Subsurface Flow and Non-reactive Transport Modeling at the Oak Ridge FRC: Site-wide and Local Area 3 Models

Fan Zhang[1]*, Jack Parker[1], David Watson[1], Eungyu Park[2], Kenneth Lowe[1], Kirk Hyder[1], and Scott Brooks[1]
[1] Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, *zhangf@ornl.gov
[2] Kyungpook National University, Daegu, Korea

Abstract

The computer program HYDROGEOCHEM 5.0 (Yeh et al, 2004) was used to develop models for three-dimensional groundwater flow and chemical transport at the Oak Ridge Field Research Center (FRC) site. Initially, work was undertaken to develop a site-wide model encompassing an area of approximately 280 acres, which includes FRC Areas 1, 2 and 3, the former S3 Ponds and the Bear Creek watershed from its head waters to the tributary NT2. Refinements in the model were undertaken to incorporate new data and improvements in the conceptual model of the site. Nonlinear optimization using the PEST code was performed to recalibrate the steady state flow model to stream gauging data and water levels from 74 wells. Rock and saprolite were modeled as anisotropic media with a maximum permeability along strike, minimum permeability in the cross-bed direction and intermediate permeability along the dip direction. Field-scale dispersivities and effective porosities were calibrated by simulating non-reactive nitrate plume evolution from the S3 Ponds considering density-dependent flow effects.

A smaller scale model was developed for Area 3 to facilitate interpretation of flow and tracer studies in the vicinity of FW106 and to help design subsequent studies. A sub-model domain was delineated and a numerical mesh developed to accommodate the finer resolution needed to simulate flow and transport at the field plot scale. Boundary conditions on the sub-model domain were obtained from the site-wide model results. Material properties were initially mapped from the site-wide model, and then refined to account for finer level details relevant to the experimental data interpretation. The fine scale model will be utilized to assess potential interactions between current experiments in Area 3 and proposed new studies and to adjust experimental plans if necessary to avoid adverse effects on neighboring field plots.

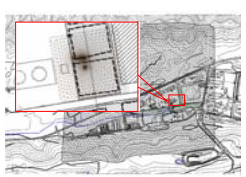


Fig 1. Simulation Domain of the Models

Site-wide Model and Refinements

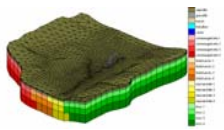


Fig 2. Material Type in Site-wide Model

The refined site-wide FRC model is discretized into 8 layers of 21,304 elements and 9 layers of 12,312 nodes. Four types of bedrock, including a "potential high permeability zone" identified by geophysical testing, are overlain by saprolite, gravel fill, a permeable trench and a rock saprolite "transition" zone. The modeling effort was undertaken with the following goals:

- Provide a means to interpret FRC site characterization data in an integrated manner to develop a more comprehensive understanding of the site.
- Identify knowledge gaps to guide ongoing characterization efforts and to identify research priorities.
- Quantitatively evaluate the validity of working hypotheses within the site conceptual model.
- Provide a tool for NABIR PIs to define boundary conditions for plot areas and provide a modeling template for more detailed plot-scale modeling efforts.

The modeling effort was undertaken beginning in FY04. Refinements in the model have been undertaken to incorporate new data and improvements in the conceptual model of the site. These refinements include:

- Modify the gravel fill zone that extends from slightly west of Area 3 to Bear Creek to incorporate information from new soil borings. Data indicates that the gravel fill overlays the saprolite directly locally and is more extensive than previously understood. This may significantly affect shallow groundwater flow and contaminant transport towards Bear Creek. To better accommodate the fill effects in the model, the upper model layer is being refined vertically and material property assignments are being refined.
- Modify the areal extent of the rock-saprolite transition zone based on new drilling results and geophysical testing [Waston, 2005]. The data indicates the zone is not as extensive as previously assumed.
- Incorporate the permeable barrier trench in FRC Area 2 in the model.
- Add a "potential high permeability zone" in the bedrock inferred from recent geophysical testing [Waston, 2005].

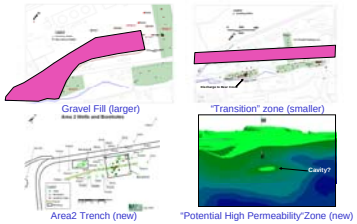


Fig 3. Site-wide Model Refinements

Site-wide Model Calibration

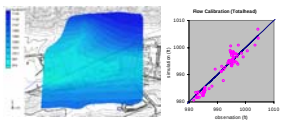


Fig 4. Site-wide Model Flow Calibration Results

Parameters calibrated

- Recharge: Hill slopes – 0.426 ft/yr, Valley – 0.496 ft/yr, Paved areas – 0 ft/yr
- Conductivity (K_S along strike, K_D along dip, K_C cross bedding)

Saprolite: K_S = 2.31e-4 cm/s, K_D = K_C = 2.31e-5 cm/s
Transition zone and potential high permeability zone:
K_S = 2.78e-3 cm/s, K_D = 9.27e-5 cm/s, K_C = 2.78e-4 cm/s
Gravel fill and trench: K_S = K_D = K_C = 0.01 cm/s
Top rock layer conductivity and depth reduction factor f [$K(z)=K(0)\exp(-fz/z_T)$]

- Conasauga Group/Rome Formation: K_S = 6e-6, K_D = 1.2e-7, K_C = 6e-12 cm/s, f = 3
- Maynardville Limestone: K_S = 8.21e-4, K_D = 1.92e-5, K_C =8.21e-7 cm/s, f = 5
- Knox Group: K_S = 1.31e-3, K_D = 7.36e-5, K_C = 1.31e-6 cm/s, f = 3
- Nolichucky Shale: K_S = 5e-4, K_D = 2.5e-4, K_C = 5.8e-5 cm/s, f = 5

In the transport simulation, the S3 pond area was separated into four parts to enable simulation of variable discharge and contaminant release characteristics during pond operation.

Parameters calibrated

- Dispersitivites: A_L = 10 m, A_T = 0.1 m
- Porosity θ= θ(0)exp(-f z/zT)

Saprolte: 0.2
Transition and potential high permeability zone: 0.2
Gravel fill and trench: 0.2
Rock units:

- Average porosity for top rock layer: 0.16
- Average depth reduction factor: 3.38

Density-driven flow moves nitrate plume deeper near source as observed in field

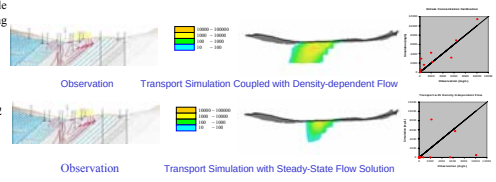


Fig 5. Site-wide Model Transport Calibration Results

Area 3 Model and Calibration

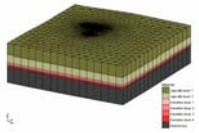


Fig 6. Material Type in Area 3 Model

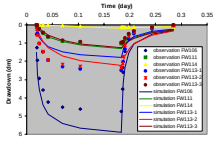


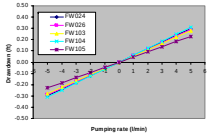
Fig 7. FW106 Pumping Test Calibration

Table 1. Layer Depths and Calibrated Parameters

Layers	Depth(ft)	K_S(cm/s)	K_D(cm/s)	K_C(cm/s)
Saprolite 1	16.5 ~ 26.3	5.56E-04	5.56E-05	1.11E-04
Saprolite 2	11.0 ~ 17.5	3.99E-04	3.99E-05	3.99E-05
Transition 1	1.13 ~ 2.25	9.70E-04	3.23E-05	9.70E-05
Transition 2	1.50 ~ 3.00	1.00E-05	5.00E-07	1.00E-06
Transition 3	0.75 ~ 1.50	1.00E-05	5.00E-07	2.00E-06
Transition 4	1.13 ~ 2.25	3.83E-03	3.83E-04	3.83E-06
Nolichuncky	30.0 ~ 30.0	5.00E-04	2.50E-04	5.80E-05

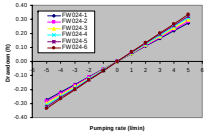
Fig 8. Location of the Wells

Area 3 Model Pumping Test and Tracer Test Simulations



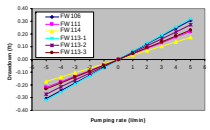
Well	Distance to FW106
FW024	33 ft
FW026	35 ft
FW103	36 ft
FW104	33 ft
FW105	50 ft

Fig 9. Effect of Pumping at FW106 on FW024 et al.



Well	Depth
FW024-1	43 ft
FW024-2	41 ft
FW024-3	40 ft
FW024-4	39 ft
FW024-5	37 ft
FW024-6	36 ft

Fig 10. Effect of Pumping at FW106 on FW024



Well	Depth	Distance to FW024
FW106	40 ft	33 ft
FW111	29 ft	34 ft
FW114	18 ft	32 ft
FW113-1	45 ft	34 ft
FW113-2	37 ft	34 ft
FW113-3	50 ft	34 ft

Fig 11. Effect of Pumping at FW024 on FW106 et al.

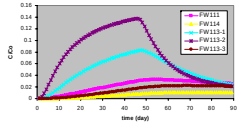


Fig 12. BT curve of FW106 tracer test (D = 4e-4 m^2/d)

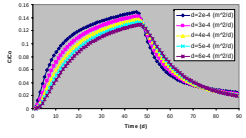


Fig 13. BT curve of FW106 tracer test at FW113-2

Note: Apparent dispersivities used in the simulations shown in Fig 12 and 13 were calculated assuming diffusion-limited fracdture-matrix mass transfer based on Parker and Valocchi (1986).

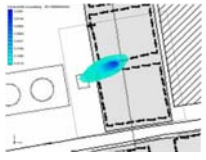


Fig 14. FW024 Tracer Test Simulation

The difference of simulated tracer concentration (C/Co) for the cases without and with pumping at FW106 ranges from -0.028 To 0.018.

Acknowledgements

This research was conducted at Oak Ridge National Laboratory (ORNL) with funding from the US Department of Energy NABIR Program. ORNL is managed by UT-Battelle LLC for the U.S. Department of Energy under contract DE-AC05-00OR22725.

References

- Doherty, J., 2002, PEST: Model Independent Parameter Estimation, Watermark Numerical Computing.
- Parker, J.C. and A.J. Valocchi, 1986, Constraints on the validity of Equilibrium and First-Order Kinetic Transport Models in Structured Soils, Water Resources Research, 22(3): 399-407.
- Waston, D., 2005, Current Opportunities and Future Research Directions at the FRC, NABIR PI annual meetings, April 18-20, 2005.
- Yeh, G.T., J.T. Sun, P.M. Jardine, W.D. Burger, Y. L. Fang, M.H. Li, and M.D. Siegel, 2004. HYFROGEOCHEM 5.0: A Three-Dimensional Model of Coupled Fluid Dlow, Thermal Transport, and HYFROGEOCHEMical Transport through Variable Saturated Condition – Version 5.0. ORNL/TM-2004/107, Oak Ridge National Laboratory, Oak Ridge, TN 37831