SIGNIFICANCE OF MESH DENSITY IN AQUIFER STORAGE AND RECOVERY MODELING USING THE WASH123D NUMERICAL MODEL

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ABSTRACT

Aquifer Storage and Recovery (ASR) is a means to store fresh water deep underground in brackish water aquifers and to recover the stored water at a later date during emergencies or times of water shortage. ASR is expected to provide a cost-effective solution to many of the world's water management needs. However, the quality of the stored water may degrade over time due to mixing and buoyancy stratification. Water quality may further be reduced during extraction due to upconing of saline water underlying the ASR well. This water quality degradation may reduce the volume of the available fresh water during recovery to the point that the ASR well is no longer cost effective. The mixing of fresh and saline water can be modeled by both the diffusion and dispersion transport processes. An unstructured three-dimensional (3-D) finite element mesh is the framework used to solve the flow and transport equations in the heterogeneous subsurface media in this study. Because flow and concentration gradients may be high in the vicinity of an ASR well, the vertical and horizontal resolution of the 3-D mesh in the vicinity of the ASR well is important. Meshes that do not have sufficient resolution in the area of interest may not accurately simulate observed conditions in these high gradient areas. On the other hand, meshes that contain too much resolution will require more computational resources, resulting in extended run time. This paper presents a sensitivity analysis conducted to evaluate the effect of various mesh resolutions on computational speed and accuracy. The WASH123D model was used to compute coupled groundwater flow and transport for ASR simulations. During the development of WASH123D example models, meshes of various vertical and horizontal resolutions were tested. The WASH123D-ASR simulations became more computationally stable as the vertical resolution was increased in the geologic units above, below, and containing the ASR well. However, there is also a limit of vertical mesh resolution, depending on the project goals, beyond which no additional improvement in accuracy of results is obtained.

1. INTRODUCTION

Water management is key to restore the South Florida Ecosystem. Aquifer Storage and Recovery (ASR) is one of the proposed alternatives recommended by the Comprehensive Everglades Restoration Plan (CERP, http://www.evergladesplan.org/) to help with water supply, storage, and distribution for South Florida. Numerical models are used as part of the ASR Regional Study to help evaluate the effectiveness of ASR. A box model (~ 40 miles x 40 miles x 2340 ft) was developed (England et al., 2006) using the WASH123D finite element numerical model (Yeh, et al., 2006) to evaluate modeling code performance under different hydraulic conditions. To conduct effective and efficient ASR simulations, both spatial and temporal resolutions are important. This paper details a sensitivity analysis on vertical mesh resolution in the vicinity of ASR well and computational time steps of the model.

2. WASH123D CODE

WASH123D is a finite element numerical model designed to simulate water flow and contaminant transport in a watershed system that can be conceptualized as a combination of 1-D channel networks, 2-D overland regimes, and 3-D subsurface media. In this study, the capability of computing coupled subsurface flow and transport in WASH123D was used for ASR simulations. With WASH123D, the variably saturated, density-dependent water flow is described by the modified Richards' equation and solved with the Galerkin finite element method. The Lagrangian-Eulerian (LE) method is employed to solve the subsurface transport equation, where particle tracking is used in the Lagrangian step to handle the advection term, and the other terms (such as sources, sinks, diffusion, and dispersion) are calculated in the Eulerian step to determine the spatial concentration distribution at the end of each time step. The use of this methodology allows the numerical stability of WASH123D not to be restricted by the Mesh Courant number. In addition, the Mesh Peclet number is restricted only by computational accuracy, not numerical stability. More detailed discussion on various types of numerical dispersion and how the LE method deals with these types of numerical dispersion can be found elsewhere (Cheng et al., 1996; Cheng et al., 1998; Yeh et al, 2006).

3. MESH DEVELOPMENT

The DoD Groundwater Modeling System (GMS, http://chl.erdc.usace.army.mil/software/gms) was used to generate the 3-D unstructured finite element mesh and set up WASH123D-ASR simulations for the box model. The box-model mesh used for this study contained an ASR well at the center of the box (Figure 1a). The horizontal resolution at the ASR well was 10 feet. The elements at the ASR well were deleted to allow Cauchy flux boundary conditions to be assigned directly to the interior faces of the mesh, representing the well injection interval. The horizontal mesh resolution gradually expands to 5000 feet along the model perimeter. Vertical mesh resolution varied among the 8 different conceptual geologic units developed by Jacksonville District (England et al., 2006). The 3 geologic units of interest for this study are shown in Figure 1b. Sufficient vertical mesh resolution was used in the confining units directly above and below the ASR injection aquifer to help resolve the large head and concentration gradients at the interfaces of these confining units. Three vertical mesh densities were tested within the injection aquifer: three elements, six elements, and twelve elements. For the 3-element, 6-element, and 12-element vertical mesh densities, the ASR well injection interval overlaps the central one element, four elements, and eight elements, respectively. Although the vertical mesh density within the ASR well injection interval varies, the top and bottom of injection interval elevations (approximate elevation –1,014 to –1,171 ft) are the same for each model. This set-up allows the mesh to compute for convergent flow fields around the well at the interfaces of the injection aquifer and the two aquitards above and below (i.e., the upper and lower confining units in Figure 1b) without using high resolution meshes and small time steps when the density effect is strong.

4. BOUNDARY AND INITIAL CONDITIONS

The box model simulation was composed of a 30-day period of fresh water injection at a rate of 5 MGD through the ASR well injection interval, followed by a 305-day storage period, and a 30-day recovery period with an extraction of 5 MGD. At the ASR well injection interval, Cauchy flux boundary conditions were used to simulate injection and extraction flow rates of 5 MGD. These boundary conditions were applied to the element faces representing the well injection interval. A saline concentration of 150 mg/L was assigned to the injected fluid to represent fresh water. During the 305-day storage period, a zero Cauchy flux was applied on the well injection interval. Dirichlet boundary conditions were used to assign the total heads along the eastern and western model boundaries to create a west to east hydraulic gradient to mimic the ambient flow. Dirichlet boundary total heads were also assigned over the model top to ensure fully saturated flow throughout the model. WASH123D converts the assigned heads to equivalent fresh water heads during computation based on the concentration and depth of each node on the model boundary. No-flow boundary conditions were used along the northern, southern, and bottom model boundaries.

As for transport computation, Dirichlet boundary conditions were used to assign the concentration along the model perimeter. Variable boundary conditions were employed for the ASR well boundary. During the injection period, 150 mg/L was the assigned saline concentration (i.e., in-coming flux through the ASR well injection interval). The saline concentration associated with the out-going flux during the extraction period was the concentration computed by the model at the ASR well injection interval. Initial concentrations were assigned as 250 mg/L, representing mineralized water, in the upper confining unit and 35,000 mg/L (i.e., the seawater salinity) in the injection aquifer and lower confining units. The horizontal conductivity was 100 ft/d in the injection aquifer and 0.01 ft/d in the adjacent confining units (i.e., the aquitards above and below the injection aquifer). Vertical conductivities were 10% of horizontal conductivities. More information regarding boundary conditions and parameter assignments is provided in England et al., 2006.

5. EVALUATION OF RESULTS

The saline concentration of the fluid at the ASR well during storage and extraction varies with depth and time depending on the relative saline concentration in the surrounding nodes, the extraction rate, and the mixing process in the ASR well. Figures 2 through 4 plot the saline concentration contours on a cross section near the ASR well at initial conditions (0 days), the end of the injection period (30 days), the end of the storage period (335 days), and the end of the recovery period (365 days) for the coarse (i.e., 3-element vertical resolution), the intermediate (i.e., 6-element vertical resolution), and the fine (12-element vertical resolution) mesh densities, respectively.

The three figures show similar results at the end of each time period. At 30 days, the injected fresh water forms a spheroid of low concentration around the ASR well as it displaces the ambient salt water. During the 305-day storage period that follows injection, there is no ASR pumping, and changes in the concentration profile are driven mainly by the density variation. As shown in Figures 2c, 3c, and 4c, fresh water is present at the ASR well, but the concentrations increase further from the well with higher concentrations at depth as a result of buoyancy stratification. During the 30-day recovery period, the ASR well pumps from the aquifer, which reduces the size of the freshwater zone. Figures 2d, 3d and 4d show similar shapes of the concentration profile after recovery including slight upconing of the higher concentrations below the ASR well.

Differences in comparisons of Figures 2, 3 and 4 are evident mainly in “smoothness” of the profiles resulting from interpolation error due to mesh resolution. The coarsest mesh shows a more angular shape of the concentration profiles and the finest mesh a smoother profile. Another notable difference in the concentration profiles between the finest mesh and the coarser meshes is visible at the boundary of the injection aquifer with the upper and lower confining units. In Figure 4b at the top and bottom of the lower concentration spheroid, there are a few nodes that show much higher concentrations than their surrounding nodes. These nodes continue to show higher concentrations throughout the simulation (Figure 4c and 4d). In fact, Figure 4c and 4d show that there is a thin layer of moderately high concentrations separating the fresh water in the vicinity of the ASR well and the freshwater above the injection aquifer. These effects result from the increased mesh resolution in the injection aquifer above and below the ASR well injection interval. For the 12-element vertical mesh resolution, the ASR well injection interval overlaps the central 8 elements. This leaves 2 elements in the injection aquifer above and below the well injection interval. The central node of these two elements maintains a higher concentration throughout the simulation for two reasons. Adjacent to the ASR well, the central nodes maintain high concentrations because the no flow boundary along the face of the adjacent elements creates a null point at these nodes. Beyond the nodes adjacent to the ASR well, the central nodes are affected by boundary effects of the confining unit above the injection aquifer that act to slow the migration of freshwater to these nodes. Further studies should be conducted to investigate how the vertical mesh resolution, for the zones above and below the well injection interval but still within the injection aquifer, would influence the ASR simulation results and subsequently the ASR performance.

A comparison of the saline concentrations during the 30-day recovery period for the different vertical mesh densities was made at a location just east of the ASR well and at approximately 120 feet east of the ASR well. The saline concentrations were averaged over the nodes within the ASR well injection interval at the eastern side of the well for each vertical mesh configuration. Since computational accuracy is dependent on the time step size used in the simulation, several time step sizes were analyzed to evaluate the impact on model results. Time step sizes varied between 0.05 and 5 days (Figure 5). Figure 5 shows that using a 5-day time step size does not provide accurate average concentrations when gradients are large near the ASR well. The 0.5 and 0.05 day time steps provide similar results indicating that no additional accuracy is achieved by decreasing the time step size smaller than 0.5 days. However, using a 0.05 day time step size, the run time was 10 times longer than using a 0.5 day time step. At a distance of 120 feet east of the ASR well, no obvious difference in concentrations is observed due to the variations in time step size.

Vertical mesh resolutions were also evaluated during the recovery period using a time step size of 0.5 days (Figure 6). All of the vertical mesh densities provide similar average concentration values near the ASR and at 120 feet east of the ASR well; however, the finest density mesh provides slightly higher average concentration values than the coarser mesh densities. The average concentration value for the fine mesh during the recovery period is obtained by averaging over the 9 nodes adjacent to the ASR well injection interval. The nodes near the bottom of the ASR well injection interval show concentration values very similar to those for the coarser meshes; however at the top of the ASR well injection interval, the concentration values are higher than those for the coarser mesh nodes. The higher concentrations at the top of the ASR well injection interval increase the average concentration values for the fine mesh. These higher average concentration values are a result of the vertical resolution of the fine mesh above the ASR well injection interval as described previously. Regarding run time, for a 0.5-day time step, an increase in vertical mesh density increases the run time in the range of 20-50%.

6. CONCLUSIONS

Vertical mesh resolution and time step size were evaluated at an ASR well using a WASH123D box model. Vertical mesh resolution does not have a dramatic impact on the concentration profiles or values in the vicinity of the ASR well. However, it is recommended that sufficient vertical mesh density be used to accurately depict concentration profiles. It is also recommended that consideration be given to the vertical mesh density within the injection aquifer but above and below the well injection interval and its impacts on the concentrations near the ASR well. Time step size has a more pronounced affect on near well concentrations than vertical mesh density. A sensitivity analysis should be performed to determine the appropriate time step size for a given model. There is an optimal time step and mesh resolution relationship which will provide an optimal run time and depends of the accuracy required for the scale of the problem under consideration.

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(a)

(b)

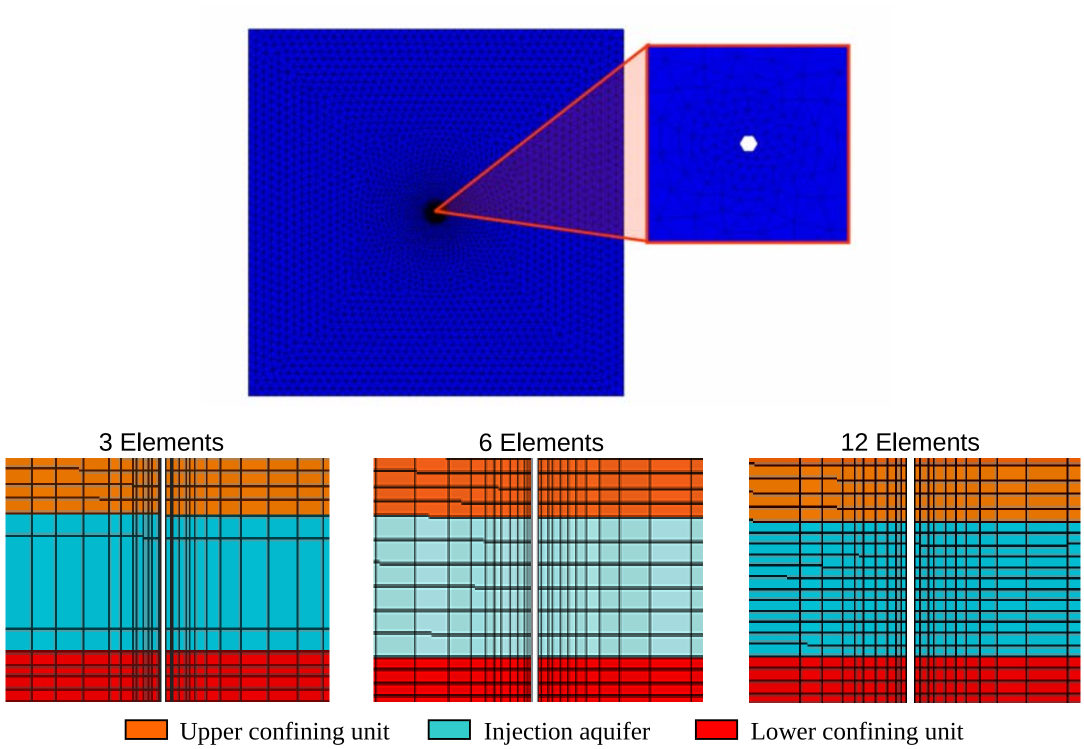

FIGURE 1. (a) Horizontal mesh resolution and (b) Vertical mesh resolution of the box model

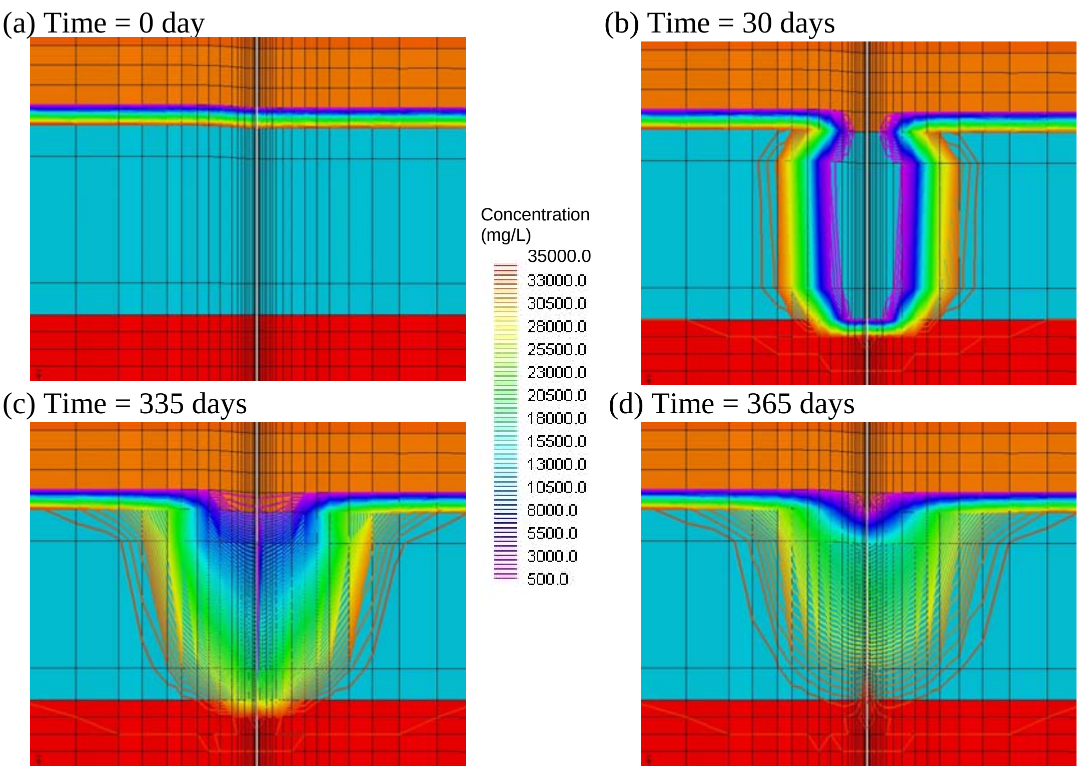

FIGURE 2. Coarse mesh cross-sectional concentration distribution at various times

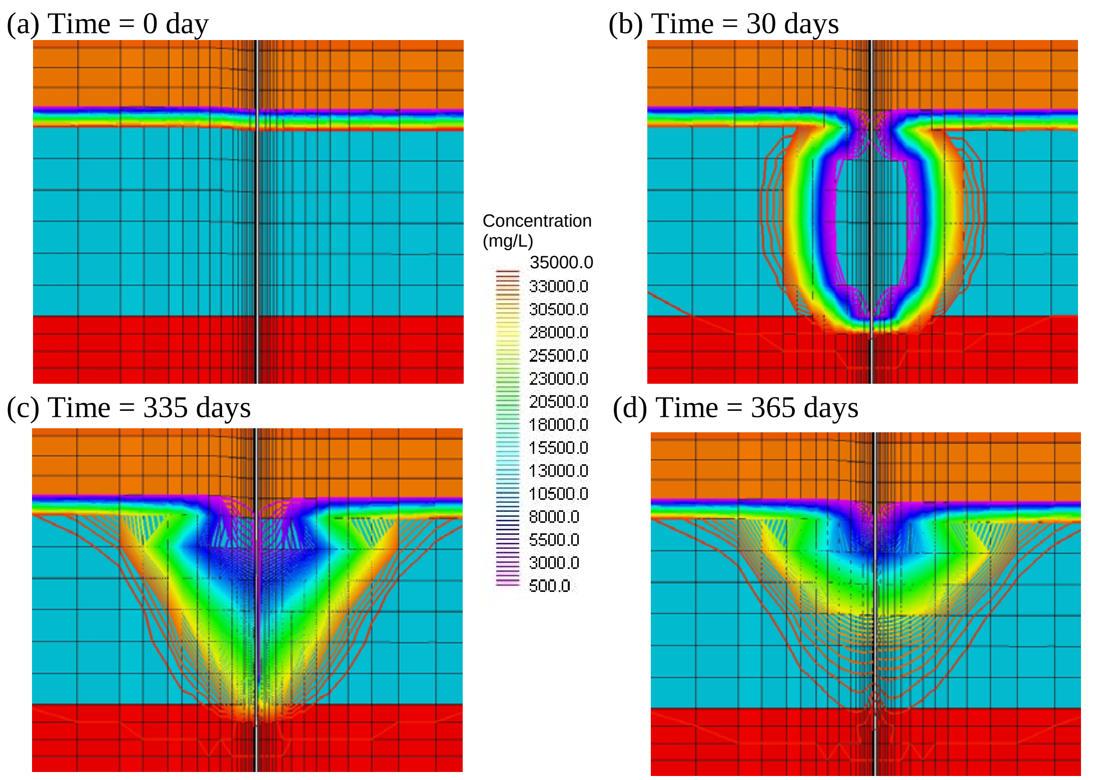

FIGURE 3. – Intermediate mesh cross-sectional concentration distribution at various times

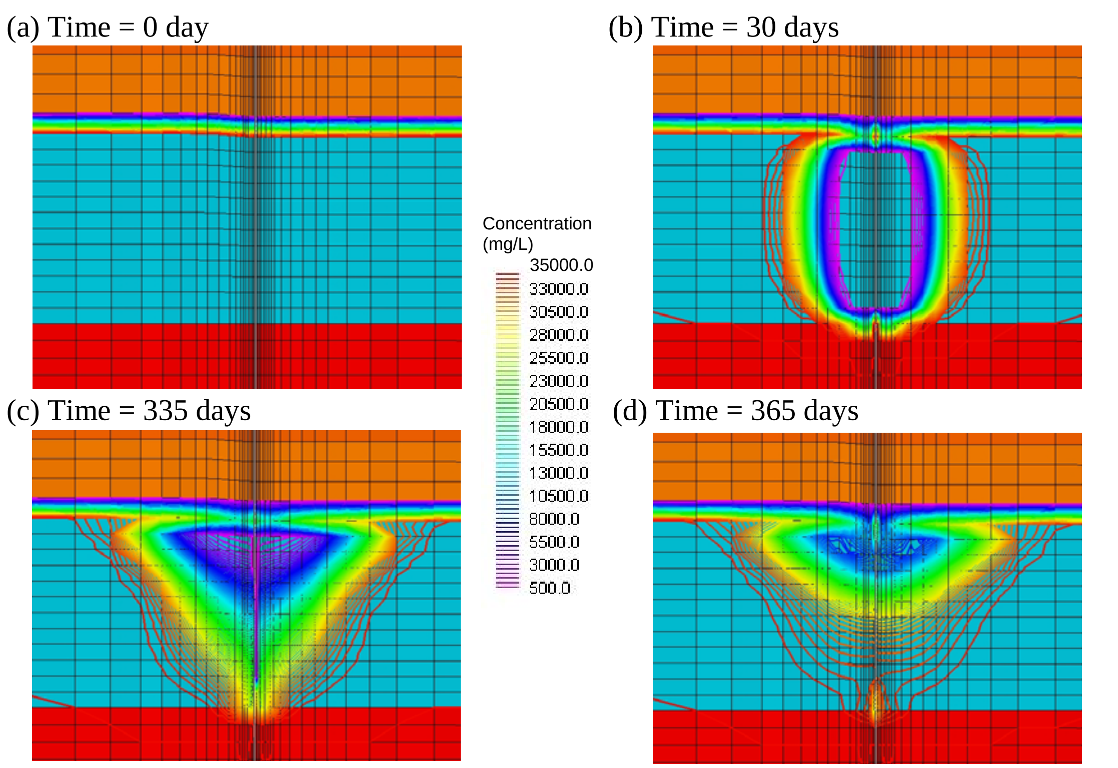

FIGURE 4. – Fine mesh cross-sectional concentration distribution at various times

a) b)

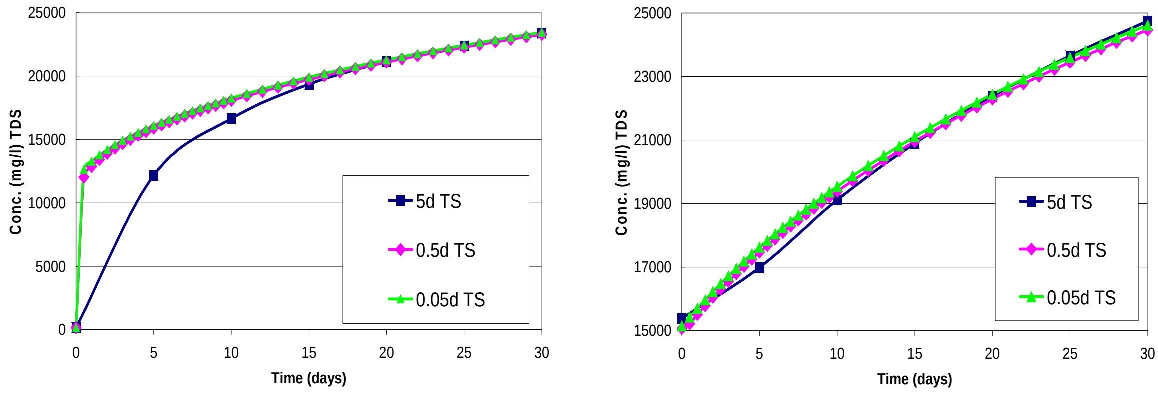

FIGURE 5. – Results of time step variation for the model with 6 element vertical mesh resolution a) at ASR well and b) at 120 feet from ASR well

a) b)

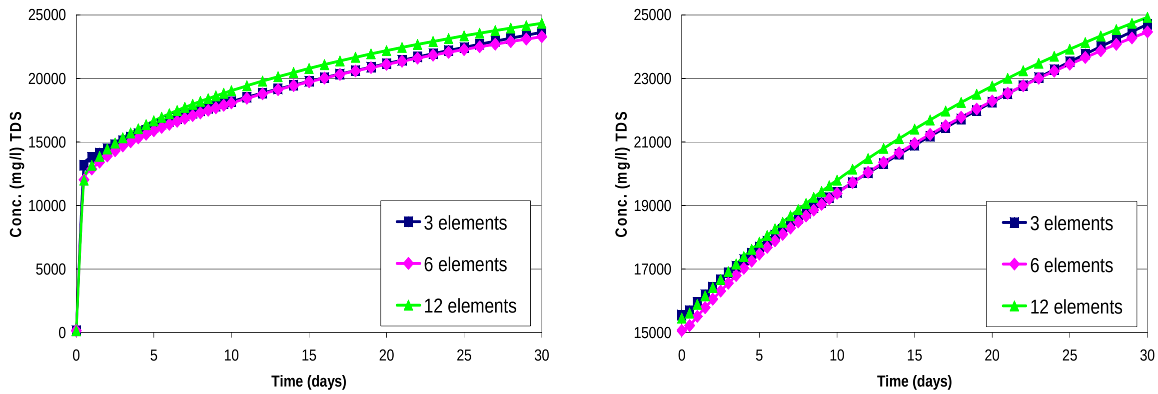

FIGURE 6. – Results of vertical mesh resolution variation at a constant time step size of 0.5 days a) at ASR well and b) at 120 feet from ASR well