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Re: F-Tank Farm Performance Assessment Velocity **Field Abstraction from PorFlow to GoldSim**

1.0 Introduction

The modeling effort supporting the F-Tank Farm (FTF) Performance Assessment (PA) used the hybrid approach. The hybrid approach is one in which both deterministic and probabilistic models are used to develop a defensible PA. The hybrid approach has many advantages, notable ones being the development of two independent models of the same physical reality and engendering a better understanding of the system behavior than could obtained with just a single model. The hybrid approach for the FTF PA used a PorFlow model for the deterministic portion of the analysis and a GoldSim model for the probabilistic portion.

In order to run a probabilistic analysis using Monte Carlo methods in a reasonable amount of time it is necessary simplify the models used. 2- and 3-D models are used for the deterministic calculation of groundwater flow and transport. These multidimensional representations of the unsaturated and saturated zones use classic finite difference or finite volume methods to solve the equations. To develop good solutions these models have to be finely meshed and that meshing leads to long run times. A 1-dimensional model was implemented to simulate the multidimensional behavior. This memo describes the abstraction of the flow field data from the 2- and 3-D models to the 1-D model.

Abstraction is the process by which the phenomena important to the simulation are extracted from the multidimensional model and implemented in the 1-D model. The phenomenon which needed to be extracted from the multidimensional model was the flow field. It should be noted that the flow field is treated similarly between the multidimensional model and the 1-D model. That is, the flow field is calculated independently of the contaminant transport. The multidimensional models impose the flow field on essentially the same mesh, while in the 1-D model it is implemented in a 1-D representation. The abstraction will be discussed in following sections.

2.0 Flow Field Abstraction

The flow field for both the PorFlow and GoldSim transport calculations is taken from the PorFlow flow calculation. The PorFlow flow calculation is a set of 40 steady-state flow periods, each period representing a unique time range. The flow field from the PorFlow flow calculation is imposed on essentially the same nodalization in the PorFlow transport model. The PorFlow flow field is abstracted

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from a multidimensional representation to a 1-D representation. This section will describe that abstraction for both the unsaturated and saturated zones.

2.1 Unsaturated Zone Flow Field Abstraction

Figure 1 shows the flow field for a Type III tank. Type I tanks show the same behavior. Type IV tanks will be discussed later. This figure, from early in simulation time, shows that the flow is directed around the intact waste form. Note that the velocity in the waste form, both grout and water layer, is zero. This says that while the waste form is intact that no waste can leave the waste. The conceptual model for FTF has the concrete failing, I.e., assuming physical characteristics of sandy soil, at 500 years and the closure cap failing some time later. However, the carbon steel tank liner stays intact for many thousands of years, longer than the closure cap's lifetime. Tank Types I and III have carbon steel tops so no water can get to the waste until those steel components fail. Once the steel fails, as far as the model is concerned, it no longer exists. Therefore, the grout and waste layer now have the same physical characteristic as the sandy soil surrounding the tank. The inlet flow boundary condition is applied uniformly across the top of the model, therefore, the flow field is uniform as can be seen in Figure 2.

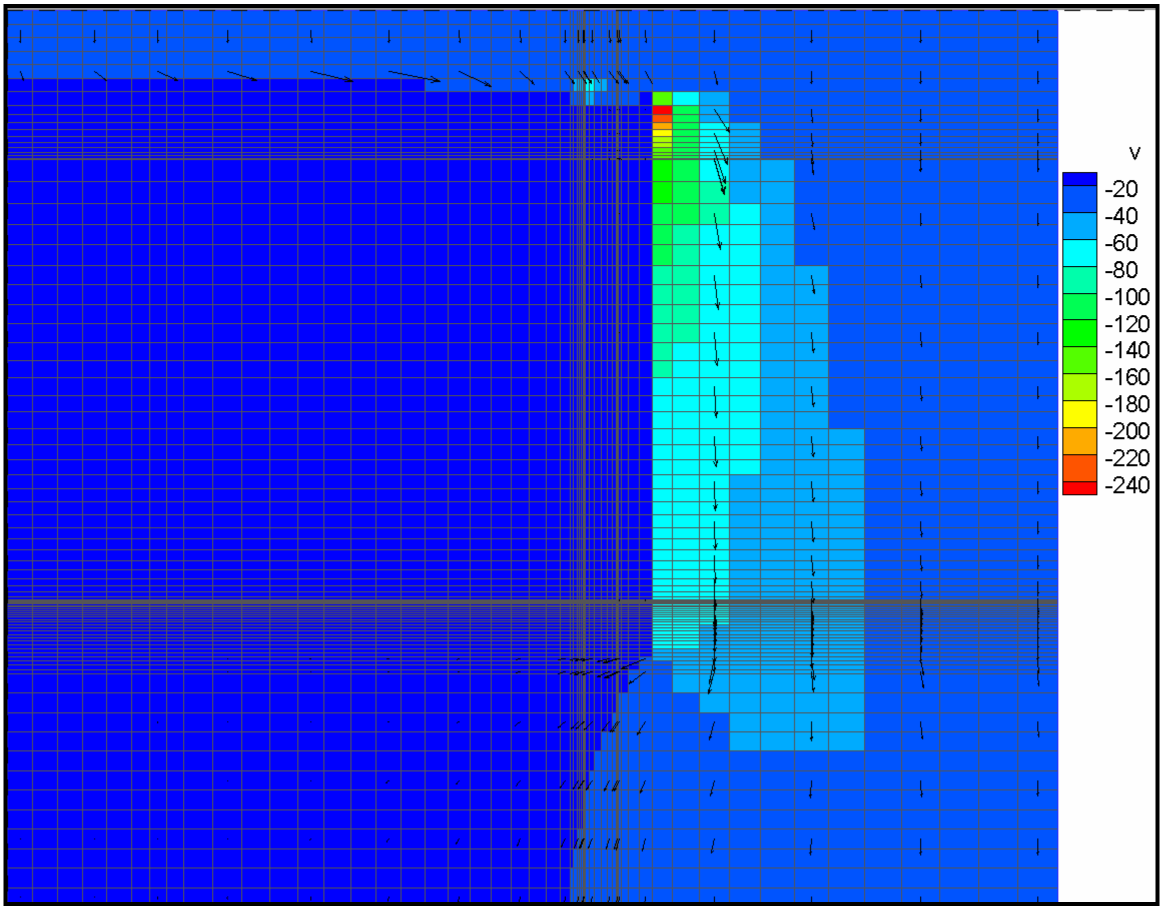

Figure 1 Tank Type III Flow Field pre-liner failure

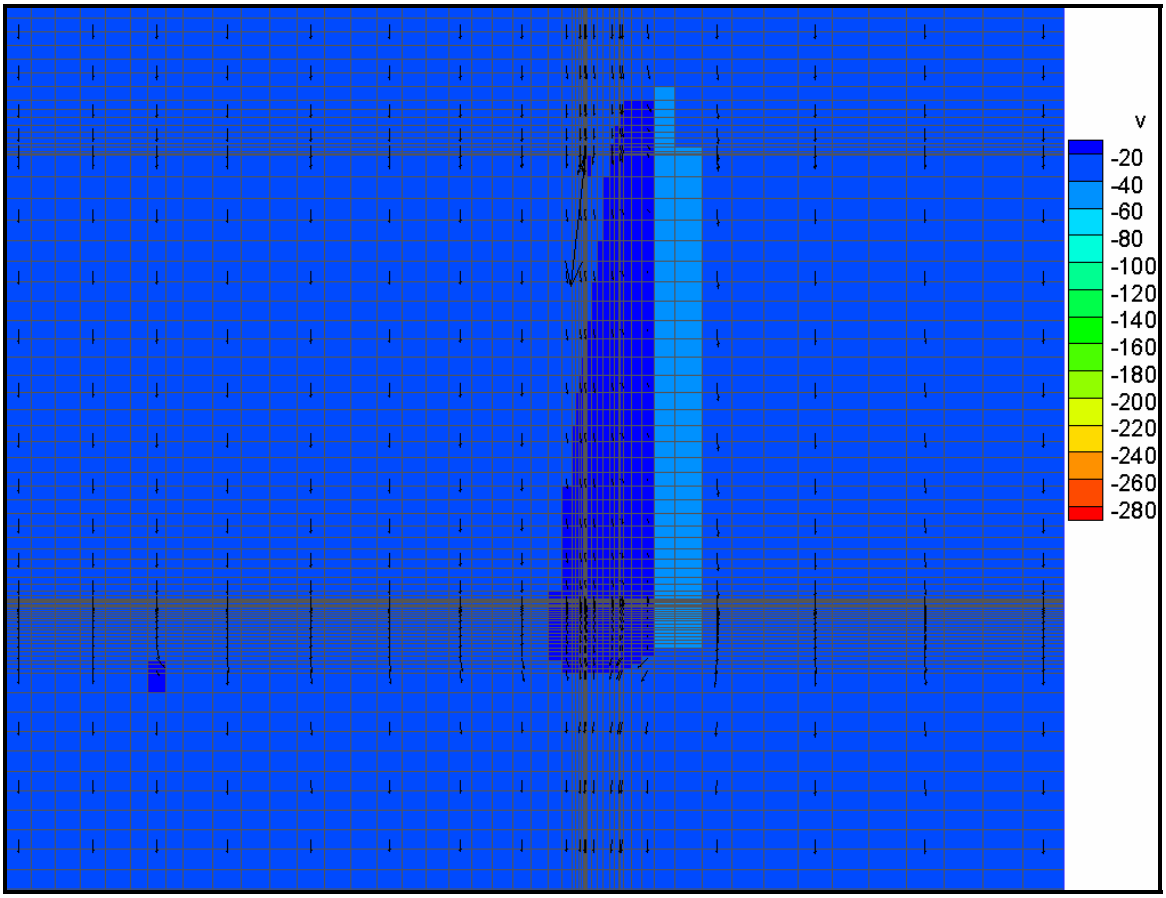

Figure 2 Tank Type III Flow Field post-liner failure

The abstraction of these data is fairly simple due to the fact that during the period of interest, once the waste is released to the environment, the flow field is essentially one dimensional. The abstraction algorithm is as follows

1. Select the row of cells approximately 0.5 m beneath the lower edge of the base mat.
2. Sample 5 data points along that row which are evenly spaced beneath the waste
3. Do a geometric average of those data and use that as the inlet flow condition for the GoldSim model.
4. Perform the first three steps for each of the 40 time periods for each of the tank types for each of the configurations.

Table 1 shows an example of the abstraction. In the row “time intervals” the values are the PorFlow node numbers, with “3” being nearer the center of the axi-symmetric tank model. Velocities are in cm/yr.

Table 1 Tank Type I Case A Unsaturated Zone Flow Field Abstraction

Type 1							
time interval	21	18	12	8	3	geometric mean	harmonic mean
1	-4.12E-04	-1.85E-04	-3.51E-05	-1.42E-05	-8.75E-06	5.06214E-05	-2.26213E-05
2	-1.01E-03	-4.52E-04	-8.47E-05	-3.34E-05	-2.01E-05	0.00012102	-5.27982E-05
3	-1.50E-02	-6.64E-03	-1.18E-03	-4.24E-04	-2.28E-04	0.00162588	-0.000640272
4	-4.35E-02	-1.92E-02	-3.37E-03	-1.19E-03	-6.22E-04	0.004610537	-0.001773137
5	-1.68E-01	-7.49E-02	-1.30E-02	-4.51E-03	-2.33E-03	0.017662549	-0.006692181
6	-3.31E-01	-1.45E-01	-2.57E-02	-8.86E-03	-4.56E-03	0.03463423	-0.013123591
7	-4.84E-01	-2.07E-01	-3.71E-02	-1.28E-02	-6.58E-03	0.050017858	-0.018942845
8	-6.83E-01	-2.90E-01	-5.18E-02	-1.79E-02	-9.19E-03	0.070058914	-0.026469412
9	-9.25E-01	-4.02E-01	-6.97E-02	-2.43E-02	-1.25E-02	0.095328636	-0.035953606
10	-1.10E+00	-4.77E-01	-8.26E-02	-2.90E-02	-1.49E-02	0.113369197	-0.042841627
11	-1.25E+00	-5.28E-01	-9.18E-02	-3.24E-02	-1.66E-02	0.126650801	-0.047758983
12	-1.44E+00	-5.95E-01	-1.02E-01	-3.61E-02	-1.85E-02	0.142308788	-0.053228907
13	-1.79E+00	-7.13E-01	-1.19E-01	-4.23E-02	-2.16E-02	0.169221964	-0.062265336
14	-2.04E+00	-7.88E-01	-1.28E-01	-4.57E-02	-2.34E-02	0.185566544	-0.067395787
15	-2.16E+00	-8.24E-01	-1.32E-01	-4.72E-02	-2.42E-02	0.193082297	-0.069675664
16	-2.24E+00	-8.48E-01	-1.35E-01	-4.82E-02	-2.47E-02	0.198127305	-0.071158376
17	-2.32E+00	-8.71E-01	-1.37E-01	-4.88E-02	-2.50E-02	0.202170274	-0.072077045
18	-2.37E+00	-8.82E-01	-1.38E-01	-4.92E-02	-2.52E-02	0.204499536	-0.072664017
19	-2.46E+00	-9.07E-01	-1.40E-01	-4.98E-02	-2.55E-02	0.208779567	-0.073585786
20	-2.57E+00	-9.34E-01	-1.42E-01	-5.05E-02	-2.58E-02	0.213548189	-0.074555993
21	-2.71E+00	-9.67E-01	-1.44E-01	-5.13E-02	-2.62E-02	0.219298359	-0.075747602
22	-2.96E+00	-1.02E+00	-1.48E-01	-5.26E-02	-2.69E-02	0.229180851	-0.077807553
23	-3.28E+00	-1.08E+00	-1.53E-01	-5.42E-02	-2.77E-02	0.241042497	-0.080233615
24	-3.51E+00	-1.13E+00	-1.57E-01	-5.55E-02	-2.83E-02	0.250076528	-0.082111259
25	-3.51E+00	-1.14E+00	-1.58E-01	-5.57E-02	-2.84E-02	0.251193572	-0.082432354
26	-3.33E+00	-1.10E+00	-1.55E-01	-5.50E-02	-2.81E-02	0.244707639	-0.081393443
27	-3.66E+00	-1.17E+00	-1.60E-01	-5.64E-02	-2.88E-02	0.256620709	-0.083569216
28	-3.25E+00	-1.09E+00	-1.54E-01	-5.47E-02	-2.79E-02	0.24214997	-0.080850599
29	-3.39E+00	-1.11E+00	-1.57E-01	-5.54E-02	-2.83E-02	0.247368111	-0.082032378
30	-3.77E+00	-1.19E+00	-1.63E-01	-5.73E-02	-2.92E-02	0.261530707	-0.084833273
31	-3.80E+00	-1.20E+00	-1.63E-01	-5.77E-02	-2.94E-02	0.263108649	-0.085359064
32	-4.12E+00	-1.27E+00	-1.69E-01	-5.96E-02	-3.03E-02	0.275838767	-0.088138182
33	-1.95E+01	-2.50E+01	-2.95E+01	-2.96E+01	-2.96E+01	26.30728404	-25.94061674
34	-1.95E+01	-2.50E+01	-2.94E+01	-2.96E+01	-2.96E+01	26.28942429	-25.92510848
35	-1.95E+01	-2.50E+01	-2.94E+01	-2.96E+01	-2.96E+01	26.28942429	-25.92510848
36	-1.95E+01	-2.50E+01	-2.94E+01	-2.96E+01	-2.96E+01	26.28942429	-25.92510848
37	-1.95E+01	-2.50E+01	-2.94E+01	-2.96E+01	-2.96E+01	26.28942429	-25.92510848
38	-1.95E+01	-2.50E+01	-2.94E+01	-2.96E+01	-2.96E+01	26.28942429	-25.92510848
39	-1.95E+01	-2.50E+01	-2.94E+01	-2.96E+01	-2.96E+01	26.28942429	-25.92510848
40	-1.95E+01	-2.50E+01	-2.94E+01	-2.96E+01	-2.96E+01	26.28942429	-25.92510848

Type IV tanks behave somewhat differently before liner failure. They do not have a steel cap. Therefore, when the closure cap fails the grout is exposed to an infiltration flow along a pathway which follows the inner lining of the tank. The tank becomes a giant bathtub with the waste layer now being attacked by water. This infiltration water provides a pathway, both diffuse and advective, for the waste to migrate into the reducing grout above the waste layer. Once the steel liner fails the physical material properties are as stated above.

The result of the flow field abstraction is to impose a 1-D flow field on the unsaturated zone. As can be seen from Figure 2, the flow field in the y-direction is essentially uniform. This is to be expected as the materials properties are very similar, and, assuming continuity one would expect the flow's magnitude to be approaching that of the boundary condition imposed on the model.

The unsaturated zone flow field is the connection between the unsaturated and saturated zones. It is a hard connection in the GoldSim model in that the two zones exist within the same model. In the PorFlow model, the saturated zone is a separate model from the unsaturated zone. The flow, in terms of a mass flux, is the output from the unsaturated zone used as an inlet boundary condition to the saturated zone. This has implications on the benchmarking and will be discussed in that section.

2.2 Saturated Zone Flow Abstraction

The saturated zone abstraction presented challenges which were not present in the unsaturated zone. Primarily, the flow is multi-dimensional (See Figure 3 and Figure 4.) The tack taken in this abstraction was to first determine what information was really needed. The saturated zone supplies the well from which the dose is calculated. The things which are important to the dose calculation are timing and concentration. Timing will be discussed in the following sections. Concentration is a benchmarking concern. In the following sections, the abstraction of the data is inseparable from the benchmarking, hence, the terms can be, and are, used interchangeably.

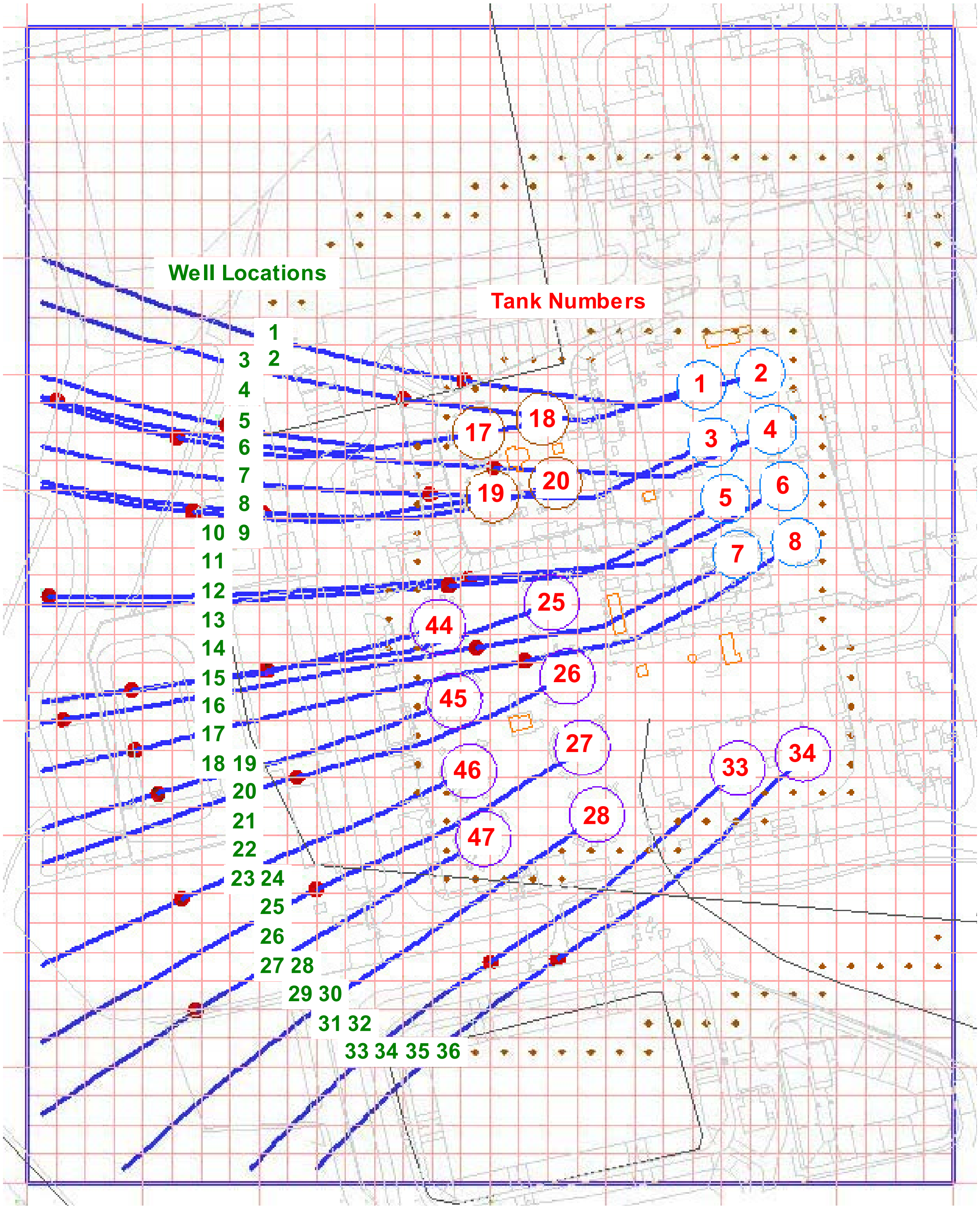

Figure 3 FTF Plan view with tank streamlines

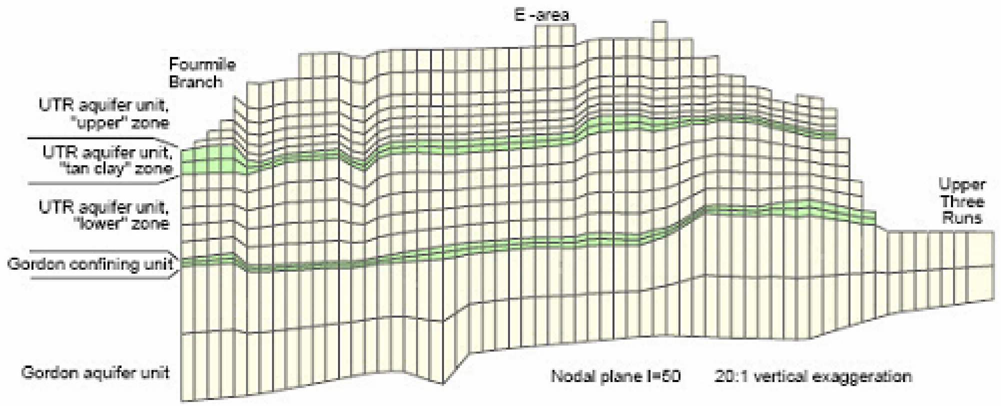

Figure 4 Aquifer cross section

2.2.1 Saturated Zone Timing

The abstraction of the contaminant arrival time was quite straightforward. The parent radionuclide's timing was the data of interest. It was implicitly abstracted by the concentration vs. time curve.

The timing benchmarking consisted of two parts: correcting the numerical diffusion and then fine tuning using the saturated zone velocity.

2.2.2 Numerical Diffusion

The saturated zone timing benchmarking was quite an interesting exercise. The GoldSim calculation showed the contaminants arriving before PorFlow thought they should. Changing the zone's velocity really had no effect on moving the arrival time. It was postulated that the reason for this was that PorFlow had some clay it its saturated zone whereas GoldSim was strictly sandy soil. A combination of clay and sandy soils was used, with interesting results. Running the ^{239}Pu series, the Pu timing was quite affected by the addition of the clay but the ^{235}U arrival time did not change. The distribution coefficient for Pu goes from 270 ml/g in sandy soil to 5900 ml/g in clayey soil. Uranium's distribution coefficient goes from 200 ml/g to 300 ml/g. The implication was this was not a distribution coefficient issue.

At this point in time the issue had the appearance of numerical diffusion. The GoldSim mode was using 10 mixing cell, giving the cell a minimum length of 10 m and a maximum of 26 m. A crude noding study was performed, and for the benchmarked tanks either 40 or 50 cells were used. When these nodings were used the GoldSim and PorFlow results practically fell on each other.

2.2.3 Saturated Zone Velocity

The major change in peak timing was accomplished by eliminating the numerical dispersion in the GoldSim model. The timing was then fine-tuned by varying the saturated zone velocity. As can be seen by Figure 3, the flowstreams from the tanks are neither linear nor in the same x-y plane. By varying GoldSim's 1-dimensional velocity one is able to account for these effects. Six tanks, of different types and locations, were used to determine the velocities. These were Tanks 17, 18, 1, 3, 5, and 34. These tanks were chosen due to scoping runs for Revision A of the PA showing them to be major contributors to the dose. They represent all tank types found in the FTF. Table 2 is a summary of the tank characteristics. As can be seen in the table, the distance to the compliance point ("Dist to well") varies considerably for these tanks. Note that the distance to the well shown in the table is a planar distance, it does not consider the 3-dimensional travel path. Each of these tanks had a velocity explicitly calculated. Velocities for similar tanks were inferred from these six.

Table 2 Benchmarked Tank Characteristics

Tank	Type	Dist. To water table (ft)	Dist to well (m)	PorFlow Region
1	I	13.5	224	E
3	I	12.1	244	E
5	I	10.6	264	D
17	IV	2.5	112	E
18	IV	2.1	132	E
34	III	17.1	244	A

This is the first time this type of analysis has been done so it is suggested that the benchmarking of the remainder of the tanks be done in order to determine if it should be done in future analyses. While one is fairly confident that the velocities for all the tanks are reasonable, one cannot state definitively that this is the case. Certainly with the resources provided at the time of the analysis, the analysis was assumed sufficient. By benchmarking the remainder of the tanks one can definitively show that the method of picking certain tanks and extrapolating their behavior to others is sufficient and a more comprehensive abstraction is not necessary.

The first step in adjusting the peak timing was to examine the behavior of ^{99}Tc. ^{99}Tc was chosen because it is a non-sorbing radionuclide. If the arrival times in the two models coincided then the saturated zone velocities are consistently represented. This was accomplished for the six tanks.

The next step was to use a sorbing radionuclide. Early attempts showed the peaks to arrive too early. It was hypothesized that since the Porflow model was modeling the clay layers separating the aquifers that the clay should have an affect on the arrival time. The GoldSim model was modified to include a mixture of clay and sand. The ^{239}Pu series was quite informative in that is showed that the Pu peak would move substantially while the U peak did not move. The magnitude of the distribution coefficient for Pu changes from 270 ml/g in sand to 5900 ml/g in clay. That of U varies from 200 ml/g in sand to

300 ml/g in clay. This showed that it was not a distribution coefficient effect, but something else. That something else was the numerical dispersion of the GoldSim model.

Once the numerical dispersion issue was dealt with, by increasing the noding, the peaks of the sorbing radionuclide fell into reasonable agreement with the Porflow peaks using the same velocities as determined by the ^{99}Tc comparisons. This is another indication that the conceptual model is giving consistent results when modeled by two independent models.