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Date: January 3, 2018

To: Tom Butcher

From: Greg Flach

Reviewer: Sebastian Aleman

3.5.2 Aquifer Model

Recommendation #139, 146

Recommended Aquifer Grid Resolution for E-Area PA Revision Transport Simulations

Scope Abstract: This memorandum addresses portions of Section 3.5.2 of SRNL (2016) by recommending horizontal and vertical grid resolution for aquifer transport, in preparation for the next E-Area Performance Assessment (WSRC 2008) revision.

Results / Conclusions: The recommended horizontal and vertical grid sizes are 25 ft and 3 ft, respectively. The horizontal resolution can approximately represent longitudinal dispersion with dispersivity (α_L) equal to 10 ft, the lowest value expected in upcoming deterministic simulations. The vertical resolution is 3 times smaller than a typical well screen (10 ft) and average plume thickness expected in E-Area (~10 ft). For overlapping model domains, each extending over about 1/3 of E-Area, these grid resolution recommendations lead to mesh sizes on the order of a half-million PORFLOW nodes, which is computationally feasible.

Discussion

An E-Area Performance Assessment (PA) revision will require aquifer transport simulations involving physical dispersion occurring over a range of scales depending on the disposal unit, and reflecting uncertainty in the appropriate dispersivity for a given scale. The objective of this effort is to select a PORFLOW grid resolution that can accommodate the smallest scale of physical dispersion expected in deterministic simulations, including sensitivity analysis (SA) and uncertainty quantification (UQ).

Horizontal grid resolution

Based on studies including Lallemand-Barres and Peaudecerf (1978) and Gelhar et al. (1992), groundwater modeling practitioners generally assume a longitudinal dispersivity that is 10% of the plume travel distance (e.g. de Marsily 1986, Section 10.1.3 and Fetter 1993, Section 2.11)

$$\alpha_L = 0.1L = 10^{-1}L \tag{1}$$

unless site-specific data are available. Figure 1 is a reproduction of Figure 2 from Gelhar et al. (1993) annotated to show Equation (1) as a solid red line. Because the more reliable data in Figure 1 are biased low compared to the overall population, the dashed line corresponding to

$$\alpha_L = 0.032L = 10^{-1.5}L \tag{2}$$

is within the uncertainty range for average longitudinal dispersivity, and expected in SA/UQ simulations.

The minimum plume travel distance per DOE Order 435.1 is 100 meters:

$$L = 100 \text{ m} \tag{3}$$

Combining Equations (2) and (3), the minimum longitudinal dispersivity expected in deterministic PORFLOW simulations is approximately

$$\alpha_L = 0.032(100 \text{ m}) = 3.2 \text{ m} = 10 \text{ ft} \tag{4}$$

Therefore, the horizontal grid resolution (Δx) should be fine enough to accommodate $\alpha_L = 10$ ft.

In general, numerical dispersion is less than physical dispersion when

$$\alpha_L \leq \Delta x \leq 2\alpha_L \tag{5}$$

depending on the numerical scheme (Zheng and Bennett 2002, Equation 7.45). PORFLOW-specific testing indicates numerical dispersion to be small when

$$\Delta x \leq 2\alpha_L \tag{6}$$

and negligible when

$$\Delta x \leq \alpha_L \tag{7}$$

Considering Equations (4) and (7), horizontal grid size would ideally be set to

$$\Delta x = \alpha_L = 10 \text{ ft} \tag{8}$$

to achieve negligible numerical dispersion. However, this mesh resolution would result in grid sizes well over one million PORFLOW nodes, which is judged to require excessive computer runtimes and storage. Instead,

$$\Delta x = 25 \text{ ft} \approx 2\alpha_L \tag{9}$$

is recommended for computational efficiency. This setting will produce a small and acceptable level of numerical dispersion, and corresponds to an 8×8 refinement of the GSA_2016 grid (Flach et al. 2017). The resulting number of PORFLOW nodes for a model cutout extending over about 1/3 of E-Area is on the order of a half-million.

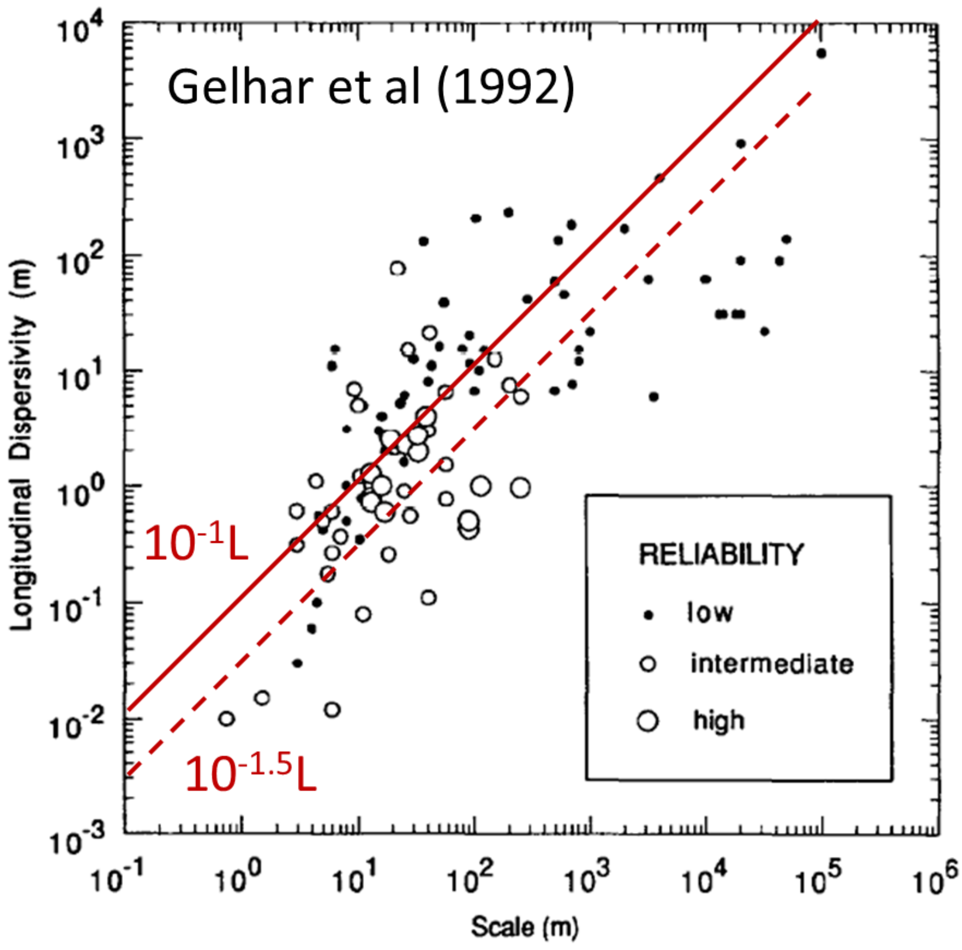

Figure 1. Longitudinal dispersivity versus scale; modified from Figure 2 of Gelhar et al. (1992).

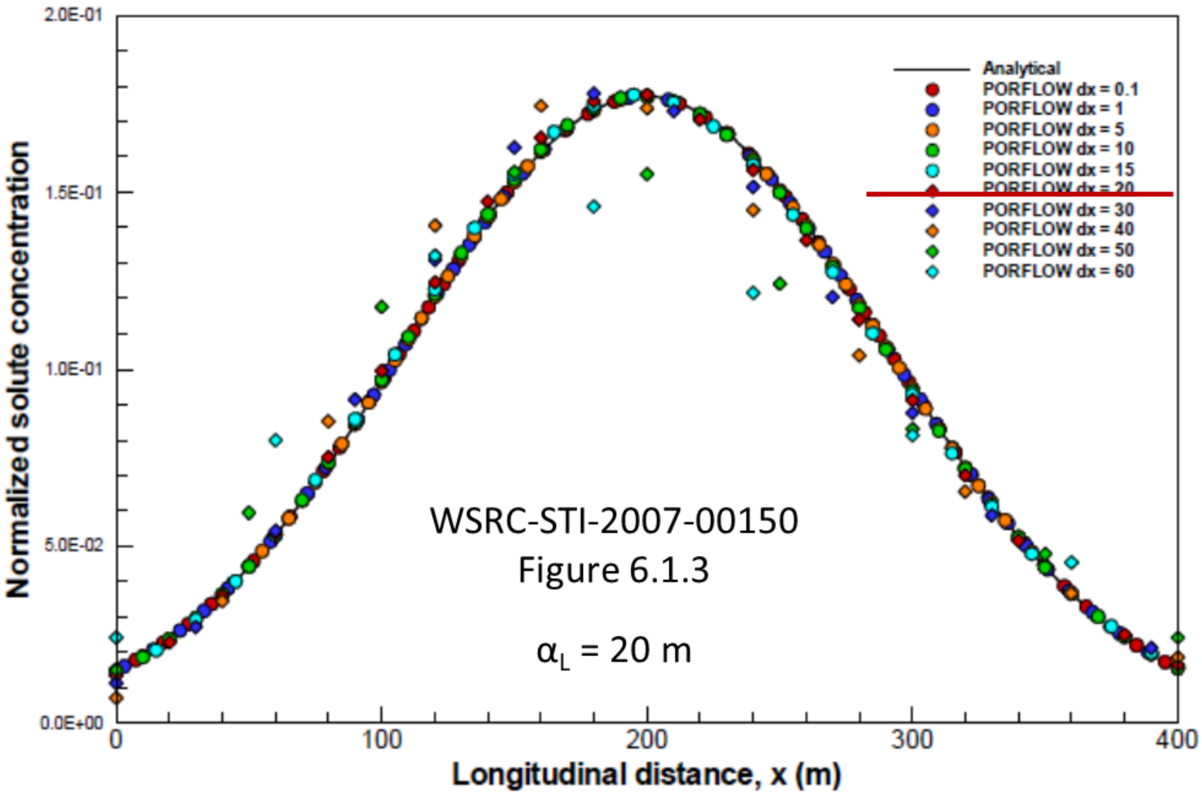

Figure 2. PORFLOW numerical dispersion as a function of grid resolution; modified from Aleman (2007).

<u>Vertical mesh resolution</u>

As a rule of thumb, horizontal transverse dispersivity is typically one order of magnitude lower than (horizontal) longitudinal dispersity, and vertical transverse dispersivity is typically two orders of magnitude lower (Zheng and Bennett 2002, Section 11.3.2). In terms of the four-parameter dispersion model implemented in PORFLOW (Hamm and Aleman 2000, Equations 2.2.24; Aleman and Flach 2010) shown in Figure 3, the corresponding dispersivity values are

$$\alpha_{LH} = \alpha_L = 10 \text{ ft} \tag{10}$$
$$\alpha_{TH} = \alpha_{LV} = 0.1\alpha_L = 1 \text{ ft} \tag{11}$$
$$\alpha_{TV} = 0.01\alpha_L = 0.1 \text{ ft} \tag{12}$$

Although explicit testing has not been performed, a vertical transverse dispersivity of 0.1 ft presumably requires a PORFLOW vertical mesh resolution on the order of 0.1 ft to achieve negligible numerical dispersion. This cell thickness would result in PORFLOW grid sizes exceeding one million nodes in E-Area, which is not computationally feasible for baseline PA simulations.

However, plume definition at a vertical resolution of 0.1 ft is not necessary from a practical monitoring perspective. A typical groundwater monitoring well at the Savannah River Site has a screen height of 10 feet if below the water table, and 10 feet or more if straddling the water table. Therefore, field measurements represent a concentration average over at least 10 ft.

Another consideration is the expected thicknesses of plumes emanating from E-Area disposal units. Figure 4 presents a calculation of plume thickness based on a mass balance concept ignoring dispersion. Plume thickness is expected to range from approximately 4.5 to 18 feet. The geometric mean of this range is 9 feet.

Figure 5 compares the vertical grid size for negligible dispersion, range of plume thicknesses, and monitoring screen lengths. Based on these reference scales, a vertical mesh resolution of 3 feet is recommended for the upcoming PA revision:

$$\Delta z = 3 \text{ ft} \approx 1 \text{ m} \tag{13}$$

This grid size is at least three times smaller than a typical monitoring well screen height, and thus provides higher resolution of plume concentration than would typically be measured in the field. The grid size is also three times smaller than the geometric mean of the plume thickness range, which will allow PORFLOW to approximately resolve the vertical concentration profile of a plume. This vertical resolution will also allow accommodate mesh resolutions on the order of a half-million nodes, which is computationally feasible.

A numerical test supporting Equation (13) is reported below.

$$D_{xx} = \alpha_{LH}\frac{v_x^2}{|\underline{v}|} + \alpha_{TH}\frac{v_y^2}{|\underline{v}|} + \alpha_{TV}\frac{v_z^2}{|\underline{v}|} + D^* \qquad D_{xy} = \left(\alpha_{LH} - \alpha_{TH}\right)\frac{v_x v_y}{|\underline{v}|}$$

$$D_{yy} = \alpha_{TH}\frac{v_x^2}{|\underline{v}|} + \alpha_{LH}\frac{v_y^2}{|\underline{v}|} + \alpha_{TV}\frac{v_z^2}{|\underline{v}|} + D^* \qquad D_{xz} = \left(\hat{\alpha}_L - \alpha_{TV}\right)\frac{v_x v_z}{|\underline{v}|} \qquad \hat{\alpha}_L = \frac{\alpha_{LH} + \alpha_{LV}}{2}$$

$$D_{zz} = \alpha_{TV}\frac{v_x^2}{|\underline{v}|} + \alpha_{TV}\frac{v_y^2}{|\underline{v}|} + \alpha_{LV}\frac{v_z^2}{|\underline{v}|} + D^* \qquad D_{yz} = \left(\hat{\alpha}_L - \alpha_{TV}\right)\frac{v_y v_z}{|\underline{v}|}$$

Figure 3. Four-parameter dispersion model implemented in PORFLOW via the STRAtified aquifer modifier.

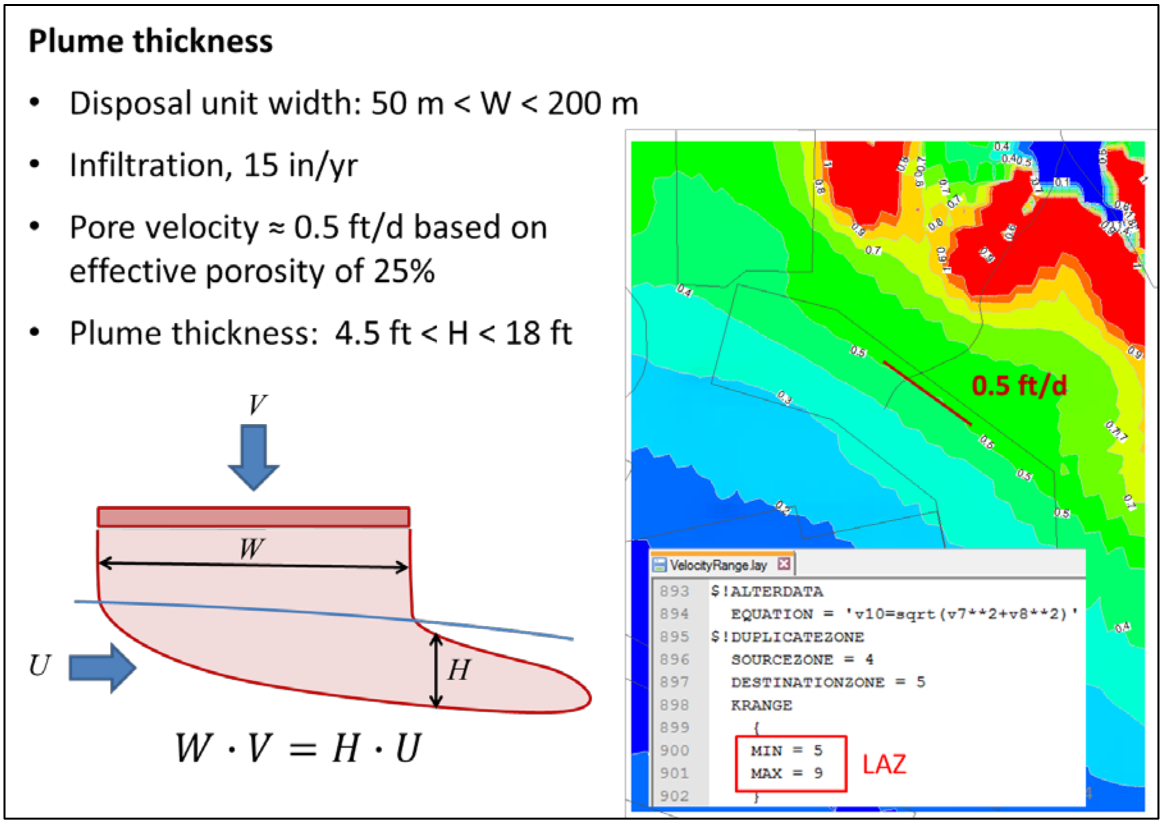

Figure 4. Estimated range of plume thicknesses in E-Area.

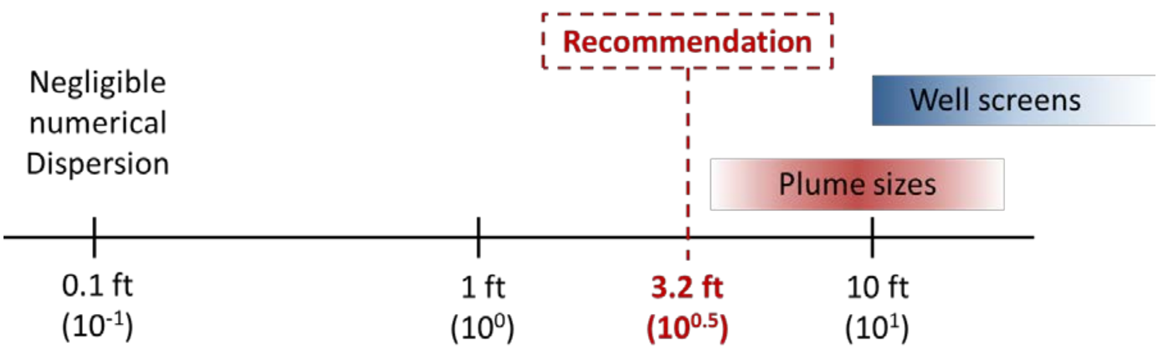

Figure 5. Scales of well screens, plume sizes, and vertical mesh resolution for negligible numerical dispersion.

Example refined grid cutouts

Figures 6 and 7 illustrate potential refined grid cutouts for E-Area based on the recommended grid resolutions given by Equations (9) and (13). The PORFLOW grid sizes are

Cutout	I nodes	J nodes	K nodes	Total nodes
East	74	138	48	490,176
Center	114	106	44	531,696
West	90	106	42	400,680

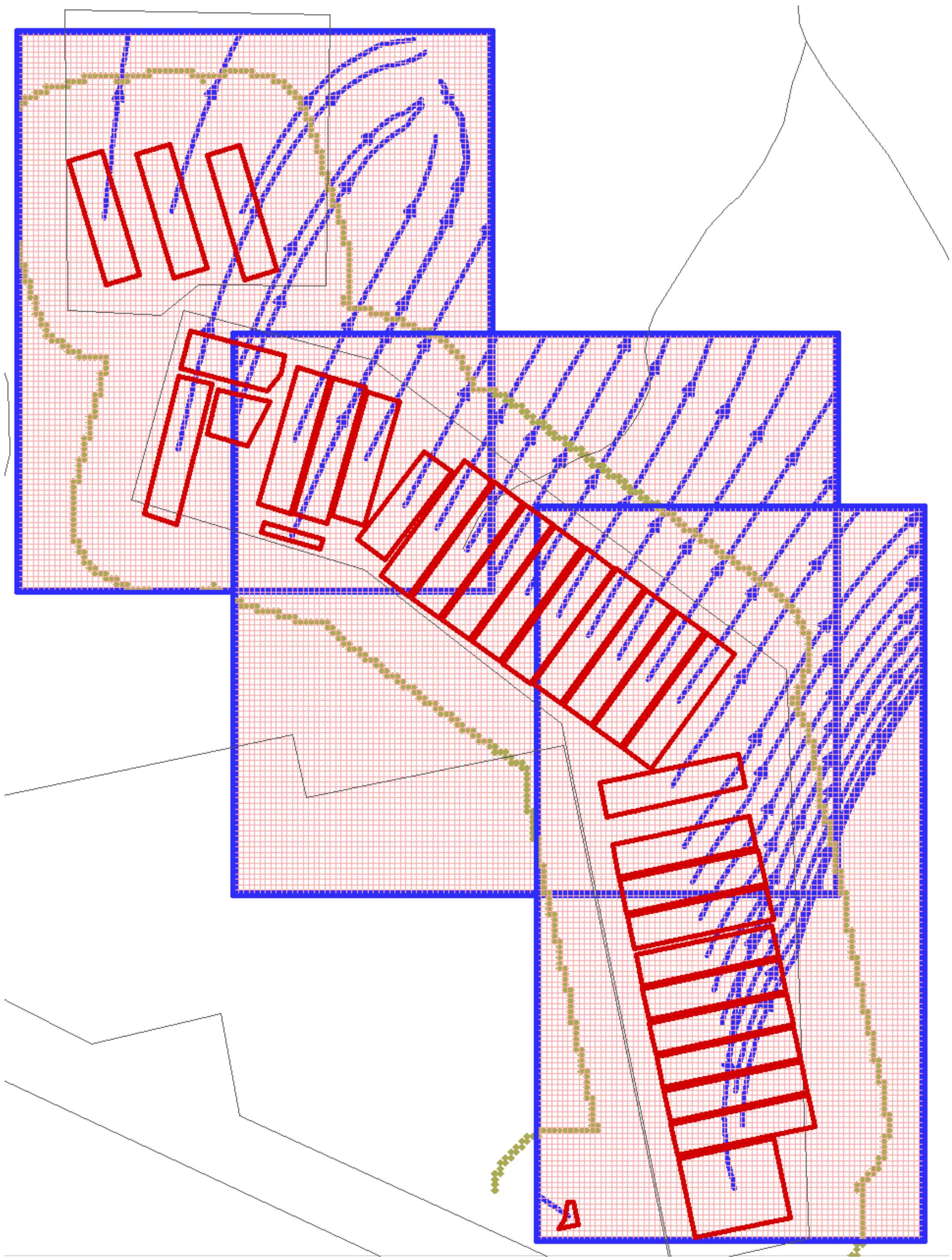

Figure 6. Example refined grid cutouts of GSA_2016 groundwater flow model for E-Area.

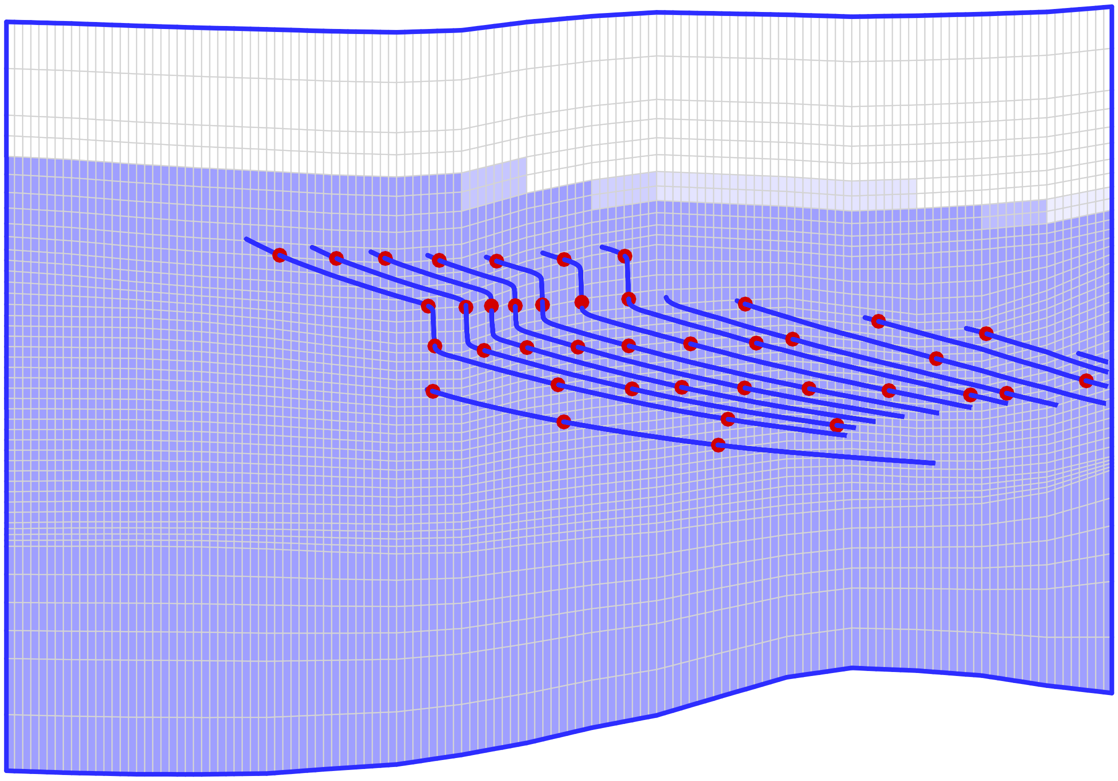

Figure 7. Example vertical refinement (10:1 vertical exaggeration).

Vertical mesh resolution test

To test the adequacy of the vertical mesh refinement recommendation summarized by Equation (13), tracer transport simulations were run with longitudinal dispersivity set to 32.8 ft and then 10 ft. The other dispersivities are defined from longitudinal dispersivity according to the general rules of thumb shown in Equations (11) and (12). In each set of simulations, one mole of a tracer species was placed just beneath the water table at disposal unit ST05, and peak concentration recorded at the 100-meter boundary. In one simulation, the GSA_2016 grid was refined vertically using kSplits = "2 4   2 2   4 4 4 4 4   2 2   2 2 2 2 2 1 1" to approximately satisfy Equation (13) where the plume is present. Figure 7 illustrates this vertical refinement. In a second simulation, the vertical mesh size was doubled by halving the kSplit factors (1 2   1 1   2 2 2 2 2   1 1   1 1 1 1 1 1 1). In a third simulation, the vertical mesh size was halved in the region of the plume, but coarsened below the plume to keep the mesh size below PORFLOW mesh size limits (1 2   1 1   8 8 8 8 8   4 4   4 4 4 4 4 1 1). Figures 8 and 9 compare the 100-meter breakthrough curves for the two sets of simulations.

Figure 8 involves the longitudinal dispersivity used most commonly in practice and in the 2008 E-Area PA, α_L = 32.8 ft, and likely the best-estimate for the E-Area PA Revision. The fine-mesh and recommended-mesh results are nearly identical, which implies negligible numerical dispersion due to vertical mesh resolution in these simulations. The peak coarse-mesh concentration is only 7% lower, suggesting non-zero but low dispersion. The recommended mesh size given by Equation (13) is clearly adequate for capturing peak concentration when α_L = 32.8 ft.

Figure 9 involves the lowest longitudinal dispersivity expected in PA sensitivity analysis, α_L = 10 ft. Peak concentration is observed to increase with decreasing vertical mesh size, an indication of numerical dispersion being present in at least the recommended-mesh and coarse-mesh simulations. The ratio of coarse-mesh peak concentration to recommended-mesh concentration is 0.84 (-16%), while the ratio of the fine-mesh to recommended-mesh concentration is 1.13 (+13%). Thus, the recommended mesh size of Δz = 3 ft leads to numerical dispersion causing at least a 13% bias in peak concentration when α_L = 10 ft.

Due to PORFLOW limitations on total mesh size, the mesh resolution required to effectively eliminate numerical dispersion could not be precisely determined while maintaining the same areal footprint. However, the required resolution can be estimated. From Figure 8, numerical dispersion is negligible when

$$\frac{\Delta z}{\alpha_L} = \frac{3\text{ ft}}{32.8\text{ ft}} \approx 0.1 \tag{14}$$

which suggests that $\Delta z \approx 1$ ft corresponds to negligible numerical dispersion due to vertical mesh resolution when α_L = 10 ft. The fine-mesh resolution in Figure 9 is approximately Δz = 1.5 ft in the region of the plume, which suggests low dispersion. Therefore, the numerical dispersion bias introduced by the recommended-mesh resolution is probably not much greater than 13% when α_L = 10 ft.

To confirm and quantify this expectation, an additional simulation was performed on a smaller areal footprint, that still captures the ST05 disposal unit and 100-meter perimeter, and with kSplits = "1 2   1 1 16 16 16 16 16   8 8   8 8 8 8 8 1 1". The latter is double the vertical resolution of the fine-mesh in the region of the plume, and termed “finer-mesh”. Figure 10 illustrates the combined results of the coarse-, recommended-, fine- and finer-mesh simulations. The fine-mesh and finer-mesh results are practically the same, which implies negligible numerical dispersion due to vertical mesh resolution in both simulations. The recommended-mesh peak concentration is 13% lower than the peaks from the two finer grids.

Figures 11 and 12 compare tracer simulations when a constant tracer source is specified, resulting in a steady-state plume. When α_L = 32.8 ft, the peak concentration is nearly the same for all three mesh resolutions. When α_L = 10 ft, the fine-mesh and recommended-mesh results are practically identical, and the coarse-mesh concentration is only slightly lower. Thus, for a steady source, numerical dispersion due to vertical mesh resolution is negligible when Δz = 3 ft for both dispersivity levels.

To summarize, numerical dispersion is negligible for the recommended resolution of Δz = 3 ft when α_L = 32.8 ft and/or the source term is steady. For α_L = 10 ft and a pulsed source, numerical dispersion associated with Δz = 3 ft introduces a small bias to peak plume concentration at 100 meters, estimated to be around 15%. This level of bias is acceptable to gain computational efficiency, because α_L = 10 ft is the lowest expected dispersivity and well below the expected best-estimate value of α_L = 32.8 ft.

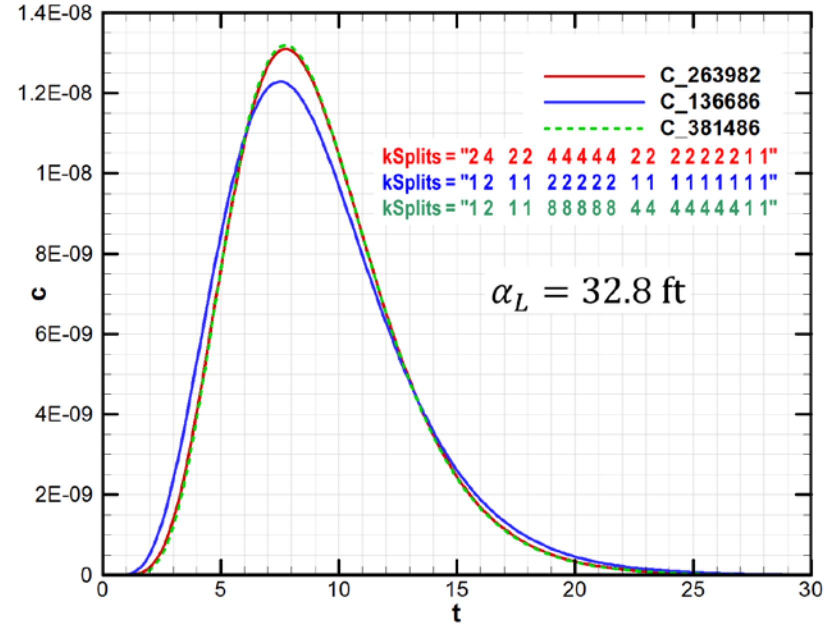

Figure 8. Tracer breakthrough curves at 100 meters for disposal unit ST05 for three vertical mesh resolutions, a pulsed source, and $\alpha_L = 32.8$ ft.

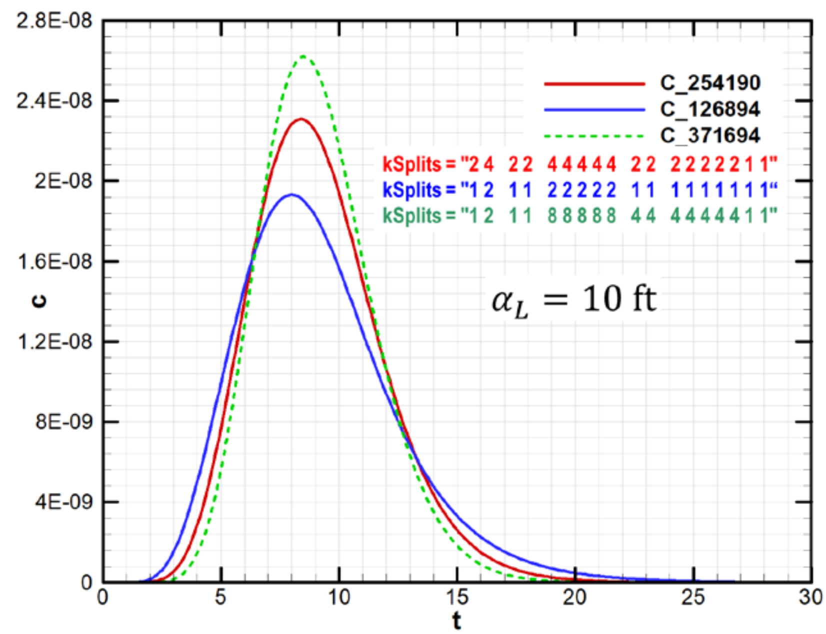

Figure 9. Tracer breakthrough curves at 100 meters for disposal unit ST05 for three vertical mesh resolutions, a pulsed source, and $\alpha_L = 10$ ft.

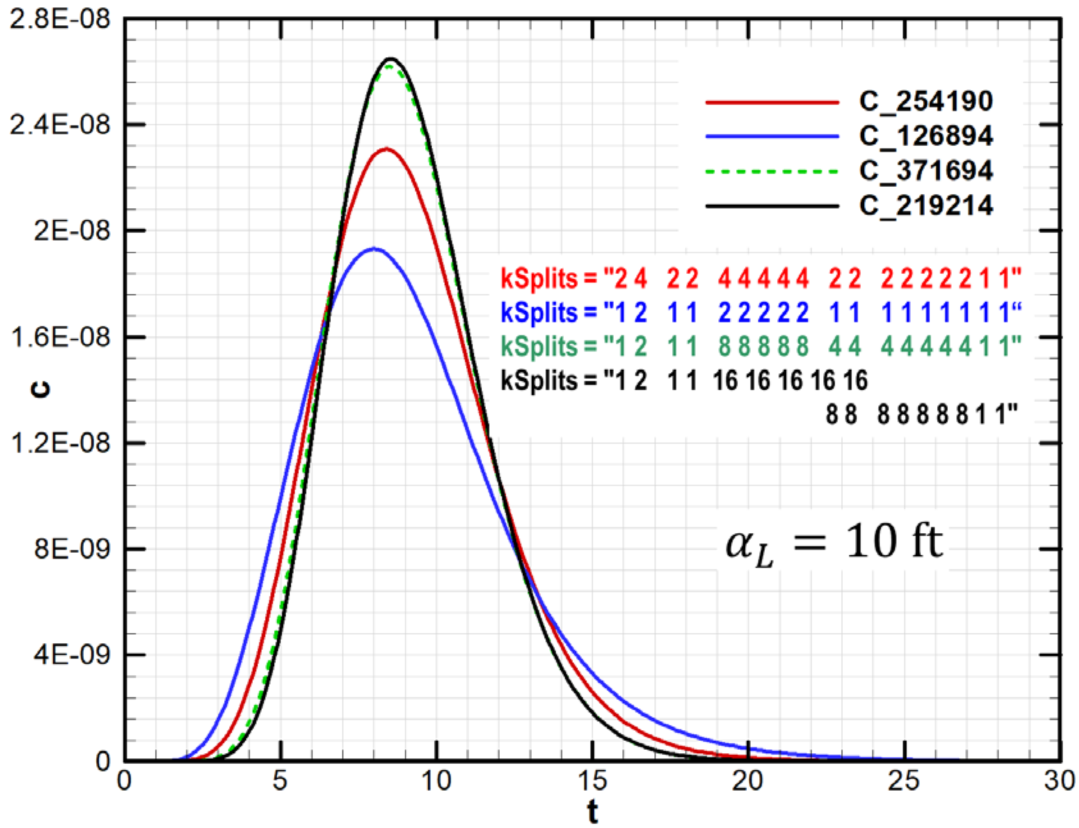

Figure 10. Tracer breakthrough curves at 100 meters for disposal unit ST05 for four vertical mesh resolutions, a pulsed source, and $\alpha_L = 10$ ft.

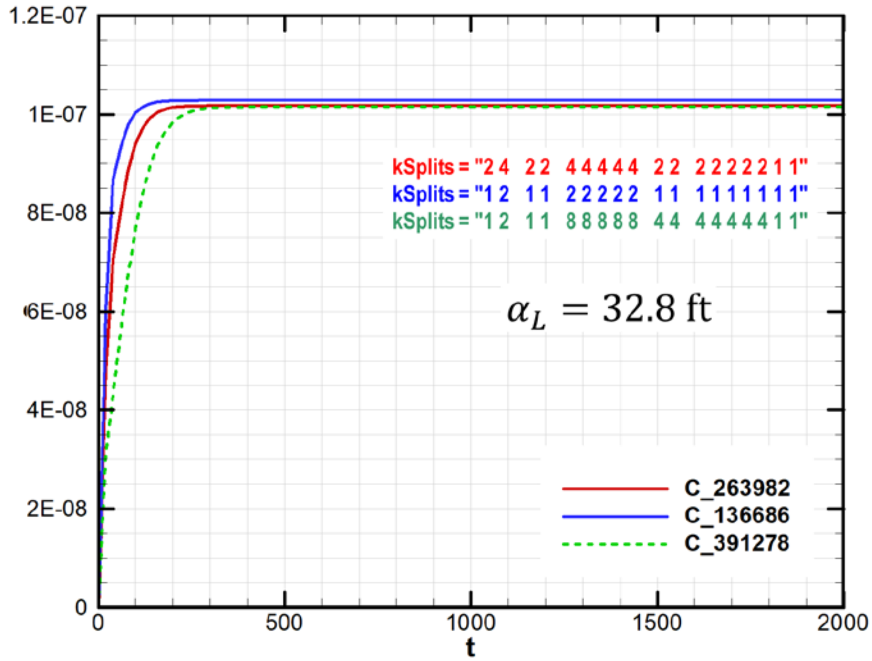

Figure 11. Tracer breakthrough curves at 100 meters for disposal unit ST05 for three vertical mesh resolutions, a steady source, and $\alpha_L = 32.8$ ft.

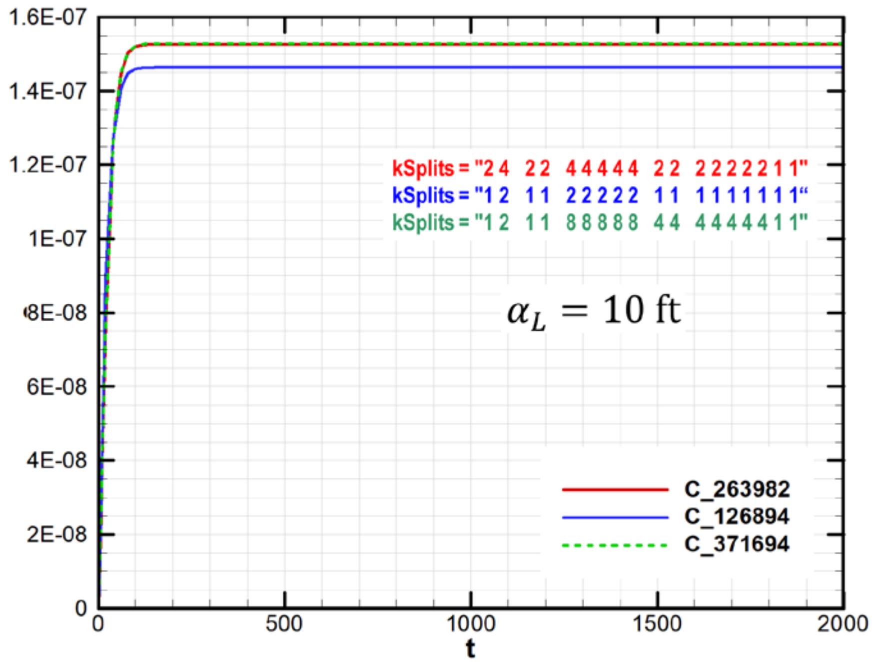

Figure 12. Tracer breakthrough curves at 100 meters for disposal unit ST05 for three vertical mesh resolutions, a steady source, and $\alpha_L = 10$ ft.

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