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Retention:
Permanent

Software Quality Assurance Plan for Aquifer Model Refinement Tool (MESH3D)

Author: Greg Flach

FEBRUARY, 2007

Savannah River National Laboratory
Washington Savannah River Company
Savannah River Site
Aiken, SC 29808

Prepared for the U.S. Department of Energy Under
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LIST OF ACRONYMS

ACRONYMS

CQF	Cognizant Quality Function
CTF	Cognizant Technical Function
DOE	U.S. Department of Energy
EPA	U.S. Environmental Protection Agency
PA	Performance Assessment
SQAP	Software Quality Assurance Plan
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
WSRC	Washington Savannah River Company

1.0 INTRODUCTION

The Environmental Analysis and Performance Modeling group of Savannah River National Laboratory (SRNL) conducts Performance Assessments (PA) of the Savannah River Site (SRS) low-level waste facilities to provide a reasonable assurance that the Performance Objectives of DOE Order 435.1 will be met. Each PA includes an analysis of contaminant transport through the saturated zone between the disposal unit and compliance boundary. The aquifer transport analysis is based on the velocity and saturation fields produced by a General Separations Area (GSA) regional groundwater flow model referred to as GSA/PORFLOW (Flach 2004). PORFLOW refers to a commercial code used to simulate groundwater flow (ACRi). Although the GSA/PORFLOW flow field can be used directly for PORFLOW aquifer transport simulations, typical practice is to use flow information defined on a localized grid of smaller extent but higher resolution using the MESH3D program. MESH3D extracts a sub-region of the GSA coarse mesh, and subdivides the coarse mesh to produce a higher-resolution grid. MESH3D also transfers velocity and saturation data from the original GSA/PORFLOW grid to the refined mesh through an interpolation process.

Although current usage of MESH3D focuses on refinement of the GSA/PORFLOW model for E-Area PAs, software capabilities and potential uses are more general and not intended to be limited by this SQAP. MESH3D can generally be used to refine any PORFLOW flow field, and is suitable for other programmatic uses (e.g. tank closure PAs).

2.0 SCOPE

This document describes the Software Quality Assurance Plan (SQAP) for the MESH3D model. This SQAP follows the guidelines and minimum content requirements specified in Washington Savannah River Company (WSRC) 1Q, Quality Assurance Manual, Procedure 20-1, Revision 8, Software Quality Assurance (QAP 20-1). The MESH3D model has been classified as Level “C” software per QAP 20-1 Attachment 1, which classifies “software applications used to comply with regulatory laws, environmental permits or regulations and/or commitments to compliance” as Level “C” software. The MESH3D model together with other PA software is used to provide a reasonable assurance that the Performance Objectives of DOE Order 435.1 will be met and to establish radionuclide limits for the various waste disposal units. This SQAP addresses the life cycle requirements for the MESH3D model as Level “C” software.

3.0 ROLES AND RESPONSIBILITIES

Oversight and assignment of all PA related work, including MESH3D modeling, is provided by the Manager, Environmental Analysis & Performance Modeling. The Cognizant Technical Function (CTF) associated with HELP modeling is Greg Flach of the Environmental Science and Bio Technology section of SRNL. The Cognizant Quality Function is Steve Loflin of the Quality Engineering group in SRNL. Should other SRNL business programs choose to use MESH3D at the same Level "C" functional classification, oversight will be provided by the appropriate Manager. The CTF, CQF and this SQAP can remain unchanged.

4.0 SOFTWARE LIFE CYCLE

WSRC Manual 1Q, Procedure 20-1 will used to assure quality throughout the Software Life Cycle. Software specific implementation of 1Q, 20-1 for MESH3D is discussed below as needed to supplement 1Q, 20-1.

4.1 FUNCTION

The functional requirements phase defines the software capabilities required to perform the task of interest that will be designed into the software by in-house or vendor software designers. The MESH3D model has been classified as Level “C” software by the Manager, Environmental Analysis & Performance Modeling.

The MESH3D code was developed by Greg Flach as a personal calculation tool, and first applied to a Special Analysis for the Intermediate Level Vault (Flach and Hiergesell 2004). The existing code is now being considered for use as general purpose software.

In reference to WSRC Manual 1Q, Procedure 20-1, Attachment 2, MESH3D is thus further classified as "Level C Existing Software". Required components of the SQAP are "Evaluation" and "Configuration Control", with other elements optionally applied using a graded approach.

4.2 EVALUATION

Following initial code development and multiple uses controlled by design-checking of each application, the MESH3D code was found to have general applicability to E-area PA analyses. MESH3D is existing software currently used solely by the software developer, Greg Flach. Therefore many of the optional elements in Attachment 2 of 1Q 20-1 are not required to assure software quality. Additional optional components deemed appropriate for MESH3D are Design, (Verification and Validation, V&V) Testing, Acceptance Testing and Access Control. Requirements and Implementation are not warranted because MESH3D is existing software. Formal User Instructions, Operation and Maintenance procedures, and Error Impact procedures are not warranted, provided the developer (Greg Flach) continues to be the sole user of MESH3D. The SQAP will be modified should additional Users be desired. The selected optional elements are discussed further below. Software Design and initial V&V and Acceptance Testing are documented as part of this SQAP.

4.3 DESIGN

The primary function of MESH3D is to interpolate flow field results from a coarse mesh onto a finer grid created by subdivision of the original mesh. Figure 1 illustrates the concept using an example application to the Intermediate Level Vault. The interpolation method (Flach and Hiergesell 2004, Appendix A) is described in this section. Although the algorithm is not constrained to a specific coarse mesh PORFLOW, the GSA/PORFLOW model (Flach 2004) will be used as an example.

Cells in the refined mesh are assigned the saturation value of the parent coarse-mesh cell in which they reside. The resulting saturation field retains the coarseness of that computed from the GSA/PORFLOW model, but this attribute is of little consequence because plume migration occurs below the water table where cells are 100% saturated. Material type is transferred to the fine mesh in the same manner.

The Darcy velocity field computed from the GSA/PORFLOW model is in the form of volumetric flowrates defined at faces between adjoining cells ("FC" variable). For steady-state and constant properties, flowrates across the six faces of a cell satisfy the mass balance

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where flow in the positive coordinate direction is positive. In developing an interpolation scheme to transfer flowrates from the coarse-mesh to the refined-mesh, each face flow is assumed to be uniformly distributed across its face. The flowrate across an arbitrary plane perpendicular to the X-axis and within the cell of interest can be written

$$FC_x = FC_{X-} + \xi(FC_{Y-} - FC_{Y+} + FC_{Z-} - FC_{Z+})$$

where

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ranges between 0 and 1. Letting **Error! Objects cannot be created from editing field codes.** and **Error! Objects cannot be created from editing field codes.** denote the number of subdivisions in the Y and Z directions, a coarse-mesh **Error! Objects cannot be created from editing field codes.** face is comprised of **Error! Objects cannot be created from editing field codes.** faces in the refined mesh. The flowrate across each of these smaller faces at position **Error! Objects cannot be created from editing field codes.** becomes

$$fc_x = \frac{FC_x}{ny \cdot nz}$$

Similar expressions can be written for the other two coordinate directions. The interpolation scheme produces mass conservation on a cell-by-cell basis (assuming the coarse mesh preserves mass). Velocities on the fine resolution mesh are computed directly from face flowrates.

In some cases, the structured MESH3D will include "inactive cells". These grid blocks encompass space above the ground surface that is not represented in the unstructured GSA/PORFLOW model, and are added for the convenience of a structured mesh. Volumetric flow rates across inactive cell faces are thus not directly available from GSA/PORFLOW. FC assignments for inactive cells take advantage of the specific way GSA/PORFLOW boundary conditions are imposed over the top surface of the unstructured mesh. No flow conditions are imposed on all vertical (xz and yz) faces. Boundary flow occurs only across horizontal (xy) faces. For inactive MESH3D cells, FC for vertical faces is set to zero and flow across horizontal faces is set to that of the underlying horizontal face. In other words, the flow across an exposed horizontal face is propagated upward through a columns of non-interacting inactive cells. This approach conserves mass in inactive cells.

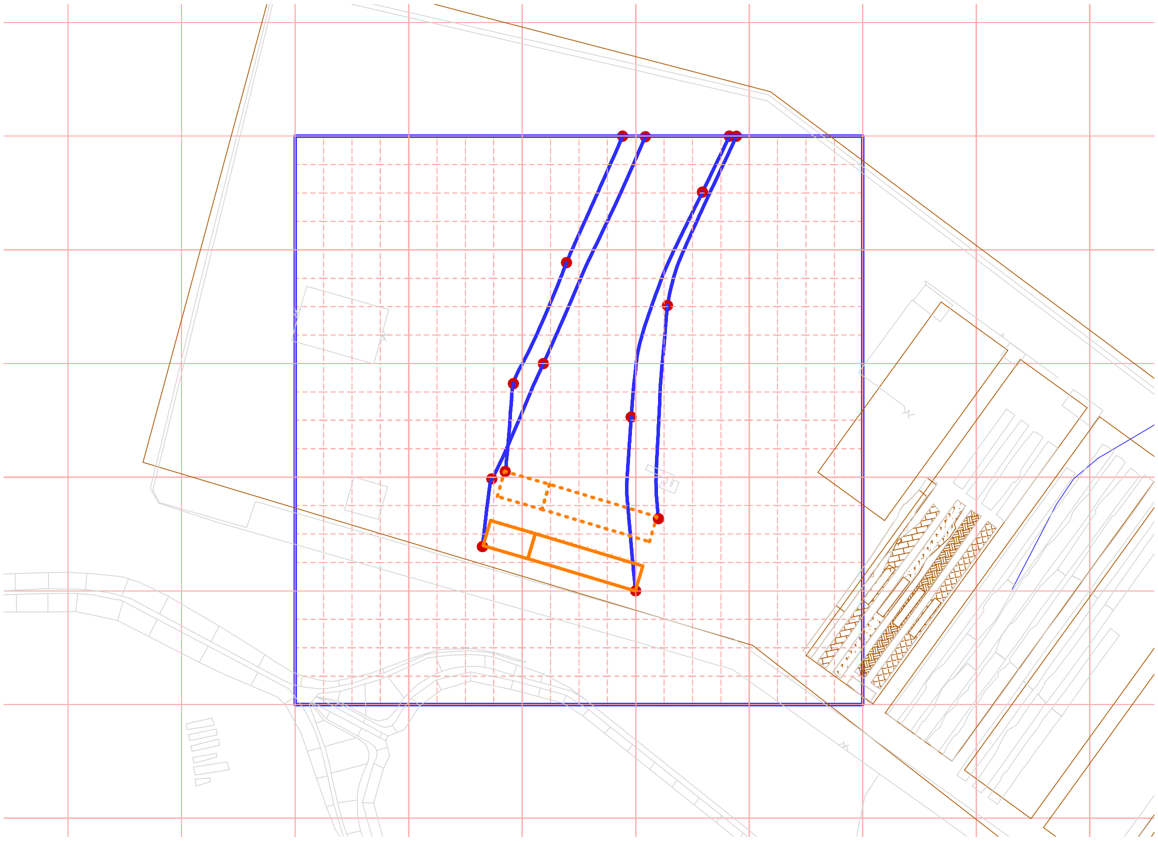

Figure 1 Example MESH3D application showing mesh refinement for Intermediate Level Vault.

4.4 TESTING

Three groups of verification and validation (V&V) tests were devised for MESH3D. The test cases use Slit Trenches #1 (SLIT1) as the example application.

Grid and Darcy flow

The first set of tests is a visual comparison of Tecplot generated particle tracking results for the GSA/PORFLOW grid and original UVW velocity components (Figure 2), the GSA/PORFLOW grid with UVW velocity components computed from FC by MESH3D (Figure 3), a MESH3D cutout without mesh refinement (Figure 4), and a MESH3D mesh with 3×3×3 refinement (Figure 5). Each figure shows particle tracks emanating from the four

corners of SLIT1 at an elevation of 230 ft, which is near the water table. Time markers are shown every two years, assuming an effective porosity of 25%. Shading delineates saturated and unsaturated conditions based on computed pressure head.
MESH3D computes U, V and W darcy velocity components from the convective flux field (FC), using a simple averaging algorithm that apparently differs from that embedded in PORFLOW. The resulting UVW values are thus not identical as those output from PORFLOW, and somewhat different particle tracks are observed in Figures 2 and 3. Figure 4 shows particle tracking results for a SLIT1 cutout grid generated by MESH3D, without mesh refinement. Within the extent of the SLIT1 grid, the pathlines are the same as shown in Figure 3, as expected. Figure 5 shows a higher resolution SLIT1 grid, created by subdividing the original grid by a factor of 3 in each coordinate direction. The corresponding particle tracks in Figure 5 differ from those in Figure 4 because of mesh refinement.

PORFLOW uses the FC variable to simulate advective transport of contamination, and the UVW variables are used in the hydrodynamic dispersion term. Therefore the discrepancy in velocity information between PORFLOW and MESH3D output affects only contaminant dispersion. The effect is quantified in subsequent V&V tests involving solute transport.

Inspection of Figures 2 through 5 suggests that the saturation state of the coarse mesh is correctly transferred to the cutout mesh, without (Figure 4) and with (Figure 5) mesh refinement. Because MESH3D results are used to simulate aquifer transport in PA applications, saturation (S) is uniformly 1.0 in the region of interest. Also, the Darcy velocity components UVW are unaffected by S.

Tracer transport

Transport simulations of a conservative (non-decaying, non-sorbing) tracer, using the flow simulations described above, compose the second group of V&V test cases. Again SLIT1 is chosen as the focus of the simulations. Tracer simulations are performed using the original GSA/PORFLOW flow solution (Figure 2), the unrefined MESH3D cutout (Figure 4), and the refined MESH3D cutout (Figure 5). Figures 3, 4 and 5 identify the chosen source and 100 meter monitoring nodes for each model. The source term is a uniform flux of 5 years duration, and transport is simulated for 15 years total.

Concentration results for simulations without specified physical dispersion are shown in Figure 6 (GSA/PORFLOW), Figure 7 (MESH3D without refinement), and Figure 8 (MESH3D with 3×3×3 refinement). In these simulations transport is affected only by advection and numerical dispersion. All three modeling runs include monitoring nodes positioned 100 meters downstream of the source zone that capture the plume centerline. The GSA/PORFLOW (Figure 6) and coarse mesh MESH3D (Figure 7) results are identical for the plume centerline monitoring nodes in common to the two runs, as expected. Higher concentrations are observed for the refined MESH3D grid (Figure 8), due to lower numerical dispersion.

Analogous results are presented in Figures 9 through 11 for specified physical dispersion. In these runs, the longitudinal dispersivity is set to 10% of 100 meters or 32.8 ft, and the transverse dispersivity is set to 1% or 3.28 ft. Ideally, identical results would be observed for the GSA/PORFLOW and MESH3D simulations, as was the case above for no physical dispersion. The GSA/PORFLOW (Figure 9) and coarse mesh MESH3D (Figure 10) results are similar, but not identical, for the plume centerline monitoring nodes in common to the two runs. The discrepancy, about 3% for the peak concentration in time and space, is due to differing UVW fields. The GSA/PORFLOW transport simulation uses UVW values computed internally by PORFLOW. The coarse mesh MESH3D simulation uses UVW velocity components computed external to PORFLOW using the FC field. Both models use the same FC input. These velocity field differences have been discussed in the previous section in the context of particle tracking results. Figure 11 shows the results for the refined MESH3D cutout. The peak concentration is significantly larger for the refined mesh, due to lower numerical dispersion.

Interpolation and mass balance checks

The peak concentration in Figures 9, 10 and 11 occurs at PORFLOW elements 54610 (GSA/PORFLOW), 876 (MESH3D cutout without refinement) and 23177 (MESH3D cutout with 3×3×3 refinement) respectively. The centriods of all three elements are co-located as evidenced by the following excerpts from saturation output files (S.out):

```
  element    X            Y            Z              S
    54610    1.29000E+04  1.23000E+04  2.02043E+02    1.000000E+00
      876    1.29000E+04  1.23000E+04  2.02042E+02    1.000000E+00
    23177    1.29000E+04  1.23000E+04  2.02044E+02    1.000000E+00
```

The coordinates above refer to the element center, where a "node" in PORFLOW parlance is located. Elements 54610 and 876 are identical in dimensions, and 23177 is a much smaller cell, the central element among the 27 total sub-cells composing the 3×3×3 refinement. Volumetric flow rates (L^3/T; not flux) for the three elements have been extracted from FC output files below (FC.out):

```
ELEMENT#       X-          X+          Y-          Y+          Z-          Z+
   54610    1.2761E+05  1.1948E+05  2.3493E+05  2.5910E+05 -8.0309E+04 -9.6336E+04
     876    1.2761E+05  1.1948E+05  2.3493E+05  2.5910E+05 -8.0307E+04 -9.6334E+04
   23177    1.3878E+04  1.3577E+04  2.6999E+04  2.7894E+04 -9.5158E+03 -1.0110E+04
```

Note that the six face flows are essentially identical between element 54610 and 876. The slight difference is an artifact of number of significant digits included in PORFLOW output. The data for element 54610 comes from a PORFLOW archive file (FLOW2.sav), in which FC is printed using an `±X.XXXXXXXXe±XX` format. The FC data for element 876 is derived from a PORFLOW OUTPut command, for which the format is `±X.XXXXe±XX` (FC.out). The differing precision is manifest in the above numbers. The comparison provides verification that MESH3D transfers FC from the GSA/PORFLOW mesh to the cutout mesh when there is no mesh refinement.

The FC values shown for smaller element 23177, one of 27 embedded in the larger parent element, can be verified through a spreadsheet calculation as shown in Table 1. The X-, Y- and Z- faces for the small element are located 1/3 the distance from the left and right faces of the parent cell. Similarly, the X+, Y+, and Z+ faces are located 2/3 the distance from the negative and positive faces. The table shows the two-step process described previously. The first step is to interpolate between negative and positive coarse mesh faces to achieve an intermediate coarse mesh flow rate. The second step is to equally subdivide the intermediate face flow into smaller face flows. The spreadsheet calculation confirms that MESH3D correctly interpolated FC information from the parent coarse mesh cell for element 23177.

Table 1 FC interpolation calculation for element 23177.

element 876	FC_{X-}	FC_{X+}	FC_{Y-}	FC_{Y+}	FC_{Z-}	FC_{Z+}
observed	1.2761E+05	1.1948E+05	2.3493E+05	2.5910E+05	-8.0307E+04	-9.6334E+04
element 23177	FC_X @ $\xi=1/3$	FC_X @ $\xi=2/3$	FC_Y @ $\eta=1/3$	FC_Y @ $\eta=2/3$	FC_Z @ $\zeta=1/3$	FC_Z @ $\zeta=2/3$
calculated	1.2490E+05	1.2219E+05	2.4299E+05	2.5104E+05	-8.5649E+04	-9.0992E+04
	$1/9 \cdot FC_X$ @ $\xi=1/3$	$1/9 \cdot FC_X$ @ $\xi=2/3$	$1/9 \cdot FC_Y$ @ $\eta=1/3$	$1/9 \cdot FC_Y$ @ $\eta=2/3$	$1/9 \cdot FC_Z$ @ $\zeta=1/3$	$1/9 \cdot FC_Z$ @ $\zeta=2/3$
	1.3878E+04	1.3577E+04	2.6999E+04	2.7894E+04	-9.5166E+03	-1.0110E+04
element 23177	FC_{X-}	FC_{X+}	FC_{Y-}	FC_{Y+}	FC_{Z-}	FC_{Z+}
observed	1.3878E+04	1.3577E+04	2.6999E+04	2.7894E+04	-9.5158E+03	-1.0110E+04

After transferring and interpolating FC data from the coarse mesh GSA/PORFLOW model to the cutout grid, MESH3D also performs an internal mass balance check on each cell in the cutout grid. Mass balance discrepancies exceeding 0.2% are flagged for further investigation. The screen output captured below for the 3×3×3 refined grid indicates no cells with a significant mass balance error. This outcome suggests the interpolation scheme is mass-conserving and has been correctly implemented in MESH3D.

Cell-by-cell check (MESH3D)

```
make    PartialBuild=.false.  WriteTecplot=.true.  Archive=TEMPLATE2  Zoom=ZOOM2
  EffPor=0.25  RunMesh3d        #complete build, GEOM + DATA
echo "../GSA/FACT.geom"  >tmp
echo "../GSA/FACT.id"   >>tmp
echo "../GSA/TYP2.dat"  >>tmp
echo "../GSA/S.out"     >>tmp
echo "../GSA/HEAD.out"  >>tmp
echo "../GSA/P.out"     >>tmp
echo "../GSA/FC.out"    >>tmp
echo ".false."          >>tmp
echo ".true."           >>tmp
echo "TEMPLATE2.ARC"            >>tmp
echo "MESH.dat"                 >>tmp
echo "COOR.dat"                 >>tmp
echo "ZOOM2.ARC"                >>tmp
echo "Mesh3d.tec"               >>tmp
echo "WaterTable.out"           >>tmp
echo ""50       60      3""             >>tmp
echo ""45       55      3""             >>tmp
echo ""1        17      3""             >>tmp
echo "0.25"             >>tmp
echo "365"      >>tmp
cat tmp  |../../../Tools/Mesh3d/Debug/Mesh3d.exe
   nnx, nny, nnz:          109         78          22
  total elements:       174636
 active elements:       102294
 zoom i elements:           50          59
 zoom j elements:           45          54
```

```
zoom k elements:            1          16
  zoom elements:        43200
  inactive zoom:         1728
Checking for mass balance problems with FC
writing MTYP
writing S
writing FC
writing U
writing V
writing W
writing GSA corner
writing ZOOM corner
writing GSA center
writing ZOOM center
writing water table information
```

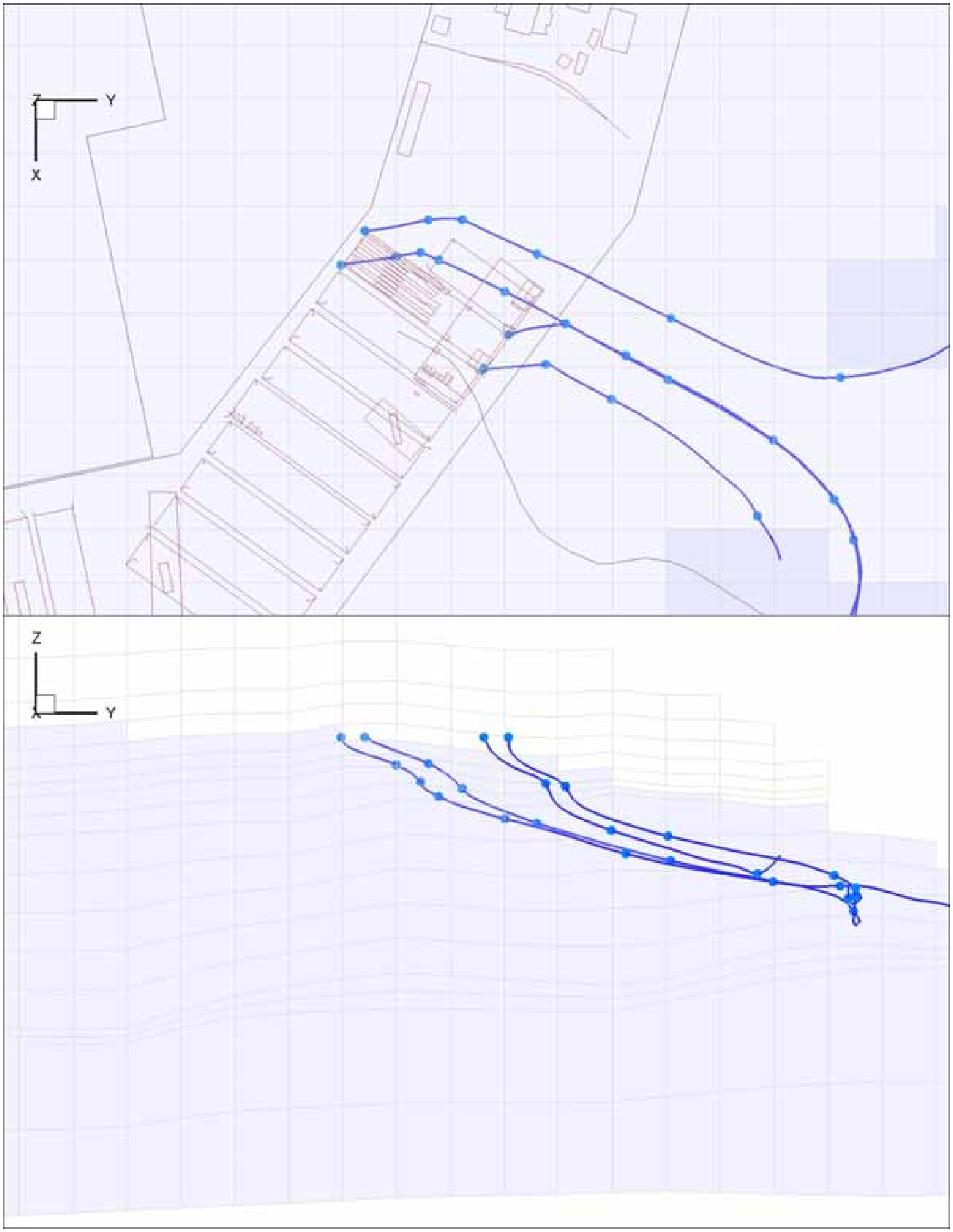

Figure 2 Particle tracking and saturation field results for GSA/PORFLOW - original UVW velocity components.

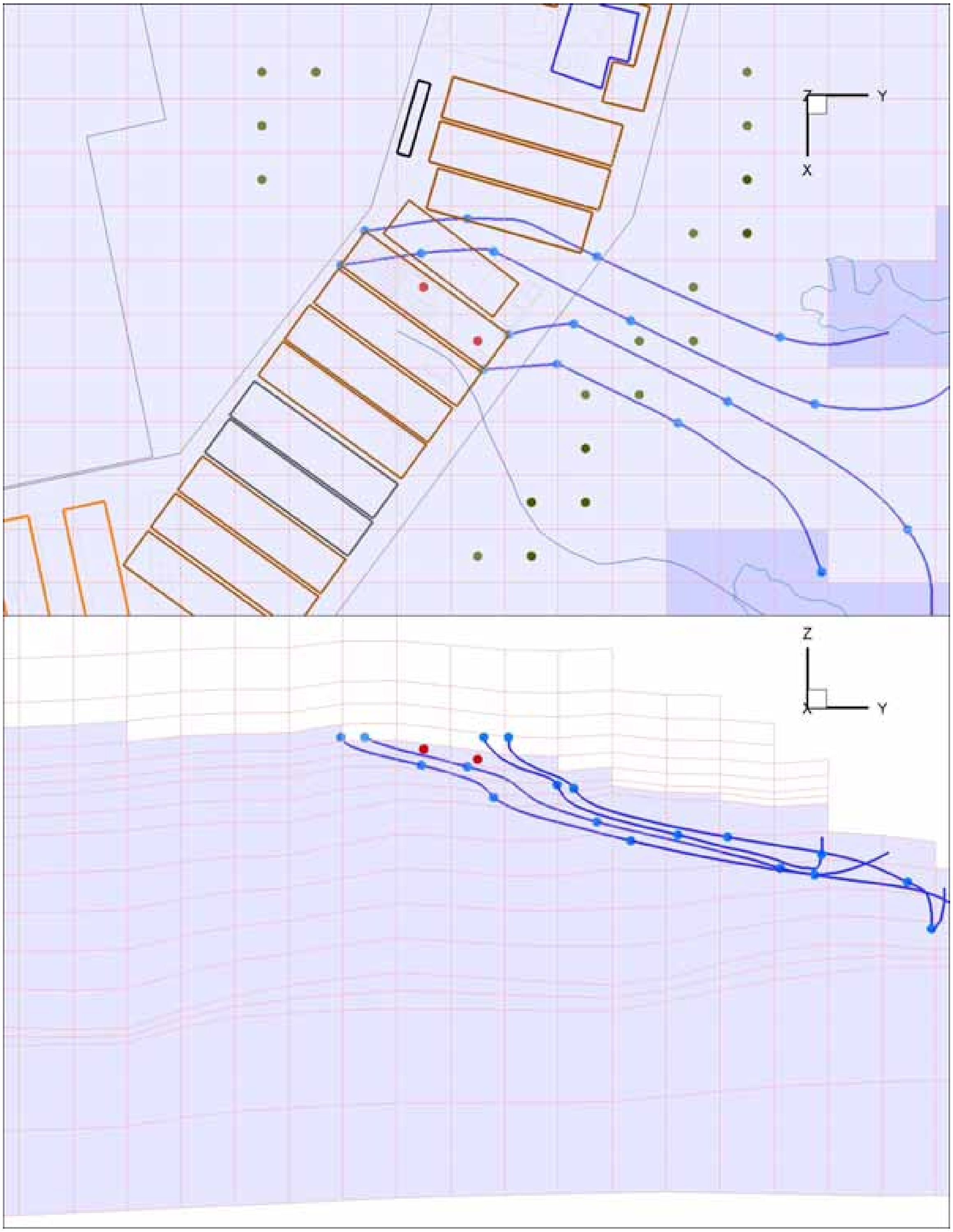

Figure 3 Particle tracking and saturation field results for GSA/PORFLOW - UVW velocity components computed from FC.

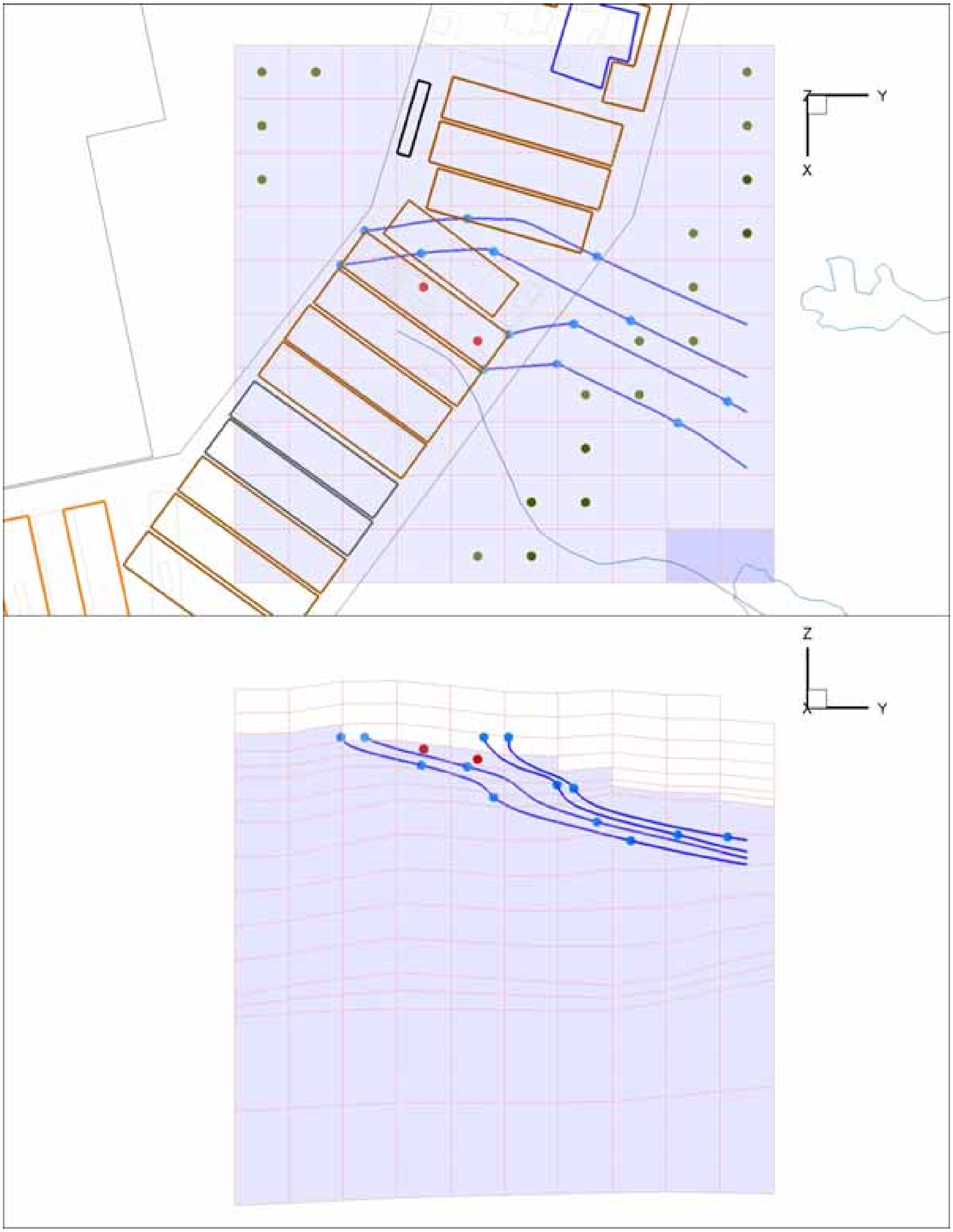

Figure 4 Particle tracking and saturation field results for MESH3D cutout without mesh refinement.

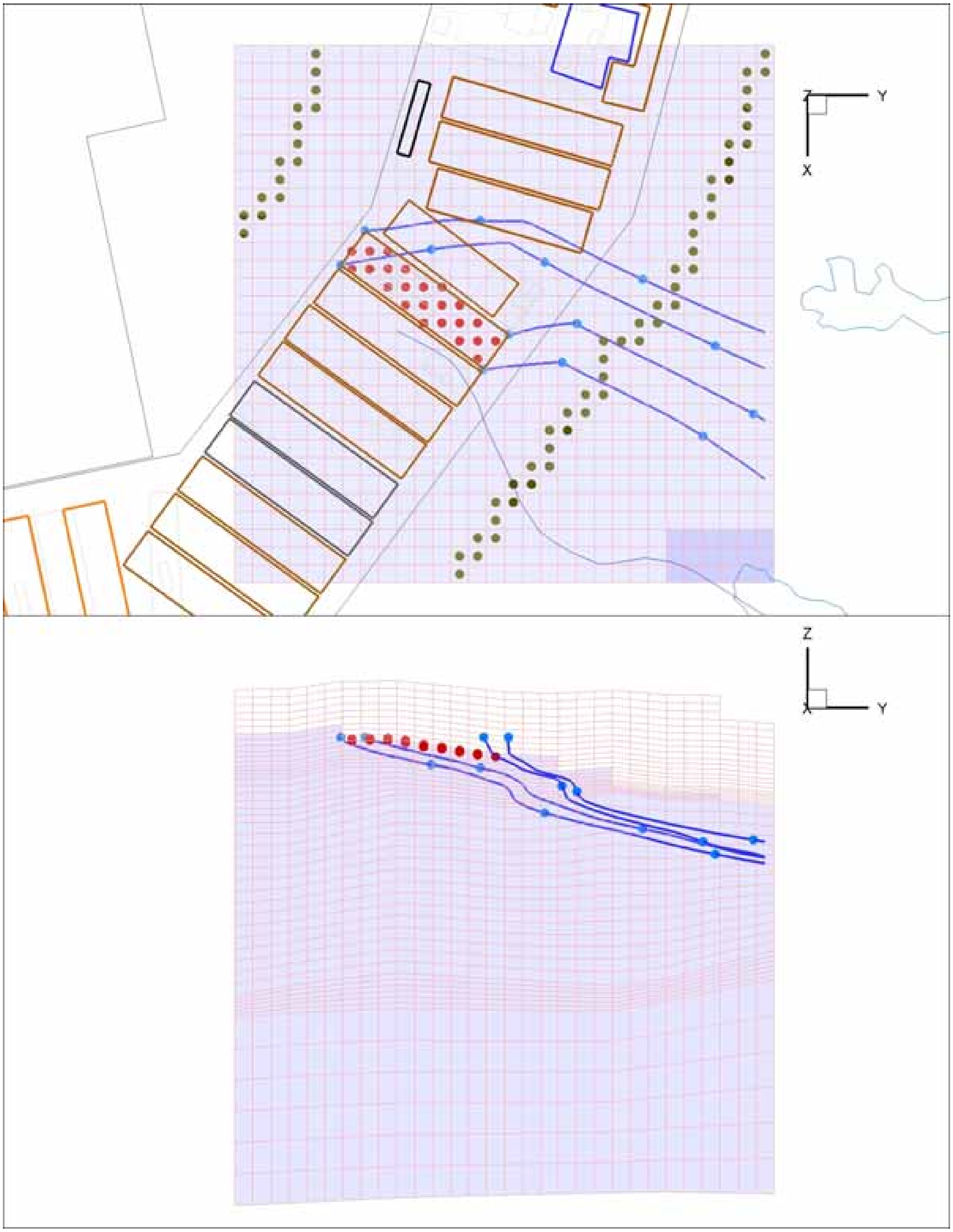

Figure 5 Particle tracking and saturation field results for MESH3D cutout with 3×3×3 mesh refinement.

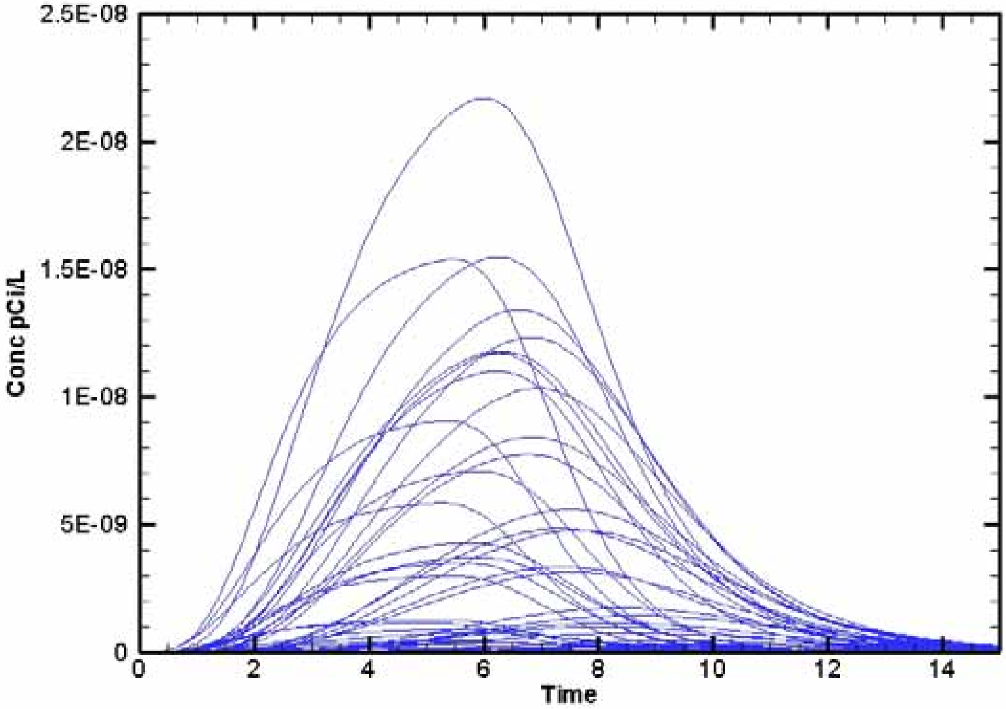

Figure 6 Concentration transients at monitoring nodes for GSA/PORFLOW; no dispersion.

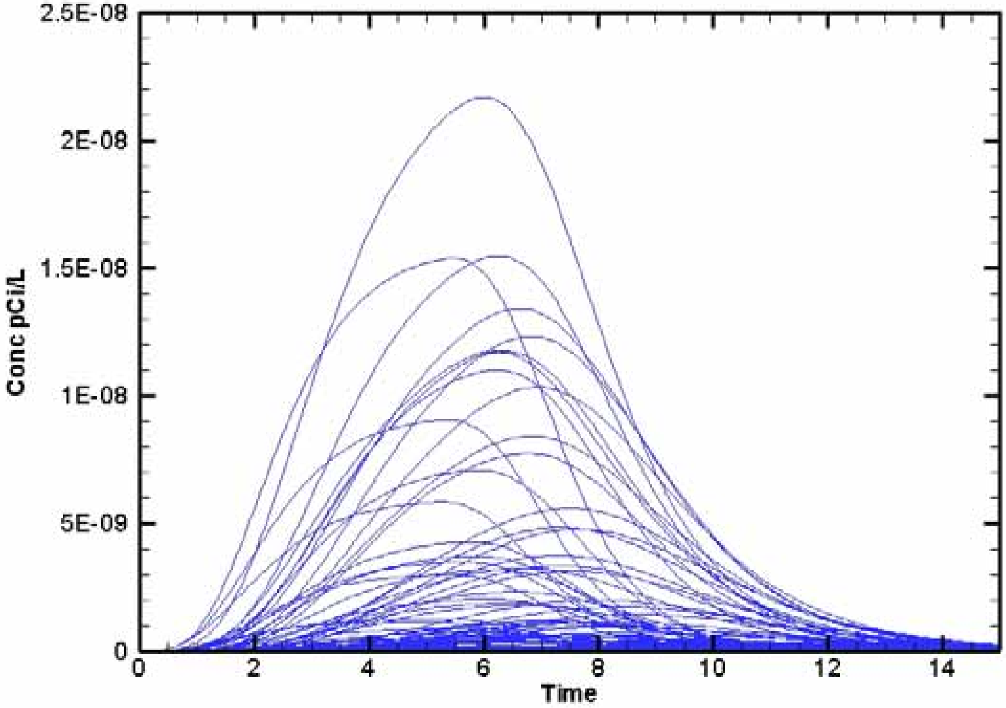

Figure 7 Concentration transients at monitoring nodes for MESH3D cutout without mesh refinement; no dispersion.

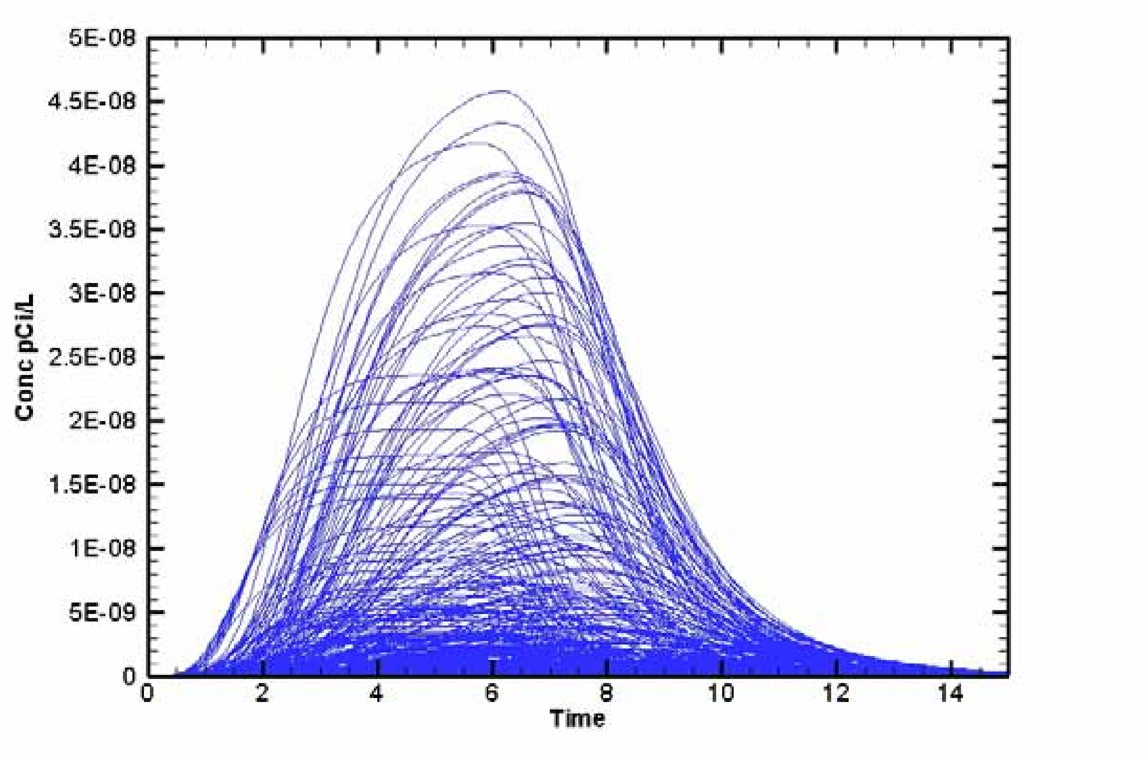

Figure 8 Concentration transients at monitoring nodes for MESH3D cutout with 3×3×3 mesh refinement; no dispersion.

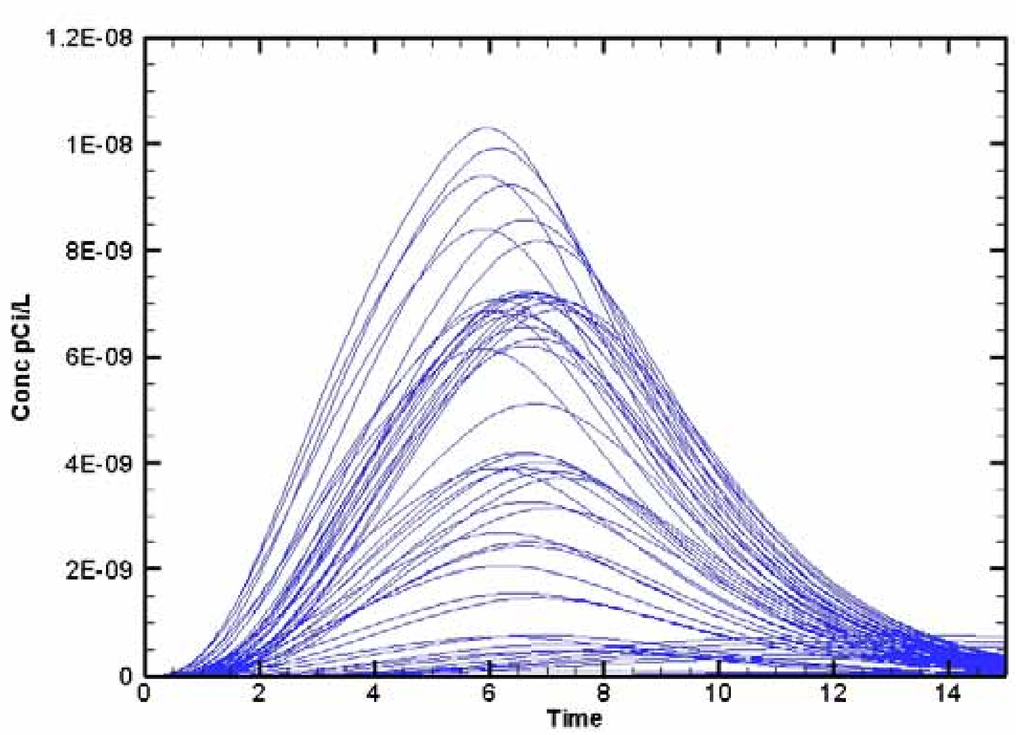

Figure 9 Concentration transients at monitoring nodes for GSA/PORFLOW; with dispersion.

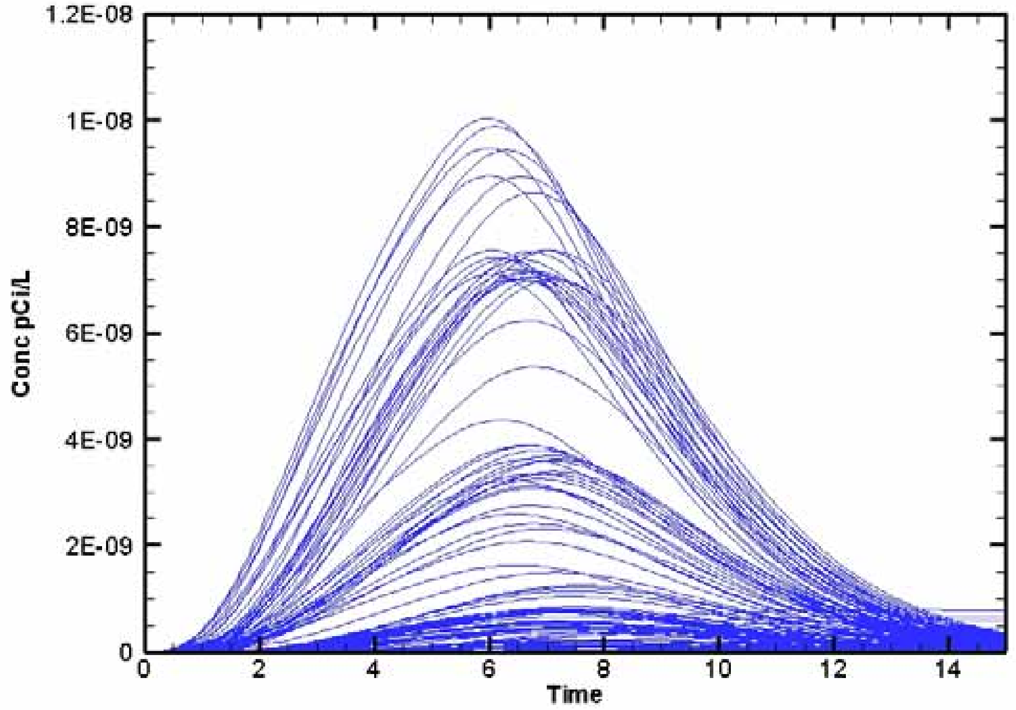

Figure 10 Concentration transients at monitoring nodes for MESH3D cutout without mesh refinement; with dispersion.

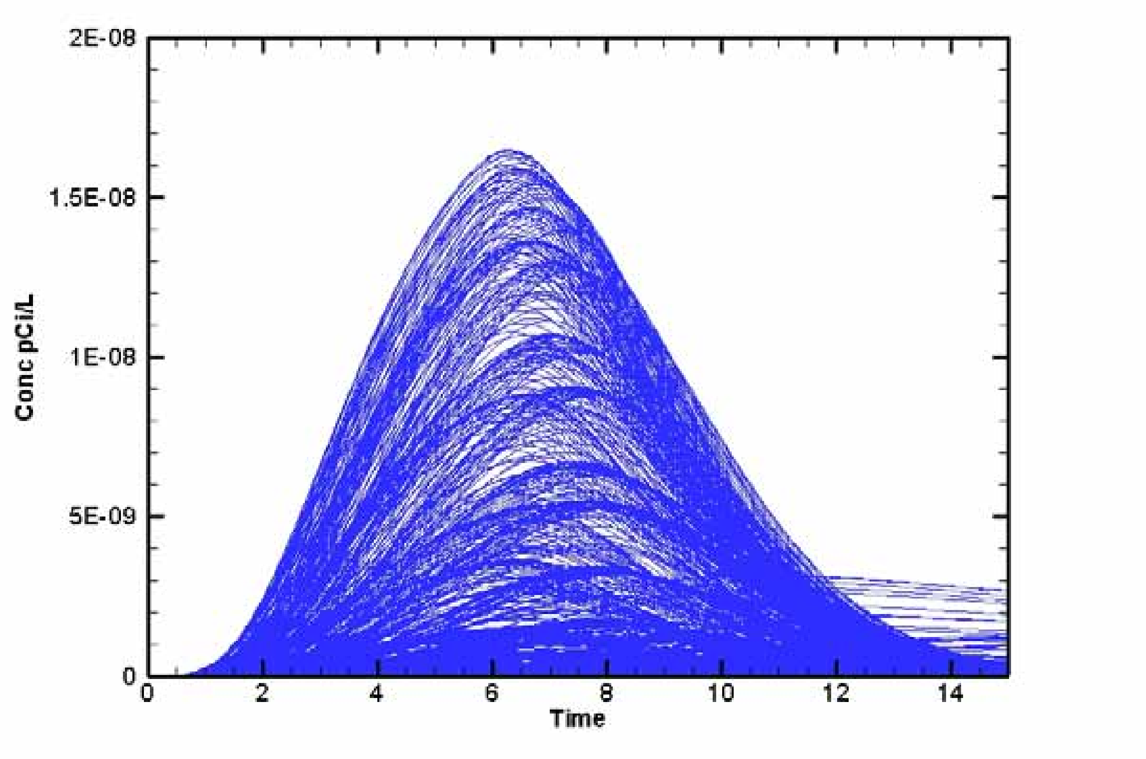

Figure 11 **Concentration transients at monitoring nodes for MESH3D cutout with 3×3×3 mesh refinement; with dispersion.**

4.5 CONFIGURATION CONTROL

Configurations of MESH3D will be identified and documented by the CTF through paper and electronic copies of the source code kept on file. Records of superseded configurations will be retained in the software file indefinitely.

4.6 ACCESS CONTROL

Operation of MESH3D will be overseen by the Manager, Environmental Analysis and Performance Modeling, who will assign tasks as needed, and by the CTF, who will ensure assigned tasks are consist with the model capabilities. Access to the software will be limited to the CTF. Access will be controlled by residence of the software on a file storage space to which only the CTF (and system administrators) has access. Should additional Users be desired, the SQAP will be modified to include development of a User Manual, and an expanded access control method. Access for other potential business programs will be controlled by the respective Manager.

4.7 PROBLEM REPORTING AND CORRECTIVE ACTION

The CTF shall report software problems/issues to the Manager, Environmental Analysis and Performance Modeling. The Manager will notify recipients of information generated by

MESH3D, and with the input from the CTF and information recipients, determine appropriate corrective action. Problem reporting and corrective action for other potential business programs will be controlled by the respective Manager.

5.0 REFERENCES

Flach, G. P., 2004, GROUNDWATER FLOW MODEL OF THE GENERAL SEPARATIONS AREA USING PORFLOW (U), WSRC-TR-2004-00106, Rev. 0.

Flach, G. P. and R. A. Hiergesell, 2004, SPECIAL ANALYSIS: REVISION OF INTERMEDIATE LEVEL VAULT DISPOSAL LIMITS (U), WSRC-TR-2004-00346, Rev. 0.

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