Paducah Gaseous Diffusion Plant Groundwater Modeling Support Activities
Phase 1 Summary Report

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ACRONYMS

DOE   U.S. Department of Energy
FD   finite difference
GV   Groundwater Vistas
MOC   method of characteristics
PGDP   Paducah Gaseous Diffusion Plant
RGA   Regional Gravel Aquifer
SVD   Singular Value Decomposition
^{99}Tc   technetium-99
TCE   trichloroethene
TVA   Tennessee Valley Authority
TVD   total variation diminishing
UCRS   Upper Continental Recharge System

1. INTRODUCTION

This report summarizes the results of Paducah Gaseous Diffusion Plant (PGDP) groundwater modeling support activities funded through the Kentucky Research Consortium for Energy and Environment for Federal Fiscal Years (FFY) 2009 through 2011. The objective the Groundwater Modeling support project is to provide an independent review of the latest PGDP groundwater flow and transport modeling efforts and to develop and operate the models to simulate potential groundwater and source area remedial scenarios that are generally outside of the scope of DOE-contractor modeling activities. Phase 1 of the Groundwater Model support project consists of two tasks. The first task is to review existing PGDP modeling documents and implement the model hardware and software. The second task is to evaluate the existing flow and transport models.

Since 1990, numerical modeling efforts have been conducted at the PGDP. The most recent one was conducted in 2008, which made significant changes from previous modeling efforts that include model discretization, boundary conditions, flow calibration, and transport simulation. The 2008 modeling efforts consists of a groundwater flow model (referred as 2008 flow model thereafter), a TCE transport model (referred as 2008 TCE model), and a ^{99}Tc transport model (referred as 2008 ^{99}Tc model). The 2008 models were received as Groundwater Vistas (.GV) files with other supplemental files including map files, initial head files, and a draft 2008 Groundwater Model Report (PGDP modeling group, 2008).

The contents of this report are organized as follows: Section 2 briefly discusses computer programs used in the 2008 model, including MODFLOW-2000, PEST-SVD, MT3D, and Groundwater Vistas. Section 3 evaluates the flow model configurations, including domain selection, spatial discretization, boundary conditions, aquifer parameters, and infiltration/recharge. Section 4 reviews the flow model calibration process. Section 5 evaluates contaminant transport models for TCE and ^{99}Tc including geochemical parameters and transport model calibration. Section 6 suggests recommendations for future PGDP modeling efforts.

2. REVIEW OF MODELING SOFTWARE

In the 2008 modeling efforts, MODFLOW-2000 (Harbaugh et. al. 2000) was used for simulating groundwater flow and MT3D (Zheng, 1999) was used for contaminant transport. Also, PEST (Doherty, 2005) was used to assist in flow and transport model calibration. Usage of these programs was facilitated by Groundwater Vistas, a graphic user interface tool.

2.1 MODFLOW-2000

MODFLOW-2000 is the third major version of MODFLOW, the U.S. Geological Survey's three-dimensional finite-different groundwater model first released in 1984. MODFLOW is regarded as a standard code for simulating groundwater flow in aquifers and is widely used by government agencies, researchers, and consulting firms. MODFLOW-2000 adds new solvers from two previous versions: MODFLOW-88 and MODFLOW-96. MODFLOW-2000 also adds functions for parameter estimation and transport simulation, but these functions are much less used due to better options for these functions existing in other programs. The most recent version of MODFLOW is MODFLOW-2005. The major addition in MODFLOW-2005 is local grid refinement, which allows multiple grids in a single MODFLOW simulation. Any of the four major versions of MODFLOW are suitable for simulating groundwater flow for the PGDP site. Using MODFLOW-2000 takes advantage of some new solvers, such as the geometric multi-grid solver (GMG) used in the 2008 flow model.

2.2 PEST

PEST (an acronym for Parameter ESTimation) is a nonlinear parameter estimation code written by John Doherty. Owing to its robustness and versatility, PEST is becoming increasingly popular among modelers for solving parameter estimation problems. PEST is model-independent, meaning it estimates parameters for a specific model without the need of changing the model code itself. Major features of PEST that pertain to calibrating a groundwater flow model include 1) allowing parameter bounds; 2) estimating different types of parameters simultaneously; 3) using multiple types of targets; 4) allowing different weights assigned to different types of targets; 6) offering convenient sensitivity analysis; and 6) estimating highly parameterized fields. Estimating large number of parameters for a complicated model can be computational prohibitive. PEST offers a "pilot points" parameterization scheme, in which parameter values at some user-specified points in a model domain are estimated and these values are then interpolated to other cells of the model grid using a spatial interpolation method, such as kriging. The underlying assumption of kriging is that within a geological unit properties of two points are more similar when the points are closer to each other. PEST further provides a SVD-assist scheme which can dramatically reduce the computation time and increase numerical stability with the cost of probably less physically realistic parameter fields. It is important to recognize that although PEST is a powerful tool, using PEST without carefully incorporating site-specific information; a "well-calibrated" model can result in erroneous parameter values.

2.3 MT3D

MT3D and its succeeding code MT3DMS are three-dimensional transport models for simulating advection, dispersion, and chemical reactions of dissolved constituents in groundwater. MT3D is designed as a transport companion to MODFLOW, in which MT3D reads water levels and cell-by-cell fluxes from MODFLOW for transport simulation. MT3D provides three transport solution methods: 1) the standard finite difference (FD) method; 2) the particle-tracking-based Eulerian-Lagrangian method called method of characteristic(MOC); and 3) the higher-order finite-volume total-variation-diminishing (TVD) method. The chemical reaction capacity of MT3D is limited to simulate equilibrium-controlled or rate-limited linear or non-linear sorption and first-order irreversible or reversible kinetic reactions for a single species. This capacity can approximate sorption and biodegradation processes experienced by TCE at the site. ^{99}TC is conservative with a half-life over 10,000 years. Therefore, MT3D is adequate for current modeling purposes of the PGDP site. If additional chemical reaction capacity is needed in the future, PHT3D (Prommer et al. 2003) can be used. PHT3D couples MT3D with PHREEQC-2 (Parkhurst and Appelo, 1999), the USGS's low-temperature aqueous geochemical reaction simulation program.

2.4 Groundwater Vistas

Groundwater Vistas (GV) is a graphical user interface program that facilitates the uses of a variety of groundwater flow and transport modeling software, including MODFLOW, MT3D, PEST, and MODPATH. MODPATH is a particle-tracking tool for MODFLOW (Pollock, 1994) and was used in the 2008 model for analyzing plume paths. GV also provides multiple tools to help model calibration and sensitivity analysis. GV processes multiple programs under one graphic interface and relieves a modeler from handling otherwise tedious input/output processes for individual programs.

3. REVIEW OF FLOW MODEL CONFIGURATION

Flow model configuration is the process of translating a site hydrogeological conceptual model into a numerical model that can be carried out in a modeling program, such as MODFLOW. As a general description of groundwater flow system for a site, a conceptual model can be translated into very different numerical model configurations depending on model purposes. For the 2008 PGDP model, the translation process includes four tasks: 1) deciding model type, i.e., a steady state model or a transient model, 2) defining numerical model domain and grid, 3) defining boundary conditions, and 4) initialization of aquifer parameters. The fourth task can also be considered as a step of model calibration, so it will be reviewed in next section. This section reviews the first three tasks.

3.1 Flow Model Type

The 2008 Flow Model used a steady-state model for PGDP groundwater flow. While recognizing natural groundwater flow is always in transient state, two arguments for choosing a steady state model were provided in the model report. The first one is a three-point analysis of RGA water level data between 1995 and 2006 which indicates that flow patterns between PGDP and the Ohio River remain relatively stable although water levels and the Ohio River stage fluctuate through time (up to 10 feet during the observation period). The other one is an observation of relatively constant locations and extents of TCE plumes through time. The practical consideration of using steady state flow is that a steady-state model requires fewer input parameters and runs much faster than a transient model, which makes model calibration more tractable. In addition, a steady-state model is commonly built to capture average behaviors of a groundwater system where temporal variation is not a major concern.

3.2 Model Domain and Grid

The 2008 Flow Model domain encompassed the PGDP plant and the area between PGDP and the Ohio River, covering an area of approximately 18.6 square miles. The domain was discretized into 582 rows and 627 columns with a uniform spacing of 50 feet. Vertically, the model domain covers the extents of the Regional Gravel Aquifer (RGA). The vertical extent of the RGA unit was divided into three layers with equal thickness. The total number of active cells is 799,389.

3.2.1 Domain and Grid Interpretation

When configuring a groundwater model domain, developers need to consider not only the hydrological conceptual model but also the intended uses of the model and the computational capacities of the modeling software.   The Groundwater Conceptual Model Report (DOE 1997b) identified three major hydrologic units at the PGDP (in descending order): the Upper Continental Recharge System (UCRS), the RGA, and the McNairy Flow System. Both the UCRS and McNairy Flow System were excluded from the 2008 flow model. The UCRS is predominately silts and clays with laterally discontinuous sand and gravel horizons. Groundwater flow in the UCRS is primary vertical. The RGA is the main aquifer consisting of gravel and coarse sand with a veneer of fine to medium sand. Discontinuous sands in the upper McNairy Formation that are contiguous with the RGA are modeled as part of the RGA. The McNairy Flow System is composed of silt, micaceous clay and fine sand which immediately underlie the

RGA from the PGDP industrial area to the Ohio River.   In the southern portion of the model domain, the upper portion of the McNairy Flow System includes the Porters Creek Clay.

In the 2008 model the UCRS was excluded as a modeled aquifer unit because the UCRS hydraulically serves as a recharge pathway to RGA. The impact of the UCRS can therefore be handled as recharge to the RGA.   The reasons to exclude the McNairy Formation included the large hydraulic conductivity contrast between the RGA and McNairy Flow Systems which limit hydraulic connection between the sediments of the two units and field sampling investigations which indicate that the RGA contains nearly all detections of groundwater contaminants of concern related to plant activities.

From a numerical modeling perspective, there are two major advantages of excluding the UCRS and McNairy Flow Systems from the model. The first advantage is that exclusion dramatically reduces the number of layers and thus computational cells in the model. This allows the use of finer grids that preferred for models utilized for remedial purposes. The second advantage is to avoid simulating re-wetting conditions in the UCRS. Re-wetting of cells in the UCRS was a modeling problem encountered in historical PGDP modeling efforts (prior to the 2008 model) because the MODFLOW-2000 code is designed to simulate saturated flow with very limited capacity for unsaturated flow. Re-wetting can significantly slow down simulations and can cause the model to diverge or fail to numerically reach a solution.

Excluding these two formations limits the models ability to simulate some potentially important scenarios. For example, it is impossible for the model to simulate a "spill" scenario, i.e., "how long it would take contamination to reach RGA if a spill occurred at the surface of the PGDP site?" Another example is the model cannot predict possible contamination in McNairy Formation. Although field investigations showed limited hydraulic interaction between the RGA and McNairy Flow System and unlikely existence of source zones in McNairy, the diffusion process due to the concentration gradient still exists and could lead to elevated concentrations in McNairy Flow System. This may be of particular concern given the fact that the highest concentrations observed in the field are near the lower boundary between the RGA and the McNairy Flow System (DOE 1997b). The 2008 model report recognized these limits and suggested the use of a cross-section model to evaluate migration potential of contaminant to McNairy Formation. Reviewing the cross-section model is beyond the scope of this study.

3.3 Boundary Conditions

The 2008 model domain was bounded by naturally occurring hydrological features in the vicinity of the PGDP. The northern domain boundary is the Ohio River. The Porters Creek Clay bounds the model domain to the south and surface water divides bound the model domain to the east and west of the PGDP. Other boundary features contributing to the groundwater system and incorporated in to the model include Bayou Creek, Little Bayou Creek, TVA ash ponds, and Metropolis Lake. Most of the boundary features were configured in the top of the model (layer 1) with the exception of the Ohio River which exists at the north side of all three layers.

The Ohio River was the main discharge feature and was simulated using drain cells. Using drain cells allows more flexibility to control fluxes. A drain cell includes a stage term and a conductance term. For the Ohio River, the stage was set at 297 feet and the conductance was adjusted during calibration. The conductance term provides resistance of water flowing from an aquifer to the drain cell. In the 2008

model, the entire Ohio River section was treated as one reach, having same stage level and conductance. In fact, MODFLOW allows multiple reaches for drain cells.

The Porters Creek Clay and surface water divides were simulated as no-flow cells. The site groundwater conceptual model (DOE 1997b) indicated that there was likely recharge from Eocene sand and Pliocene gravel deposits overlaying the Porters Creek Clay to the UCRS. However, the recharge rate was not well understood and the Eocene sand and Pliocene gravel are considered a no-flow boundary in the 2008 model. Surface water divides are commonly used to constrain the extent of a groundwater flow model. They were often treated as no-flow cells. It is worth mentioning that the bottom of the model (layer 3) was also configured as no flow, ignoring water exchange between RGA and the underlying McNairy Flow System (i.e., as an aquitard).

Bayou Creek and Little Bayou Creek were simulated using recharge cells. Streams or rivers are commonly simulated using river cells, which consist of a stage term and a conductance term. Using recharge cells instead of river cells for Bayou Creek and Little Bayou Creek reduced two parameters to one parameter: recharge rate. The recharge rate can be positive or negative, emulating water flow into or out of the aquifer. Both creeks were divided into multiple reaches and the recharge rate for each reach was adjusted during calibration.

Metropolis Lake was given a hydraulic conductivity value of 50,000 ft./day, literally allowing water to move in and out of the aquifer freely while putting no impact on groundwater mass balance.

The 2008 model handled boundary features in a practical way in which most boundary features were treated based on their actual hydraulic functions to the aquifer rather than on their surface flow characteristics. This allows better handling of hydraulic connection between these boundary features and the aquifer.

4. REVIEW OF FLOW MODEL CALIBRATION

Regardless of using traditional trial-and-error methods or more recent automatic parameter estimation methods, a model calibration process consists of three steps: 1) selection of calibration targets; 2) selection of parameters; 3) adjusting parameter values to match the targets. This section reviews the three steps as well as calibration results.

4.1 Selection of Calibration Targets

The 2008 model used three types of targets: water level, flux, and angle (also called gradient). A total of 76 water level targets were used with 44 in layer 1, 20 in layer 2, and 12 in layer 3. An Ohio River flux target of 4,837 gallons per minute (gpm) was used as the only flux target. 1704 angle targets were used.

All the water level targets used were measurements obtained in February 1995. There were water level measurements in other periods. The selected period had relative larger number of measurements and was prior to the beginning of the extraction wells pumping. The flow pattern in February 1995 was similar to other periods as shown in Fig. 4.3 in the model report. The source for the Ohio River flux value of 4,837 gpm was not presented in the model report. The angle targets were based on simulated water levels from a uniform hydraulic conductivity, which, stated in the model report, match the plume trajectories.

4.2 Selection of Parameters

During the calibration process in the 2008 model, the parameters to be estimated included horizontal hydraulic conductivity, conductance of the Ohio River drain cells, and recharge values. Technically, hydraulic conductivity is the only aquifer parameter that needs be considered in a steady state groundwater flow model. However, recharge, a boundary feature, was often treated as a parameter. In the 2008 model, recharge was used for precipitation, the PGDP site, TVA pond, Bayou and Little Bayou Creeks. Except for TVA pond, all recharge values were adjusted during calibration. The recharge rate of TVA pond was fixed as 0.0159 ft/day. The conductance of the Ohio River was a boundary term that was adjusted during calibration.

The parameter choice in the 2008 model included most important parameters which pertain to steady state groundwater flow, except a vertical hydraulic conductivity value, which was set as one-tenth of the horizontal hydraulic conductivity at the same cell. Setting vertical hydraulic conductivity as a ratio of its horizontal counterpart is very common in groundwater modeling although the ratio value is somewhat arbitrary.

4.3 Parameter Estimation

The 2008 model used PEST with SVD-assist to estimate parameters automatically. Horizontal hydraulic conductivity values were allowed to vary from cell to cell and were estimated using a pilot-point method. Recharges were estimated using a traditional zonation pattern with one value for each zone. The parameter estimation also used a regularization scheme for hydraulic conductivity.

Using the pilot-point method requires a user to specify pilot points, where hydraulic conductivity values are estimated based on target information. The values of all other active cells will then be interpolated by Kriging. The 2008 model assigned a regular grid pattern of pilot points throughout the domain with additional points added to the plume locations and locations where pumping tests have been conducted. The selection of pilot points focused on areas affecting plume migration and considered available site-specific information.

Using a zonation method requires a user to separate a parameter field to several zones. In the 2008 model, both Bayou Creek and the Little Bayou creek were divided into five recharge zones each. The PGDP industrial site was divided into a checkerboard pattern of 21 recharge zones. Lagoons, ditches, and buildings associated with the PGDP site were assigned four additional zones. All other areas were assigned to one zone corresponding to precipitation. This zonation represented overall site conditions, however, the checkerboard pattern was applied as a workaround for a complicated system of poorly characterized leaky underground utilities within the industrial site.

Though a powerful estimator, PEST can lead to unrealistic parameter values if the problem parameter is not properly constrained by available site information. In the 2008 model the hydraulic conductivity values for pilot points located where pumping tests had been conducted were constrained by pumping test results whereas pilot points at other locations were given uniform set of input values, including minimum, maximum, and initial values. The initial hydraulic conductivity values assigned to the pilot points were also used to regularize the estimation process; penalizing estimates deviating from the initial values. The regularization would generate less perfect matches to the targets while trying to force estimated values to stay closer to the initial values. The precipitation recharge was constrained within a small range (2.64 to 7.64 inch/year) but recharge zones for the PGDP site and for surface water features were allowed to vary from 0.0044 to 114.83 inch/year. Notice that the hydraulic conductivity values were regularized but the recharge values and drain cell conductance values were not regularized.

In the 2008 model, the calibration process used a weighting strategy, assigning different weights to different types of targets. Water level targets were assigned a weight value of 1.0. The Ohio River flux target was assigned a weight of 7.55×10^{-6}. The angle targets were assigned a weight of 0.01. With much higher weights than other types of targets, water level targets became dominant targets and parameters were adjusted primarily to match these targets.

4.4 Calibration Results

The calibrated model reasonably matched the targets. Model-predicted potentiometric surfaces were similar to field observations. The calibrated model also reasonably replicated plume paths. By matching the selected targets, the calibration process resulted in spatial distribution of hydraulic conductivity, recharge for pre-defined recharge zones, and conductance of the drain cells.

With constraint from pumping test data and regularization using initial hydraulic conductivity values of pilot points, the estimated hydraulic conductivity value has a range from 50 to 5000 ft/day. It is difficult to judge if the estimated spatial variation reflected the stratigraphy. On the other hand, the estimated hydraulic conductivity distribution showed smooth transition among all cells in each layer, indicating that no subunits within the RGA were incorporated into the model. PEST allows multiple zones with cell-by-

cell parameter variation in each zone. If multiple zones, i.e., subunits, were added, the estimated parameter fields would more likely show sharp contrast along zone boundaries.

The estimated Ohio River conductance was 3.048 ft^2/day, which is equivalent to a conductivity value of 6 $\times$ 10^{-3} ft/day given a 50 ft by 50 ft cell size with 5 ft thick drain bed. While this conductivity value is relatively low, it is still within the range for silt. The estimated recharge values were mixed. The estimated precipitation recharge seems reasonable. On the other hand, without proper constraint, the calibration generated some unrealistic recharge values at the PGDP site. For example, the estimated value for recharge zone in the vicinity of the C-400 building area was near zero and the result contradicts site thermal records from both the UCRS and vertical extent of the RGA indicating elevated groundwater temperature due to the leakage of warm water from site operations. The recharge values for Bayou and Little Bayou creeks ranged from –986.18 (at LBC seeps) to 148.89 inch/year. The recharge values for the two creeks seem to represent a reasonable fraction of the overall site mass balance.

5. REVIEW OF TRANSPORT MODEL

The 2008 transport model simulated plumes of TCE and ^{99}Tc. The transport model used the fluxes calculated from the calibrated flow model and simulated the migration history that spanned from estimated historical contaminant releases to 2008. The overall strategy applied to the transport model was to match the current (measured) plume geometry through adjustment of source locations and temporal loading rates. Major steps in the transport model development included: 1) deciding transport parameters; 2) selection of a solution scheme; 3) calibration of transport models. These steps are reviewed below.

5.1 Deciding Transport Parameters

With the exception of the TCE half-life, transport parameters were predetermined and were not adjusted during transport model calibration. Some of the predetermined parameter values were adopted from previous modeling efforts and others were typical values for transport modeling.

All transport related parameters, including porosity, bulk density, distribution coefficient, half-life, longitudinal dispersivity, transverse dispersivity, and vertical dispersivity were considered homogeneous. In field conditions, these parameters were likely spatially variable. These parameters were difficult to characterize and were commonly treated as homogeneous. Even treated homogeneously, these parameters could be adjusted during transport model calibration, which may potentially improve the transport model results.

5.2 Selection of a Solution Scheme

The 2008 transport model compared three types of solution schemes available in MT3D and decided to use the finite difference (FD) method over the Total Variation Diminishing (TVD) method and Method of Characteristics (MOC). The TVD method was found to produce a steep lateral concentration gradient as observed in the field measurements but needed much longer simulation times than the FD method. The MOC produced similar plume shapes as the FD method but required longer simulation times.

The FD method is also known to generate more numerical dispersion than the other two methods, increasing plume lateral extent and expediting plume front. While using the FD method seems necessary for transport model calibration, the TVD method could be used to run calibrated transport models and reduce numerical dispersion.

5.3 Transport Model Calibration

The 2008 transport model simulated plumes of TCE and ^{99}Tc as two different models. The calibration for the TCE model started with the estimation of the TCE half-life. A 10-year half-life for TCE was adopted based on three 45-year simulations using biological half-lives of 6, 10, and 16 years, respectively. After the TCE half-life was determined, the calibration continued with individual plumes for Northwest, Northeast, Southwest plumes. All calibrated individual plumes were then combined together to form a final model. Individual plume calibration used trial-and-error and superposition method. Items adjusted during the calibration process were spatial and temporal loads of TCE source areas. Calibration targets

for Northwest and Southwest plumes were plume geometries whereas targets for Northeast plume were concentration data from a few monitoring wells.

The resulting TCE loads were two concentration boundary cells for the Northwest plume, ten groups of recharge cells for the Southwest plume, and three concentration boundary cells for the Northeast plume. Concentrations of the two concentration-boundary cells for the Northwest plume were constant through time representing a non-depleting DNAPL source. Each group of recharge cells for the Southwest plume had constant concentration through time but the concentrations varied from group to group. Concentrations of the three concentration boundary cells for the Northeast plume varied significantly through time. Source loads for the Northwest and Southwest plumes were supported by the field source zone characterization. Loads for the Northeast plume had little support from the field data as the source areas are poorly characterized.

The source loads for ^{99}Tc were three recharge zones of temporally uniform concentration and one cell of constant concentration. Although there was no evidence of ^{99}Tc source zone existing in the RGA, a constant concentration cell had to be assigned to C-400 area due to the low recharge value (1×10^{-6} ft/day) obtained during flow model calibration.

Simulated plumes from the calibrated transport models reasonably matched observed TCE and ^{99}Tc plumes. Simulated concentration values also moderately matched to observed values in the six monitoring wells but also showed multiple peaks through time. Simulated plume fronts appear to be moving faster and farther downgradient than the observed plumes near the Ohio River.

6. REVIEW SUMMARY AND RECOMMENDATIONS

6.1 Review Summary

The 2008 flow and transport model used MODFLOW-2000 for groundwater flow and MT3D for contaminant transport. The numerical model encompassed the RGA while excluded overlaying UCRS and underlying McNairy Flow System. Boundary features that introduce or extract water from the aquifer were incorporated. The handling of these boundary features was based on their functionality relative to the groundwater flow system. Through the use of the automatic calibration tool, PEST, the flow model calibration achieved reasonable matches to selected targets. The pilot point method allowed greater flexibility than traditional zonation methods for adjusting hydraulic conductivity. The transport models used uniform transport parameters. The calibration of transport models was accomplished through adjustment of spatial and temporal source loads. The transport model calibration reasonably matched the geometries of the plumes.

Overall, the model achieved a good match to site observations and the majority of parameters determined, assigned and distributed in the model were within their respective reasonable ranges. The model in current stage can be used to assist with the development of site remediation actions. However, there are some potential areas where input data could be refined: 1) The first is the calibration of anthropogenic recharges within the PGDP industrial site. The existing model calibration resulted in near zero recharge values near the C-400 building while site thermal records showed elevated groundwater temperatures that are likely the result of leaking hot water distribution and recirculation lines. The near zero recharge also caused some problems in the calibration of the ^{99}Tc plume model. A constant concentration cell was forced in the RGA for the C-400 source area although the source may be located in the UCRS; and 2) Highly temporal varying source loads for the Northeast TCE plume had insufficient support from field data.

Note that excluding both UCRS and McNairy Formations may not have a strong influence on the main plumes. However, this handling prevents the model from being used to simulate a few potentially important scenarios. For example, the existing model will not be able to simulate time needed for a contaminant released on the ground to reach RGA. Additionally, the existing model cannot evaluate contaminant mass migrated through diffusion processes into the McNairy Flow System.

6.2 Recommendations

Below are some recommendations to improve upon the success of the existing model:

- Incorporate stratigraphy data to constrain parameters in flow model calibration. Specifically, the existing model used the same range of hydraulic conductivity for every cell where pumping tests had not been conducted. A new stratigraphy dataset is expected to be available in the near future, which can be used to assign hydraulic conductivity based on materials properties and matching the materials properties at a given location to similar locations where measurements have been conducted.
- Incorporate site leakage data to constrain anthropogenic recharge. While the exact site recharge is difficult to characterize, a reasonable range of lower and upper bounds can be added to the calibration to achieve reasonable values.

- Calibrate the flow model without SVD to improve the spatial distribution of hydraulic conductivities. The SVD-assist method is known to speed up the parameter estimation significantly but can generate un-realistic parameter fields. Advances in computing power may allow the calibration to be done in a reasonable time frame without using SVD.

- Add more pilot points at possible future paths of the contaminant plumes to improve hydraulic conductivity estimation in those areas.

- Recalibrate the Northeast TCE plume. The calibration of Northwest TCE and Southwest TCE and ^{99}Tc plumes were achieved using temporally uniform source terms. If no new data are available, the calibration of the Northeast TCE plume should use similar strategy, not like the existing model that used highly temporally varying loads.

- Investigate potential mass migration into the McNairy Flow System by adding a homogeneous layer to the bottom of the existing calibrated transport model. Field data showed that the highest TCE concentrations are near the bottom of RGA and model iterations including the homogeneous base layer would suggest whether future modeling should include the McNairy Flow system

- Consider independent evaluation of the UCRS and underlying terrace gravels/Eocene sands as potential sources of UCRS recharge in the southern portion of the model domain. The Terrace Gravels and Eocene sands overlie the Porter's Creek Clay along the southern portion of the model domain.

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