Abstraction of Information from 2- and 3-dimensional PorFlow Models into a 1-D GoldSim Model- 11404

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ABSTRACT

The Savannah River National Laboratory has developed a "hybrid" approach to Performance Assessment modeling which has been used for a number of Performance Assessments. This hybrid approach uses a multi-dimensional modeling platform (PorFlow) to develop deterministic flow fields and perform contaminant transport. The GoldSim modeling platform is used to develop the Sensitivity and Uncertainty analyses. Because these codes are performing complementary tasks, it is incumbent upon them that for the deterministic cases they produce very similar results. This paper discusses two very different waste forms, one with no engineered barriers and one with engineered barriers, each of which present different challenges to the abstraction of data.

INTRODUCTION

The hybrid approach to Performance Assessment modeling used at the SRNL uses a 2-D unsaturated zone (UZ) and a 3-D saturated zone (SZ) model in the PorFlow modeling platform. The UZ model consists of the waste zone and the unsaturated zoned between the waste zone and the water table. The SZ model consists of source cells beneath the waste form to the points of interest. Both models contain "buffer" cells so that modeling domain boundaries do not adversely affect the calculation. The information pipeline between the two models is the contaminant flux. The domain contaminant flux, typically in units of moles (or Curies) per year from the UZ model is used as a boundary condition for the source cells in the SZ.

The GoldSim modeling component of the hybrid approach is an integrated UZ-SZ model. The model is a 1-D representation of the SZ, typically 1-D in the UZ, but as discussed below, depending on the waste form being analyzed may contain pseudo-2-D elements.

A waste form at the Savannah River Site (SRS) which has no engineered barriers is commonly referred to as a slit trench. A slit trench, as its implies, is an unlined trench, typically 6 m deep, 6 m wide, and 200 m long. Low level waste consisting of soil, debris, rubble, wood, etc. is disposed within the trench which is then covered with soil and a cap. The filled trench resembles the surrounding soil, albeit with a higher porosity. As a result, the flow field through the trench is essentially 1-dimensional. This dimensionality makes the abstraction of information from this waste form fairly simple.

Engineered waste forms present challenges not seen in the slit trench because of their higher dimensionality. Flow fields must conform to the barriers and are therefore subject

to changes in direction. This paper will examine one case and show how this multi-dimensional flow field can be abstracted into a 1-dimensional flow field while retaining characteristics important to the transport of radioactive contaminants.

One complication not addressed by the two preceding examples is that of multiple sources. This presents quite a challenge to the benchmarking exercise, but a fairly robust method has been developed to deal with it. While the PorFlow analyses can treat all sources as independent in space, this is not possible with a 1-D model. This problem has been addressed by constructing multiple 1-D models of the waste forms and using plume overlaps at the assessment points to address the multiple sources which can contribute to a distinct assessment point.

Why model?

Modeling is performed in order to develop an understanding of the physical system. When one model is used to analyze a physical system, the description of the behavior of the physical system is constrained by all the assumptions inculcated by the strictures of the modeling environment. The hybrid system used at the Savannah River Site uses two modeling platforms, and even though each has its own strictures, in the end one has two very independent models. When these models are compared, as they are in benchmarking, any differences in system behavior must be explained. This requires the analyst to fully understand both the physical system and the modeling environments.

Another way this could be looked at is in terms of a technical review of the models. One typical method of review is to run an independent calculation. This is exactly what is done in benchmarking. If neither model is accepted as the "truth", then, as above, differences in results must be explained. Again, this leads the analyst to a deeper understanding of the models and their results.

What to benchmark?

With many different physical processes being modeled, how does one choose which processes to be benchmarked? If one looks at the purpose of the analysis and then works backwards, it becomes fairly obvious. For a Performance Assessment, the parameter of interest is the dose at a compliance point. If one ignores the details of the dose calculation, the parameter of interest becomes the concentration of a radionuclide at the compliance point. While it may be possible to benchmark to this one parameter, it is not likely that one would obtain meaningful results due to the large number of independent variables in a typical PA. Looking back into the model's "information pipeline", the choice of another benchmarking point becomes obvious.

The SRS PA PorFlow model consists of two distinct modules. There is a 2-D UZ and a 3-D SZ. The information pipeline between these two modules is the total contaminant flux crossing the computational boundary. The complementary GoldSim model is 1-D with the UZ and the SZ being contained in a single module. Since the information pipeline in the PorFlow model is the flux between the UZ and SZ, it becomes an obvious,

and convenient, location for another benchmarking point. It also makes sense in that if one is able to benchmark the flux at the UZ-SZ interface, then SZ to compliance point benchmarking has a much better chance of being realistically benchmarked.

Now that we know what we wish to benchmark, the question is what data is needed from the PorFlow model so that the GoldSim model can perform similarly?

Flow data abstraction

Flow data must be abstracted from PorFlow as it is a flow and transport code while GoldSim is a transport code. Figure 1 shows examples of two waste forms. The slit trench consists of materials which all have approximately the same permeabilities. This leads to a flow field which is essentially uniform and 1-dimensional. The vault consists of materials in which the permeabilites vary by orders of magnitude. This gives a much more complicated flow field (as shown in Figure 2). All flow data are abstracted from the vertical velocity component only.
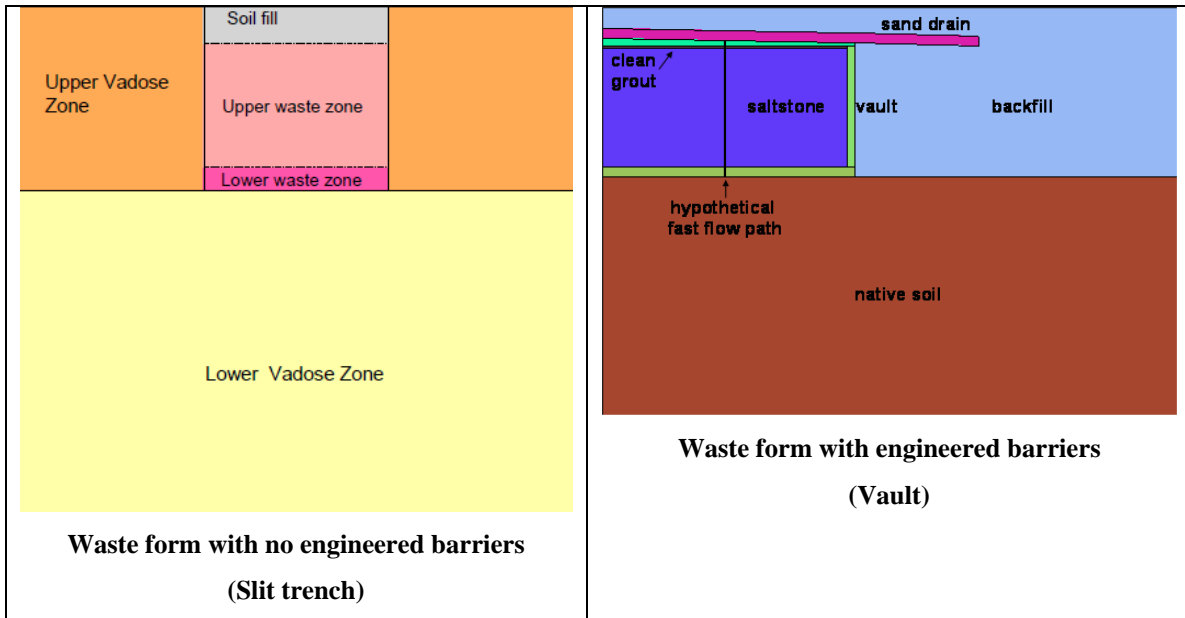
Figure 1 Examples of waste forms

The paradigm for abstracting flow data is to sample the data at various vertical and horizontal locations. Since the slit trench is a symmetric model, a regular sampling pattern could be established with multiple locations sampled in each of the material zones. The vault model represents half the waste form, so it is asymmetric. Again, data sampling was performed in each of the materials at multiple locations. The GoldSim model's top boundary elevation was the clean/contaminated grout interface so no data were sampled in the clean grout or the sand drain. However, as can be seen in Figure 2, the sand drain greatly affects the flow pattern in the backfill adjacent to the vault and this was accounted for in the sampling of that region.
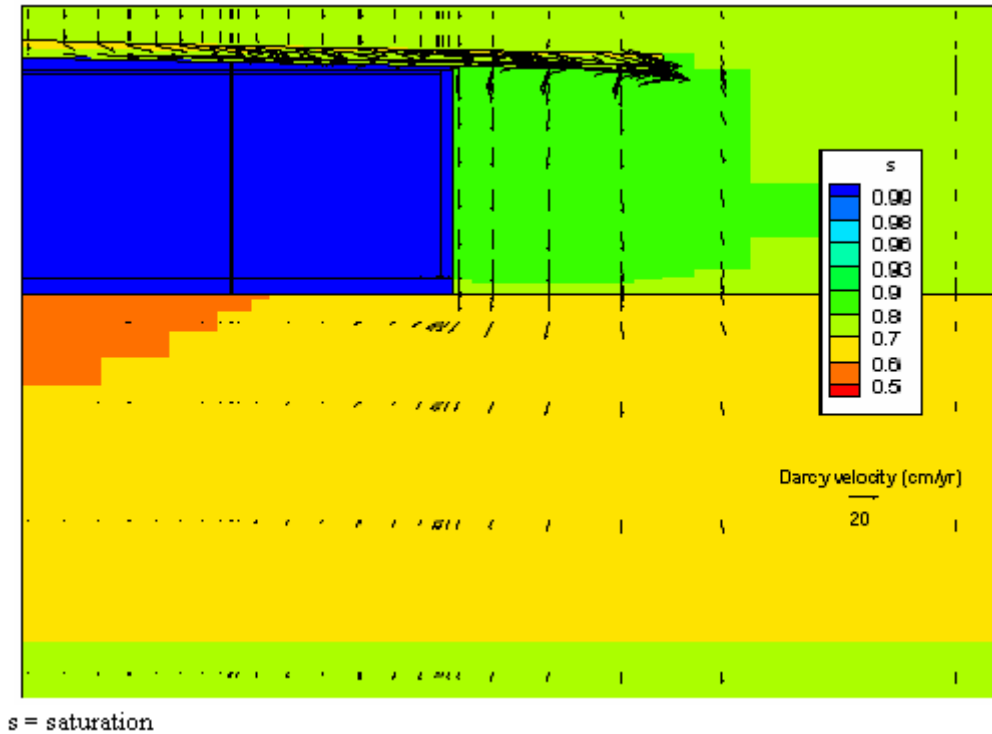
s = saturation

Figure 2 Vault flow field and saturation profile

Once the data are obtained, something must be done with it. At this point, the analyst must apply his knowledge of the system behavior to what is the best way to use the data. A common sense approach is initially to use the simplest approach. The simplest may not be sufficient and may lead to different attempts as to what approach will provide adequate results.

The simplest approach would be to use a single, uniform velocity in the GoldSim model to simulate the multidimensional PorFlow flow field. This approach works for the slit trench. (Note that because of the scenarios analyzed, advective transport was always much greater than diffusive transport.) Figure 3 shows the abstracted data. PorFlow runs a steady-state flow calculation for each of its steady-state time periods, hence the stack of data points at discrete times. The "j=" indicates elevation. When the data were examined, if one looked at a horizontal slice, the flows appeared fairly uniform. Therefore, each elevation data point represents an average value for all points sampled at that elevation. The geometric mean of the elevations' flows was used as the first attempt at benchmarking.   When the single value (the geometric mean) was applied to all the flow paths in the UZ, an example of which is shown in Figure 4, the benchmarking agreement with the PorFlow material flux was quite good. Therefore, this abstraction was deemed sufficient for the benchmarking to proceed.

The example of GoldSim vault model shown in Figure 4 is the result of several iterations of abstraction and benchmarking. From a cursory examination of the raw PorFlow data it was apparent that at least two flow paths would be needed, one for inside the vault and

one for the backfill. There also appeared to be a substantial vertical gradient in the backfill's velocity, so the idea of using a single velocity for the entire stack was deemed unacceptable. Sampling of the PorFlow data occurred at elevations corresponding to the each of the GoldSim model's mixing cells. Since a single mixing cells was used to simulate the grout and the backfill, a geometric average was used for each elevation.
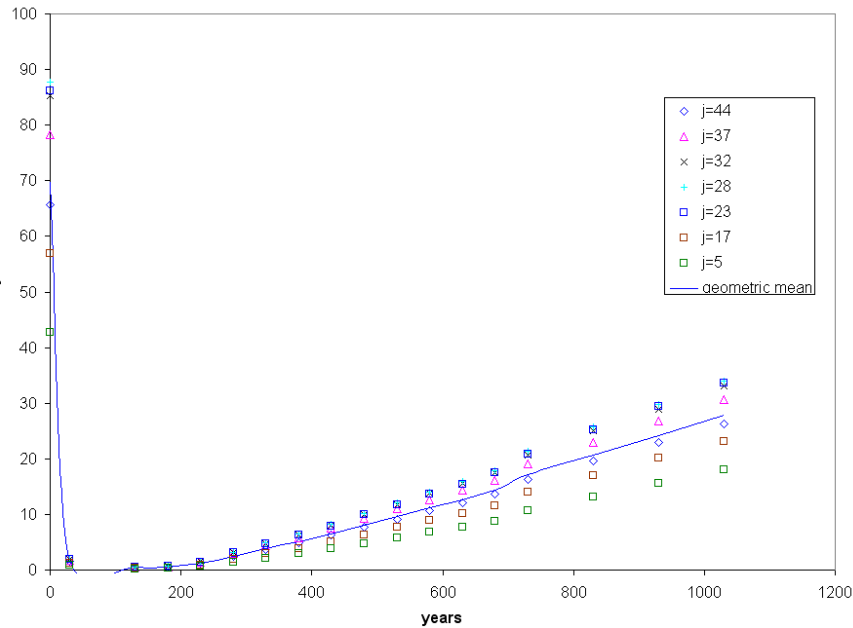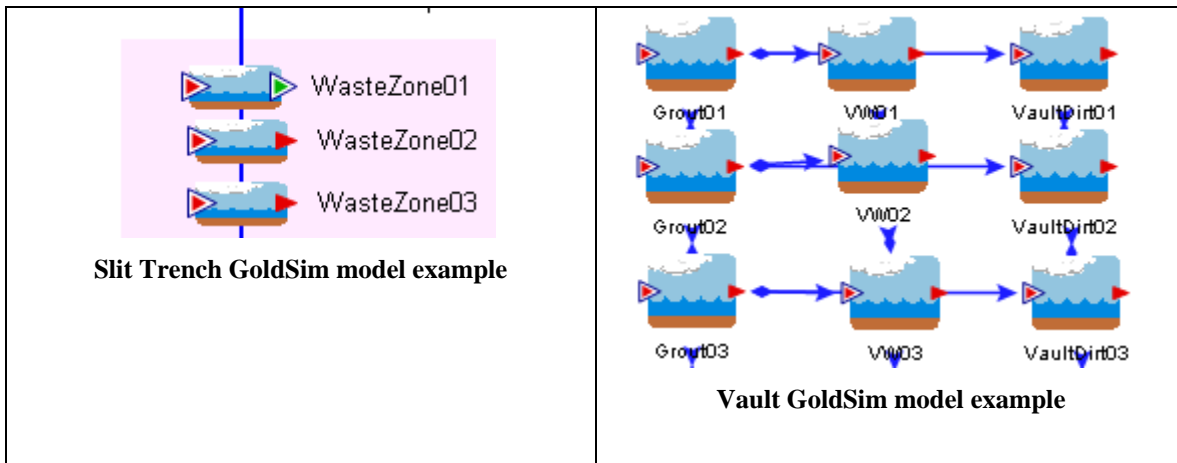

Figure 3 Abstracted Porflow flows

Figure 4 GoldSim model examples

The examination of the PorFlow model's flow field also showed extremely low velocities in the waste form for portions of the simulation. Further delving in the PorFlow model's simulation showed that at times diffusive transport was an important factor. This diffusive transport led to a contaminant deposition in the vault wall before the start date of the simulation. The contaminant was then released from the wall by diffusion to the

backfill and by advection to the native soil. In the GoldSim model, advection is modeled only in the vertical direction and diffusion only in the horizontal direction.

A column of mixing cells was added to the GoldSim model to simulate the vault wall, and a flow field for those cells was needed. The vault wall was represented by relatively few computational cells in the PorFlow model. As a result, the cells on the wall-backfill boundary had a relatively high flow rate because of the differencing scheme used in PorFlow. Therefore, data extracted from the PorFlow model were from the center of the vault wall to minimize the influence of the differencing scheme.

The final abstracted flow data for the UZ GoldSim model resulted in an $n \times 3 \times t$ matrix where n=number of mixing cells in a column, 3=number of columns (grout, wall, backfill), and t=number of time periods.

The SZ flow is not abstracted in the same manner. Its "abstraction" is really part of the benchmarking exercise. An "appropriate" value, typically some average value in the desired direction, is used as the starting point for the benchmarking. The important parameter to match in the initial benchmarking is the arrival of the contaminant, so the SZ flow rate is adjusted to give a reasonable agreement with arrival time.

Mass Flux Abstraction

Conceptually, the UZ-SZ interface mass flux abstraction is quite simple. PorFlow provides a mass flux leaving the computational domain of the UZ model. This corresponds exactly to the mass flux in the flow pathway connecting the last UZ mixing cell to the first SZ mixing cell in the GoldSim model. This is all that is required for the slit trench model. With the velocities set as described above, excellent agreement is found between the two models at the UZ-SZ interface as illustrated in Figure 5 where the solid lines represent PorFlow data and the dashed lines represent GoldSim data. The ease with which agreement can be reached is attributable to the fact that the flow field for the slit trench is essentially 1-D so its representation is similar in both models.
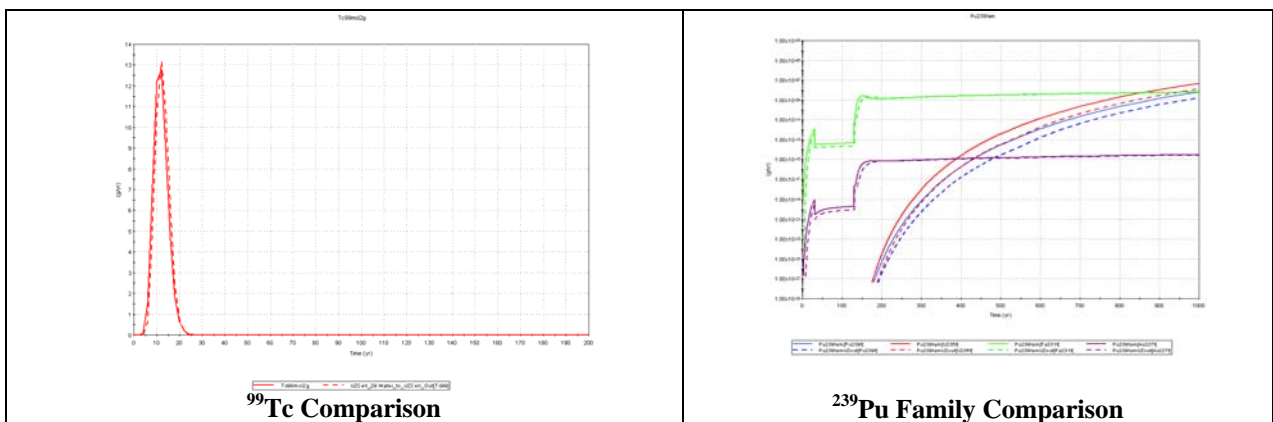

99Tc Comparison   239Pu Family Comparison

Figure 5 Benchmarking Examples

The similarity does not extend to the vault model. While the flow abstraction gives a good starting point for the benchmarking, because of the multidimensionality of the flowfield and the collapsing of many computational cells into one, the initial agreement between the two models usually leaves a great deal to be desired. Here, again, the line between data abstraction and benchmarking becomes blurred. In order to match the behavior at the boundary of the PorFlow model, a step-wise process must be followed. This is essentially the same process we started with, determining what the most important features are and proceeding from there. For engineered barriers, material fluxes must be matched entering and exiting the barrier if one wishes to have any hope of matching the material flux leaving the computational domain. Mass flux data must be abstracted from appropriate elevations of the PorFlow model and integrated to give a correspondence to the GoldSim model. By then adjusting the flow, one is able to obtain an equivalent flow field for the GoldSim model. This must be done for each of the barriers, at least in early times. In some simulations, it is assumed that the barriers degrade in time and their flow characteristics become similar to the backfill and native soil. Once this transition occurs, the simulation becomes conceptually very much like the slit trench.

Concentration Abstraction

The final step of benchmarking, and therefore the final abstraction, is matching the contaminant concentration at the compliance point. PorFlow computes concentrations for each of its computational cells, which appear as a point value to the GoldSim model. PorFlow can define regions and within these regions one can obtain maximum, minimum, and average values of the desired parameters. Conceptually, the GoldSim model's mixing cell is a PorFlow region. The mixing cell's concentration is a volume average. This would appear to be the parameter by which a comparison can be made, but again we move from abstraction into benchmarking. The size of the mixing cell in the SZ is somewhat arbitrary, so the concentration is affected by the choice of size. Therefore, the benchmarking is deemed sufficient if the behavior of the GoldSim model lies between the maximum and minimum values and hopefully near the average.

Conclusions

Data can be abstracted from a multidimensional model to a one dimensional model with the 1-D model's results providing reasonable agreement with the multidimensional model's results. However, abstraction cannot be done in a vacuum. The parameters to be benchmarked must lead the abstraction. In many cases several iterations between abstraction and benchmarking are necessary to produce a satisfactorily benchmarked model.