MODELING BRACKISH AQUIFER STORAGE RECOVERY WITH THE WASH123D NUMERICAL MODEL

S. M. England[1], H.-P. Cheng[2], G. T. Stevens[1], E. V. Edris[2], C. J. Brown[3]
[1]US Army Corps of Engineers, Philadelphia District, Wanamaker Building, 100 Penn Square East, Philadelphia, PA 19107-3390
[2]Coastal & Hydraulics Laboratory, US Army Engineer Research & Development Center, 3909 Halls Ferry Road, Vicksburg, MS 39180-6199
[3]US Army Corps of Engineers, Jacksonville District, 400 W. Bay Street, Jacksonville, FL 32202

Abstract Aquifer Storage and Recovery (ASR) is the storage of fresh water in an aquifer via injection during times when water is available, and recovery of the water from the same aquifer via pumping during times when it is needed. ASR is expected to provide a cost-effective solution to many of the world's water management needs: storing water during times of flood or when water quality is good, and recovering it later during emergencies or times of water shortage, or when water quality from the source may be poor. ASR systems can usually meet water management needs at less than half the capital cost of other water supply alternatives. When compared to other alternatives that require construction of water treatment plants and surface reservoirs to meet increasing peak demands, potential cost savings have been anticipated. Besides, ASR has been recognized to have less impact on the environment, aquatic and terrestrial ecosystems. When water is stored deep underground in brackish aquifers, however, the mixing of the saline water that is originally in the brackish aquifer and the fresh water that is injected into the aquifer, due to diffusion and dispersion, may degrade the water quality of the stored water and reduce the volume of the available fresh water in the following recovery periods of time. Although both the diffusive and the dispersive fluxes can be modeled as proportional to concentration gradient, the dispersion coefficients are highly dependent on the flow velocity, whereas the diffusion coefficients are independent of the flow velocity. Therefore in the evaluation of brackish aquifer storage recovery (BASR), whatever factor that would significantly affect the flow velocity in the brackish aquifer during both the injection and withdrawal periods should be accounted for in the associated evaluation models. In this paper, we will demonstrate how BASR can be modeled with the WASH123D numerical model that is capable of computing saline transport and density-dependent flow in 3D subsurface media. A hypothetical example that includes various model parameters, *e.g.*, pumping rate, hydraulic conductivities, porosity, and dispersivities will be employed to detail the model setup and conduct a sensitivity analysis.

INTRODUCTION

Aquifer Storage and Recovery (ASR) is one of the proposed alternatives recommended by the Comprehensive Everglades Restoration Plan (CERP, http://www.evergladesplan.org/). The goal of ASR in the South Florida Region is to help with water supply, storage, and distribution. The ASR Regional Study will include numerical groundwater models in order to evaluate the effectiveness of ASR. For this phase of the project, four box models (~ 40 miles x 40 miles x 2340 ft) were developed using the WASH123D finite element code [Yeh, et al., 2003]. Each of the four "cases" is intended to evaluate modeling code performance under different hydraulic conditions. This paper details the WASH123D model construction and summarizes the simulation results for one of the CERP box models developed in support of the United States

Army Corps of Engineers, South Florida Water Management District, and United States Geological Survey efforts on CERP.

WASH123D CODE

WASH123D is a finite element numerical model designed to simulate variably saturated, variable-density water flow, reactive chemical transport, and sediment transport in watershed systems. It is capable of conceptualizing a watershed system as a combination of 1-D river/stream, 2-D overland, and 3-D subsurface sub-domains. A modified Richards' equation is used to describe 3-D density-dependent flow and is solved with the Galerkin finite element method. WASH123D uses the Lagrangian-Eulerian (LE) method to solve the transport equations, 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., 1998; Cheng et al., 1996; Yeh et al., 1995]

MESH DEVELOPMENT

WASH123D uses an unstructured 3-D finite element mesh to solve the flow and transport equations in variably-saturated subsurface media. The box-model mesh used for this study was based on conceptual geology developed by the Jacksonville District. The horizontal resolution of the mesh at the ASR well is 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 screen. The mesh resolution expands to 5000 feet along the model perimeter. Vertical mesh resolution varied among the different conceptual geologic units. 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 the ASR system in these high gradient areas. On the other hand, meshes that contain too much resolution may make the simulation computationally too expensive. To balance between computational accuracy and efficiency, increased resolution was used in the confining units directly above and below the ASR injection aquifer (Upper Floridian). This increased resolution allowed the WASH123D model to depict the large head and concentration gradient at the interfaces of these confining units. The final 3-D mesh was composed of 112,716 nodes and 212,940 triangular-prism elements. Figure 1 illustrates the mesh resolution and conceptual geology used for the box model. The DoD Groundwater Modeling System (GMS, http://chl.erdc.usace.army.mil/software/gms) was used to generate the WASH123D mesh.

BOUNDARY AND INITIAL CONDITIONS

Boundary conditions were assigned to the finite element model to simulate ASR pumping into the Upper Floridian aquifer. At the ASR well, 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 screen within the Upper Floridian Unit (approximate elevation –1,014 to –1,171 ft). The saline concentration of the injected fluid was 150 mg/L. 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. Dirichlet boundary conditions were used to assign the total head along the eastern and western model boundaries. WASH123D converts these assigned heads to equivalent fresh water heads based on the concentration and depth of each node. No-flow boundary conditions were used along the northern and southern model boundaries. Dirichlet boundary conditions were also used to assign the concentration along the model perimeter. Tables 1 and 2 show the hydraulic and transport properties, respectively, for each geologic unit in the WASH123D model.

Table 1 Hydraulic Properties and Boundary Conditions

Geologic Unit	Head BC West Tot Head (ft)	Head BC East Tot Head (ft)	Head BC North Tot Head (ft)	Head BC South Tot Head (ft)	Conductivity Horiz (ft/day)	Conductivity Vert. (ft/day)	Mod. Compress of Matrix (1/ft)	Specific Storage (1/ft)	Effective Porosity
SAS	20	20	No Flow	No Flow	100	10	1.70E-03	1.70E-03	0.25
HG	No Flow	No Flow	No Flow	No Flow	0.01	0.001	7.00E-07	1.19E-06	0.4
UF	50	30	No Flow	No Flow	100	10	7.00E-07	1.01E-06	0.25
MFCU	No Flow	No Flow	No Flow	No Flow	0.01	0.001	7.00E-07	1.07E-06	0.3
MF	40	20	No Flow	No Flow	500	50	7.00E-07	1.01E-06	0.25
LFCU	No Flow	No Flow	No Flow	No Flow	0.01	0.001	7.00E-07	1.07E-06	0.3
LF	0	0	No Flow	No Flow	5000	500	7.00E-07	1.01E-06	0.25
BZ	0	0	No Flow	No Flow	10000	1000	7.00E-07	1.01E-06	0.25

Table 2 Transport Properties and Boundary Conditions

Geologic Unit	Con. BC West (mg/L)	Con. BC East (mg/L)	Con. BC North (mg/L)	Con. BC South (mg/L)	Tortuosity	Bulk Density (slug/ft^3)	Dispersivity Long. (ft)	Dispersivity Trans. (ft)	Flow IC Tot Head (ft)	Con. IC (mg/L)
SAS	150	150	N/A	N/A	1	3.784	0	0	Based on Steady State Simulation with no pumping	150
HG	150	150	N/A	N/A	1	2.969	0	0		150
UF	35000	35000	N/A	N/A	1	3.784	0	0		35000
MFCU	35000	35000	N/A	N/A	1	3.531	0	0		35000
MF	35000	35000	N/A	N/A	1	3.784	0	0		35000
LFCU	35000	35000	N/A	N/A	1	3.531	0	0		35000
LF	35000	35000	N/A	N/A	1	3.784	0	0		35000
BZ	35000	35000	N/A	N/A	1	3.784	0	0		35000

Based on the boundary conditions at time zero and hydraulic properties in the simulation, WASH123D calculates a steady state flow field, which was later used as the initial condition for the transient portion of the simulation. Since the WASH123D model is a coupled density dependent code, the initial hydraulic head boundary conditions were converted to equivalent freshwater heads based on the depth and saline concentration at each node. For this simulation, the nodes in the geologic units above the Upper Floridian aquifer were assigned a saline concentration of fresh water (150 mg/L), while the nodes in and below the Upper Floridian aquifer were assigned a saline concentration of seawater (35,000 mg/L). The specified boundary conditions result in a west to east hydraulic gradient.

EVALUATION OF RESULTS

The box model simulation was composed of a 30-day injection period, followed by a 305-day storage period, and a 30-day recovery period. Since computational accuracy is dependent on the time step size used in the simulation, a sensitivity analysis was performed to evaluate the impact of the time-step size on model results. For this sensitivity analysis the time step of the injection and extraction cycles were varied between 0.05 and 5 days. The results of this analysis, presented in Figure 2, indicate that the change of the computational result becomes insignificant as the time step size is reduced to below 0.5 days. Therefore, a time step size of 0.5 days was used during the injection and extraction cycles for all simulations in this study. The following discusses the results of the WASH123D model during each phase of the simulation.

Injection Period

Once the initial steady state flow field is generated, the ASR pumping well injects fresh water into the Upper Floridian aquifer at 5 MGD for 30 days. During this injection cycle the hydraulic head at and immediately surrounding the ASR well increases substantially, nearly doubling in magnitude. Figure 3b shows a cross sectional view of the concentration profile in the vicinity of the ASR well at the end of the injection cycle. This figure shows that the injected fresh water has displaced the ambient saline water forming a spheroid of lower concentration water in the vicinity of the ASR well. This lower concentration water permeates into the confining units above and below the Upper Floridian aquifer.

Storage Period

After the 30-day injection cycle, the ASR well is turned off for 305 days. During this storage period, the hydraulic condition tends to stabilize and approach a steady state condition. Figure 3c shows a cross sectional view of the concentration profile in the vicinity of the ASR well at the end of the storage period. Although the concentration at the ASR well remains relatively constant, the effects of buoyancy stratification are noticeable. During the storage period, the density effect is the dominating factor in the flow field. Consequently, the concentrations at the nodes in the lower portion of the Upper Floridian aquifer increase substantially faster than the nodes at the top of the aquifer.

Extraction Period

After the storage period the ASR well extracts at 5 MGD for 30 days. During this extraction cycle the hydraulic head at and immediately surrounding the ASR well decreases substantially. Figure 3d shows a cross sectional view of the concentration profile in the vicinity of the ASR well at the end of the storage period. Up-coning of the higher concentration saline water below the ASR well was observed during extraction. It must be noted that the well screen of injection and extraction in the Upper Floridian aquifer covers the center four vertical elements, rather than all the six vertical elements in the aquifer. This setup allows the mesh to compute for convergent flow fields around the well at the interfaces of the Upper Floridian aquifer and the two aquitards above and below without using high resolution meshes and small time steps when the density effect is strong. Because of this, the salt concentration of nodes in the lower portion of the aquifer in the vicinity of the ASR well increase in concentration faster than the nodes above during the period of extraction due to both diffusion and up-coning.

FUTURE MODEL DEVELOPMENT

During the development of the box model, meshes of various vertical and horizontal resolutions were tested. The WASH123D simulations became more computationally stable as the vertical resolution was increased in the geologic units above, below, and containing the ASR well. Additional studies are anticipated that evaluate the effect of various mesh resolutions on computational speed and accuracy.

In addition to the mesh sensitivity simulations, additional modifications to the WASH123D code are anticipated. One modification will be to the algorithm used to calculate the equivalent freshwater head in variable density flow systems. In simulations where higher density fluid is overlain by fluid of a lower density, the current algorithm tends to overestimate the equivalent freshwater head in the higher density solutions. Additional upgrades to address temperature variations on thermal transport will also be incorporated to the WASH123D code. These upgrades in conjunction with WASH123D's current abilities to model variably saturated groundwater flow and surface/subsurface flow interactions will help model the dynamic flow and transport issues inherent in the CERP ASR program.

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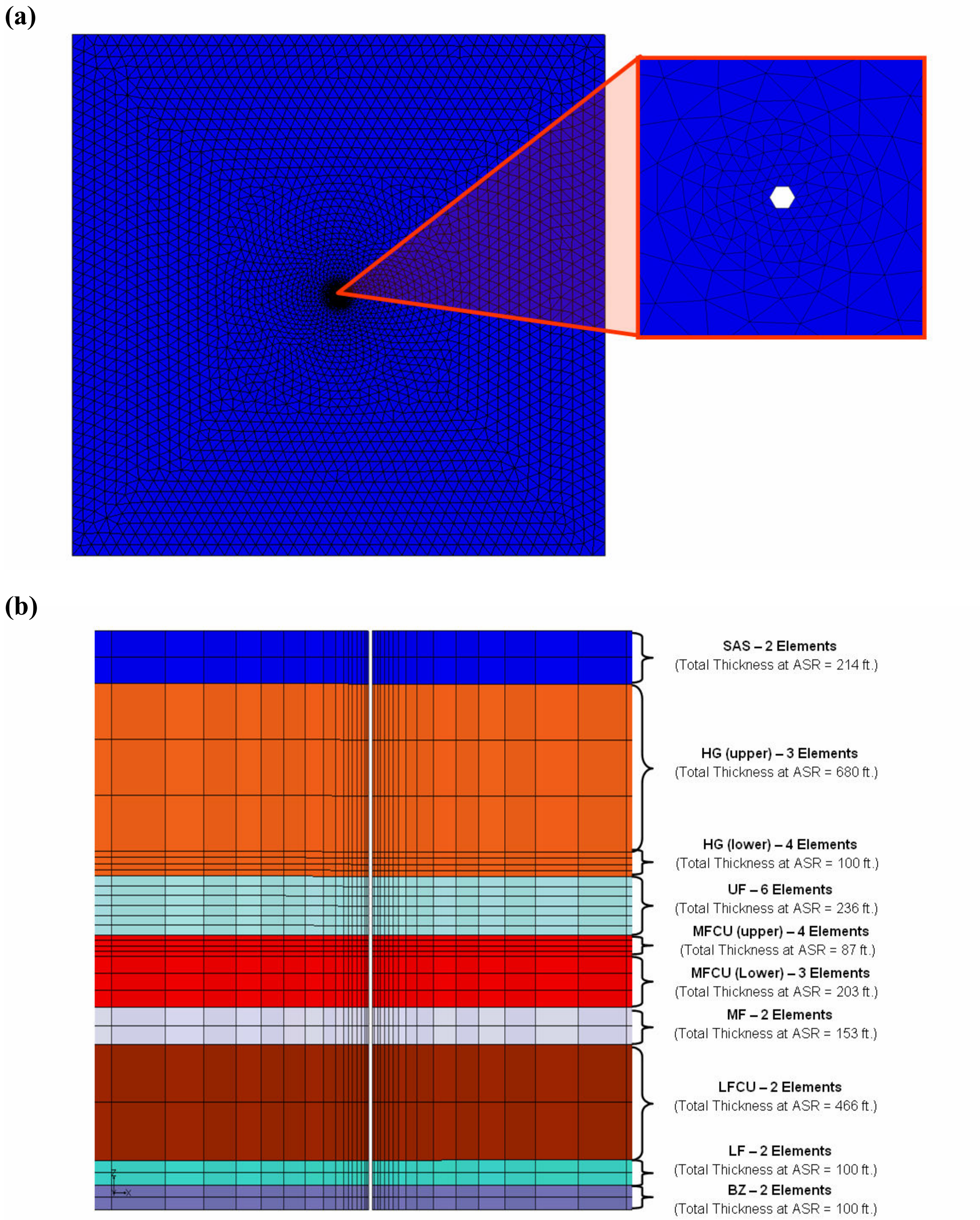
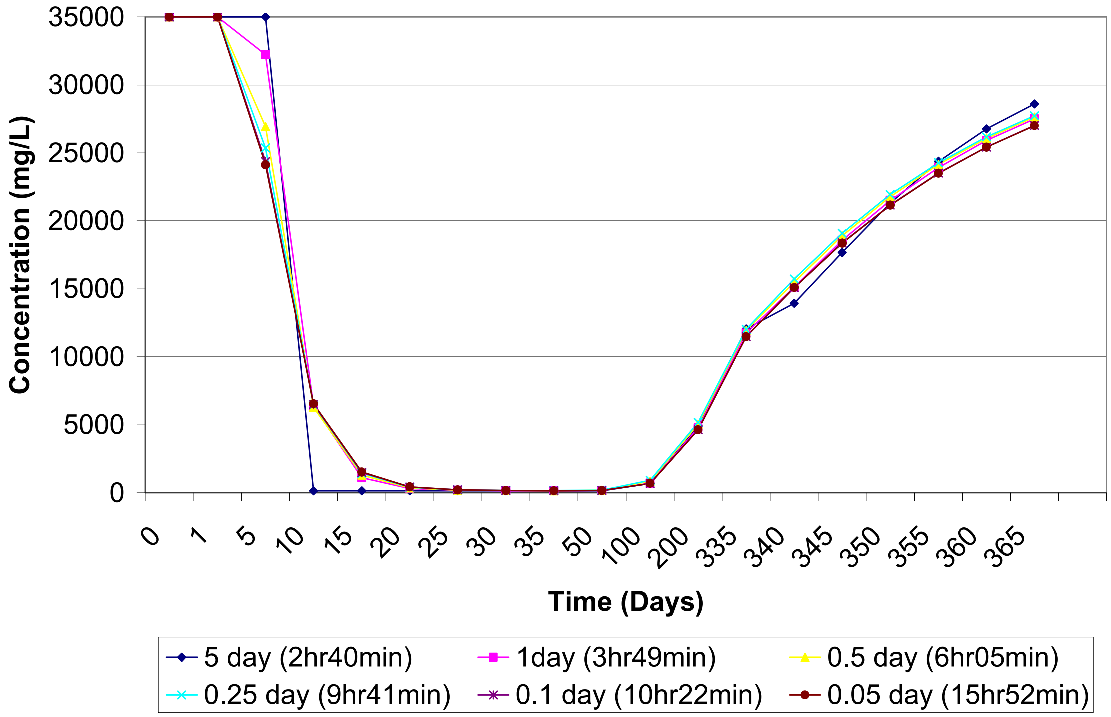


Figure 1. (a) Horizontal mesh resolution and (b) conceptual geology and vertical mesh resolution of the ASR box model



Note: Legend identifies the time step size of the injection and extraction cycles
with the associated simulation time in parentheses

Figure 2 – Sensitivity analysis results of time step size

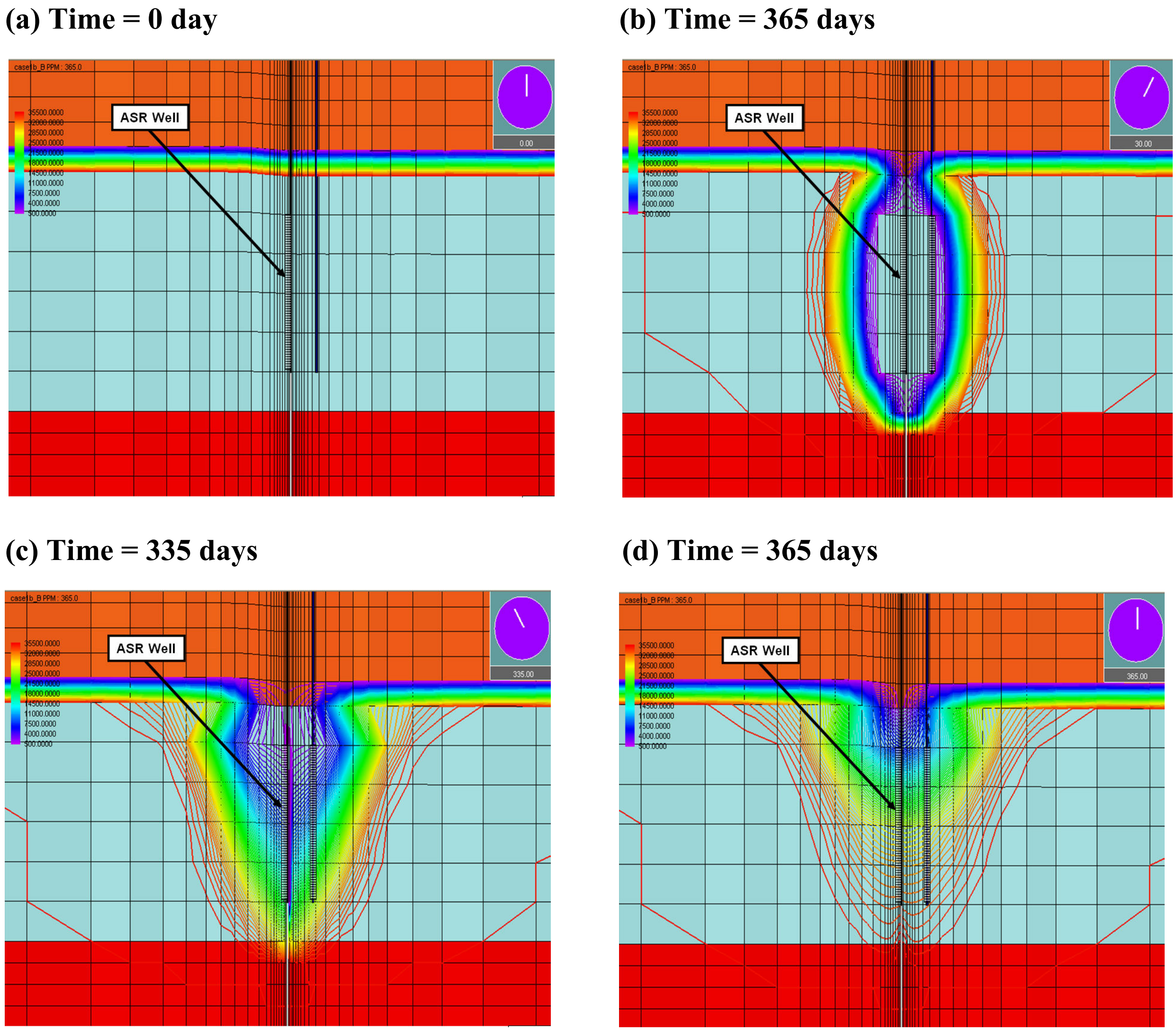


Figure 3 – Cross-sectional concentration distribution at various times