential pitfall in PA type analyses that establish facility disposal limits through performing simulations of the groundwater pathway, as is the case at SRS, exists and needs to be avoided. The potential pitfall occurs when contaminant concentrations are sufficient that the solubility limit for that element becomes a factor. When isotopes of the same element are simulated separately and are constrained independently by the solubility limit, the calculated concentrations are different than if both isotopes are simulated simultaneously in the presence of the solubility limit. In previous investigations at SRS, simulations of contaminant species were performed separately for all parent radionuclides of interest. Originally, this approach was dictated by a code limitation; however that limitation has since been rectified.

Additionally, it is not uncommon for one parent radionuclide to decay into one of the other radionuclides of interest as it proceeds through its decay chain, also creating a vulnerability to the same pitfall. An example of this is represented by the different Pu isotopes, each of which decays and produces different U isotopes, some of which are being evaluated individually as parent radionuclides. Using these radionuclides as an example, when an anticipated facility waste inventory contains both Pu isotopes and U isotopes the total mass of either Pu or U present in the system at any time cannot easily be evaluated without carefully summing up the mass of U in the system, at all times, from multiple simulations, as well as keeping track of the residual saturation in order to convert Pu and/or U mass to concentration in pore water. The determination of whether the solubility limit is approached anywhere within the transport zones must be determined external to the transport code, which is time-consuming and prone to the introduction of errors.

The following hypothetical case was evaluated to illustrate this pitfall. Two Uranium isotopes, ^{233}U and ^{234}U were simulated separately as the parent radionuclides within the PORFLOW code using the Base Case model domain and the contaminant transport parameters and conditions identified earlier. This approach was undertaken to illustrate a point, even though PORFLOW has the capability to simulate all of the radionuclides simultaneously and invoke a solubility limit on an element by element basis. The ^{233}U source term was set to 100 moles and the ^{234}U source term was set to 10 moles. Each parent was initially simulated without a solubility constraint imposed upon the system and the concentration results of these simulations are illustrated in the upper illustration if Figure 4. The peak concentration of ^{233}U was 1.82E+04 mg/L and for ^{234}U was 1.82 E+3 mg/L.

Then a parallel simulation was performed using the GoldSim code. All conditions were duplicated except for the fact that both parent isotopes, ^{233}U and ^{234}U, were simulated together, simultaneously within the same model run. As expected, the PORFLOW results were identical to the GoldSim results for both radionuclides, as illustrated in the upper part of Figure 4.

Then a solubility constraint was implemented within each model and the simulations repeated. The solubility limit of 6.0E+3 mg/L was selected because it fell between the peak concentrations that were realized for ^{233}U and ^{234}U. The results produced from these individually simulated radionuclides and simultaneously simulated radionuclides were very different. These results are shown in the lower part of Figure 4.



^{233}U and ^{234}U simulated without a solubility constraint

^{233}U and ^{234}U simulated individually and together with solubility constraint imposed

Figure 4. ^{233}U and ^{234}U simulated without solubility constraint

In this graph, the PORFLOW (individual) results are illustrated using dashed lines and GoldSim (simultaneous) results are shown using the solid lines. The PORFLOW simulated concentration profile for ^{233}U approaches the solubility limit (6.3 E+3 mg/L) while the concentration profile for ^{234}U is identical to the ^{234}U profile realized in the absence of the solubility limit and determined to be 1.82E+03 mg/L. When the concentrations ^{233}U and ^{234}U from these separate realizations are totaled together, the combined concentration profile actually exceeds the solubility limit for a period of time.

The GoldSim results, illustrated by the solid blue and red lines, both increase over time until they level off, as constrained together by the solubility limit. When the sum of the concentrations for both ^{233}U and ^{234}U are tracked through time, the total concentration approaches the solubility limit, never exceeding it. Individually, the maximum concentrations for ^{233}U and ^{234}U were calculated to be 5.44E+03 and 5.48E+02 mg/L, respectively, both concentrations significantly less than the maximum concentrations calculated in the separate, independent simulations

performed for the two U isotopes using PORFLOW. In this hypothetical case, the differences are calculated to be approximately 14% and 70% less than concentrations realized in the independent simulations of the two U isotopes. This serves to underscore the point that multiple isotopes must be simulated together in the presence of a solubility limit that impacts the concentrations of the elemental form of the isotopes in order to obtain accurate results.

A similar situation can occur when a particular parent is simulated within an individual model simulation, and a different parent (simulated separately) produces an ingrowth of the former parent radionuclide as it undergoes radioactive decay through time. Such a relationship occurs, for example with ^{238}Pu and ^{234}U, two radionuclides often found in SRS disposal facility anticipated closure inventories or already disposed within them.

It should be pointed out that recent PORFLOW versions have incorporated the capability to apply solubility limits by chemical element as well as by specific isotope of elements, thus providing a means to avoid the pitfall. That capability did not exist in earlier versions, which led to the practice at SRS of evaluating each parent radionuclide in separate simulations. This example is provided simply to underscore the importance in performing simulations of all species of a given element simultaneously, in the same simulation.

CONCLUSIONS

The code-to-code comparison of GoldSim with PORFLOW was undertaken using an identically configured model domain, material properties and boundary conditions built into each model. The main difference in the codes is that PORFLOW computes subsurface flux terms while GoldSim does not, therefore, the GoldSim models had flux terms prescribed that were identical to those computed in PORFLOW. Beyond this, the mechanisms of radioactive decay, partitioning of contaminants between solid and fluid, implementation of specific boundary conditions and the imposition of solubility controls were all tested. The results of the comparison indicate that identical results were obtained from both codes. Issues of temporal and spatial discetization were not addressed in this evaluation by virtue of the fact that time-step increments and node dimensions and numbers were kept the same. It is assumed that differences in noding and time-stepping schemes can potentially produce significantly differences results, although this line of investigation was not pursued in this study. Finally, based on evaluating identical models, it is concluded that the use of GoldSim to develop 1-D equivalent models of the PORFLOW multi-dimensional models is justified.

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