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Interim TCE Transport Model for the Paducah Gaseous Diffusion Plant Site

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Acronyms

DOE	U.S. Department of Energy
KRCEE	Kentucky Research Consortium for Energy and Environment
PGDP	Paducah Gaseous Diffusion Plant
RGA	Regional Gravel Aquifer
SP1	Stress Period 1 of the 2016 Update
SP2	Stress Period 2 of the 2016 Update
^{99}Tc	Technetium-99
TCE	Trichloroethene

1. Introduction

The PGDP sitewide groundwater flow model underwent a major update in 2016 (DOE, 2017). The 2016 update incorporated additional field data to a major version of the sitewide model completed in 2008 (DOE, 2010). While both models simulate the groundwater at the site as steady state, the 2008 model had one stress period whereas the 2016 model had two stress periods, one for before the pump-and-treat operation was initiated (SP1) and the other for post plant shutdown conditions with pump-and-treat still in operation (SP2). A review of the 2016 update (KRCEE, 2018) found that the total flow in the 2016 update was roughly half the total flow in the 2008 model. The predicted site-wide groundwater flow from the 2016 update, therefore, was expected to be much slower than the predicted flow from the 2008 model. When used for solute transport modeling, these two models would yield very different travel times even though the migration paths might be similar. Since the 2016 update only has the flow component, the impacts of the changed flow field on simulating contaminant transport remain unclear.

In addition to simulating the groundwater flow, the 2008 model also included transport models of TCE and ^{99}Tc. The 2008 transport models reasonably matched field observed plume location and geometry through adjusting contaminant source locations, temporal source loading rates, and transport parameters. The 2008 transport models provided needed data to conduct an assessment on the impacts of the changed flow field on simulating contaminant transport.

To assess the potential impacts of the changes in the flow field introduced in the 2016 update on contaminant transport, this study established an interim TCE transport model that incorporated transport parameters in the 2008 TCE transport model into the 2016 flow model. The simulated TCE plumes from the interim transport model were compared with the simulated TCE plumes form the 2008 TCE transport model and field-observed plumes.

2. Summary of the 2008 Flow Model and the 2016 Update

Brief summaries of the two models are given here. Detailed reviews of these models can be found in KRCEE (2011) and KRCEE (2018).

The 2008 model simulated groundwater flow in the regional gravel aquifer (RGA) as steady state flow with one stress period. The model was calibrated to water level data measured in February 1995 and the Ohio River Flux. Model parameters selected for calibration were horizontal hydraulic conductivity and recharges. Horizontal hydraulic conductivity values were allowed to vary from cell to cell. Recharges were configured using a zonation pattern with one value for each zone. PEST coupled with pilot points was used to estimate these parameters automatically.

The 2016 update kept the design of the 2008 model with several changes. Some of the changes were introduced to incorporate new field data and these changes included: 1) adding groundwater inflow from the Terrace Gravel; 2) revising RGA extent and thickness; 3) refining anthropogenic recharge zonation; and 4) representing surface hydrologic features using river boundaries. While keeping the stress period in the 2008 model, the 2016 also introduced one additional stress period that was calibrated to water levels measured in September 2014. The first stress period corresponded to pre-pumping condition and the second stress period corresponded to post plant shutdown.

3. Summary of the 2008 TCE Transport Model

The 2008 model included a TCE transport model that built upon the fluxes calculated from the 2008 flow model. The transport model simulated the TCE plume migration history from estimated historical contaminant releases up to 2008. All transport related parameters, including porosity, bulk density, distribution coefficient, half-life, longitudinal dispersivity, transverse dispersivity, and vertical dispersivity were considered homogeneous. Except for the TCE biodegradation half-life, transport parameters were predetermined and were not adjusted during transport model calibration. The predetermined parameter values were either adopted from previous modeling efforts or from literature. A TCE half-life of 10 years was adopted by comparing simulated Northwest plumes from three different half-lives with the 1995 plume. Table 1 shows the parameters for the 2008 TCE transport model.

Table 1. Transport Parameters in the 2008 TCE Transport Model (DOE, 2010)

Transport Parameter	Value
Bulk Density, g/cm^3	1.67
TCE Distribution Coefficient (K_d), cm^3/g	0.0188
Porosity (ft^3/ft^3)	0.30
TCE Biological Half-Life, years	10
Longitudinal Dispersivity, ft	50.0
Transverse Dispersivity, ft	5.0
Vertical Dispersivity, ft	0.5

The transport model was calibrated by adjusting source locations and temporal loading rates until the model produced simulation results that reasonably matched the measured plume geometry. The resulted 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 at 250,000 µg/L at the southern edge of the C-400 building. Each group of recharge cells for the Southwest plume had constant concentration through time (Table 2). Concentrations of the three concentration-boundary cells for the Northeast plume varied significantly through time (Table 3). 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. The 2008 model report (DOE, 2010) pointed out that the calibration of the Northeast plume was problematic due to lack of characterization data and warned that the model was unfit for evaluating Northeast plume source and dissolved-phase remedial options.

Table 2. Southwest Plume TCE Recharge Concentrations (DOE, 2010)

Source	Recharge Concentration, µg/L
SWMU-7	490
SWMU-2	16
SWMU-3	2,500
SWMU-1	5,000
SWMU-91	1,000
SWMU-4	5,000
SWMU-136	10,000
SWMU-209	10,000
AOC-211	10,000
SE Corner of C-720	10,000

Table 3. Northeast Plume Source Loadings in the 2008 TCE Model

	TCE Concentration (µg/L)								
	cell at C-333 bldg			Suspected Hotspot Source Area			Suspected Upper NE Source Area		
Year	Layer 1	Layer 2	Layer 3	Layer 1	Layer 2	Layer 3	Layer 1	Layer 2	Layer 3
1966-1973	0	0	0	0	0	0	0	0	0
1974	118	23.8	15.7	0.4895	0.4895	0.4825	8750.3	14173.15	9989.7
1975	1125	114	64.5	0.4565	0.4625	0.462	13495.7	21113.8	15355.05
1976	19731.75	880	410.5	0.417	0.425	0.4365	16619.35	26758.35	18216.85
1977	31250	12715.75	4620	0.333	0.3515	0.358	16989.55	26119.5	18125.15
1978	31250	31250	31250	0.239	0.273	0.3135	13793.2	20389.15	14016.45
1979	31250	31250	31250	0.209	0.282	0.3585	8465.3	12145.05	8702.25
1980	31250	31250	31250	0.61	0.9	1.245	4495	6277.15	4725
1981	31250	31250	31250	40.45	54.5	40.8	2490	3245	2365
1982	31250	31250	31250	100	100	100	1475	1840	1300
1983	31250	31250	31250	100	100	100	475.5	520	437
1984	31250	31250	31250	100	100	100	30.55	27.85	27.1
1985	31250	31250	31250	100	100	100	0.05	0.05	0.05
1986	31250	31250	31250	100	100	100	0.05	0.05	0.05
1987	31250	31250	31250	76	6.25	0.765	0.05	0.05	0.05
1988	31250	31250	31250	0.05	0.05	0.05	0.05	0.05	0.05
1989	31250	31250	31250	0.05	0.05	0.252	15.45	32.3	35
1990	31250	31250	31250	48.8	100	100	3350	6633.85	5822.25
1991	31250	31250	31250	100	100	100	835	1395	1710
1992	0.05	31250	31250	100	100	100	0.05	0.05	0.05
1993	0.05	10.9	250	0.331	1.775	12.35	5.45	16.05	9.05
1994	0.05	0.68	0.545	47765.45	2890	125	1610	500	375.5
1995	58.5	60	5.45	1520	32.45	0.1255	0.05	0.05	0.05
1996	31250	31250	31250	157894.5	24260.05	5414.6	6.6	11.65	8.85
1997	31250	31250	31250	184.5	69	34.8	3005	1280	910
1998	31250	31250	31250	352.5	14.3	0.129	1.21	0.515	0.815
1999	31250	680	27392.35	30643.45	218	1.03	2.19	3.64	3.245
2000	1.905	0.247	1.99	15081.45	34.85	0.05	16.1	9.3	9.35
2001	0.05	0.05	0.05	23366.45	162	0.59	8.95	13.75	10.25
2002	0.05	0.0575	0.05	4655	55	0.264	130.5	129	82
2003	0.1395	0.3125	0.2015	8695.2	105.5	0.57	2.26	1.185	1.585
2004	0.4545	0.484	0.456	8618.45	70.5	0.219	164.5	775	350
2005	0.5	0.5	0.5	6348.75	81.5	0.4785	6923	2250	1470
2006	0.5	0.5	0.5	9017.3	170.5	1.86	0.945	0.615	0.69
2007	0.5	0.5	0.5	9.35	5.9	6.95	0.5	0.5	0.5
2008	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5

4. Interim TCE Transport Model Configuration

The interim TCE transport model was built upon the 2016 update of the flow model and incorporated transport parameters and TCE source loadings from the 2008 TCE model. The interim model simulated a period from 1966 to 2018 to allow comparison of the model results with field-observed TCE plumes for recent years.

A transport model requires flow fields throughout the simulation period. Stress period 1 (SP1) of the 2016 update was used to represent the flow field during the period between 1996 and 2013 and stress period 2 (SP2) of the 2016 update for the more recent period of 2014-2018. The pumping data in the 2008 model and SP2 of the 2016 update were configured into the interim model as follows (Table 4).

Table 4. Pumping Data Incorporated into the Interim Model

Well Name	Pumping Rate (ft^3/d)	Years in Operation
N_NW_Field_229	-7700	1995-2011
N_NW_Field_228	-9625	1995-2011
S_NW_Field_230	-12127	1995-2011
S_NW_Field_231	-10203	1995-2011
NE_Field_331	-16940	1996-2018
NE_Field_332	-19828	1996-2018
S_NW_EW232	-21175	2011-2018
S_NW_EW233	-21175	2011-2018

The transport parameters in the 2008 TCE model (Table 1) were directly added to the interim model. The two constant concentration cells for the Northwest plume in the 2008 TCE model were directly incorporated into the model. The three time-varying constant concentration cells for the Northeast plume (Table 3) were copied over for the same period between 1966-2008. Because the concentrations of the three cells in 2008 were so low (0.5 µg/L), the sources were assumed disappeared after 2008.

The TCE sources for the Southwest plume in the 2008 model were introduced using recharge cells, which relied on flow rates and concentrations to introduce TCE to the model domain. The 2016 update refined anthropogenic recharge zones and had separate calibrated recharge values for the two stress periods. To make sure the exact amount of TCE was introduced into the

interim model, for each recharge cell, TCE concentration was calculated using the following equation:

$$C_{TCE\text{-}Interim}=C_{TCE\text{-}2008}*Q_{2008}/Q_{2016} \quad (1)$$

Where

$C_{TCE\text{-}Interim}$ -- TCE concentration of the recharge cell in the interim model

$C_{TCE\text{-}2008}$ -- TCE concentration of the recharge cell in the 2008 model

Q_{2008} -- Recharge rate of the recharge cell in the 2008 model

Q_{2016} -- Recharge rate of the recharge cell in the 2016 update

The recharge rate of SP1 of the 2016 update was used for the period between 1996 and 2013 in the interim model and the recharge rate of SP2 of the 2016 update for the more recent period of 2014-2018.

The 2008 TCE model was also extended to 2018 to compare the TCE plume prediction capabilities between the two models. Pumping data (Table 4) were incorporated into the extended period of 2009-2018. TCE sources for the extended period were assumed as same as the sources in 2008. Again, because the concentrations of the three cells for the Northeast plume in 2008 were so low (0.5 µg/L), the Northeast plume sources were assumed disappeared after 2008.

5. Model Result Comparison

Simulated TCE plumes from the interim model and the 2008 model for five different years, 1995, 2002, 2008, 2014, and 2018, were shown in Figures 1 through 5. These years were selected to show how well the two models predicted plume migration in recent years. These years are roughly evenly distributed temporally to show a consistent pace of plume migrations. All the selected years, except 2008, had field observed TCE plumes for comparing model predictions with field data. The year of 2008 was selected because 1) it was the last simulation year in the original 2008 TCE model and 2) it also filled the gap between 2002 and 2014 in which no field observed TCE plumes were available to the project.

Figures 1 through 5 illustrate that simulated plumes with the interim model plumes were smaller than plumes simulated with the 2008 model. Plumes in the interim model traveled less along the groundwater flow direction and spread less comparing to the plumes in the 2008 model.

The difference in simulated plumes can be explained by the groundwater fluxes of the models. The 2016 interim model had smaller flux than the 2008 model while both models utilized the same transport parameters.

In transport modeling, movement of solute is represented by two processes, advection and dispersion. Both processes are directly related to groundwater flux.

Advection is the process in which solutes travel with moving water. The travel velocity of a solute is calculated as

$$v = \frac{q}{n} \qquad (2),$$

where

v –solute travel velocity, commonly called average linear velocity

q – Darcy velocity or specific discharge, which is calculated from a groundwater flow model

n – Porosity

Dispersion in porous media is controlled by mechanical dispersion and molecular diffusion. Mechanical dispersion is caused by small scale velocity variations as water travels through various pores in the subsurface. In transport modeling, mechanical dispersion is represented by a linear combination of average linear velocity and dispersivity. For a three-dimensional solute transport problem, the spreading effect of the solute is represented by the longitudinal dispersivity in horizontal flow direction, by the transverse dispersity in the horizontal direction perpendicular to the horizontal flow, and by the vertical dispersivity in the vertical direction (See Table 1 for dispersivity values in the 2008 model). Molecular diffusion is caused by the concentration gradient of the solute. For most solute transport problems in aquifers, the effects of mechanical dispersion are much greater than the molecular dispersion.

Because both advection and dispersion are proportional to the Darcy velocity, smaller fluxes will lead to less travel distance along the flow direction and less spreading than larger fluxes given the same porosity and dispersivity values. In comparison with field observed plumes, the interim

model underestimated the plume size and migration distance. If the 2016 flow model is used to build TCE transport model, porosity and dispersivity need be adjusted to increase plume travel velocity and spreading to better match field observed plumes.

Figures 1 through 5 illustrate that both models matched the trajectory of the Northwest plume well. For the Northeast plume, the results from the 2008 model reasonably matched plume trajectory, but the simulated plume from the interim model traveled much further west and deviated further way from plume trajectory further north. The solute travel direction is controlled by the flow field from the associated flow model. A re-calibration of the 2016 flow model may be needed if it is used to build a transport model to simulate the Northeast plume.

The southwest plume was difficult to compare between models as simulated Southwest plumes from both models merged with the Northwest plume. The recent field data (Figures 4 and 5) also showed that the high concentration region of the southwest plume was disappearing, and the low concentration areas merged with the Northwest plume.

Finally, both models showed the simulated Northwest plume shrank over recent years, which were likely responses to operation of the long-term pump & treat system. How well the modeled responses match field observed responses is not evaluated in this project.

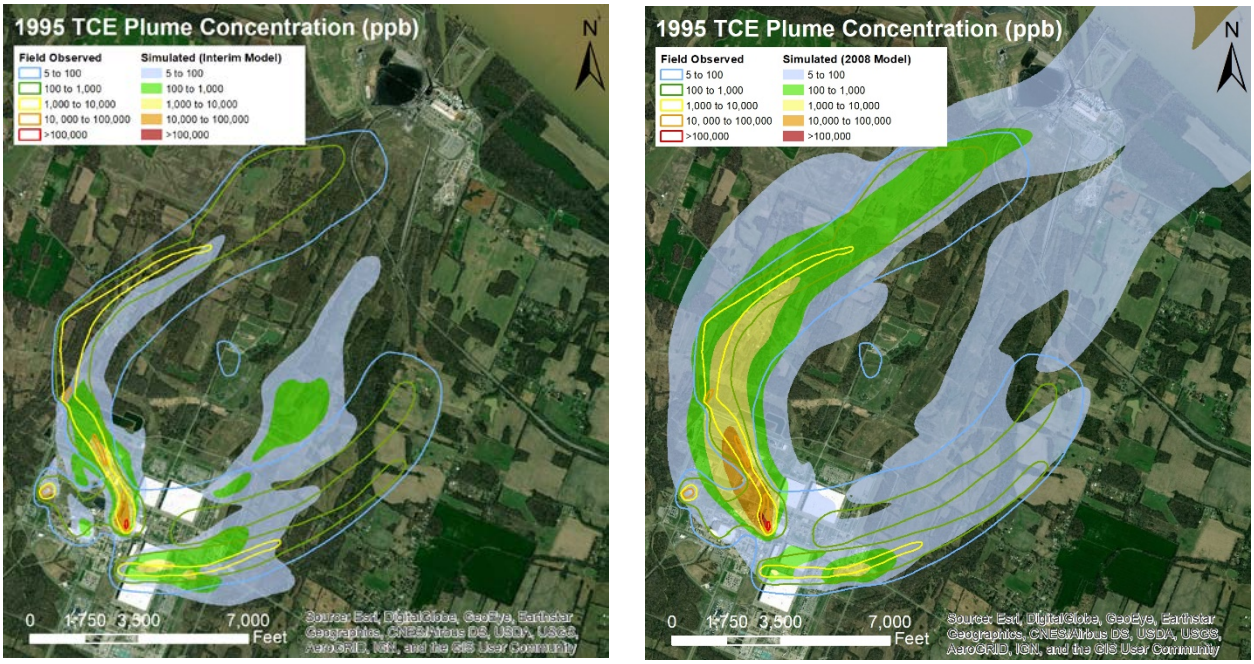

Figure 1. Comparison of TCE Plume Simulation Results for 1995 Between the Interim Model (left) and the 2008 Model (right). Color Floods Illustrate Simulation Results and Solid Lines Show Field Observed Plumes.

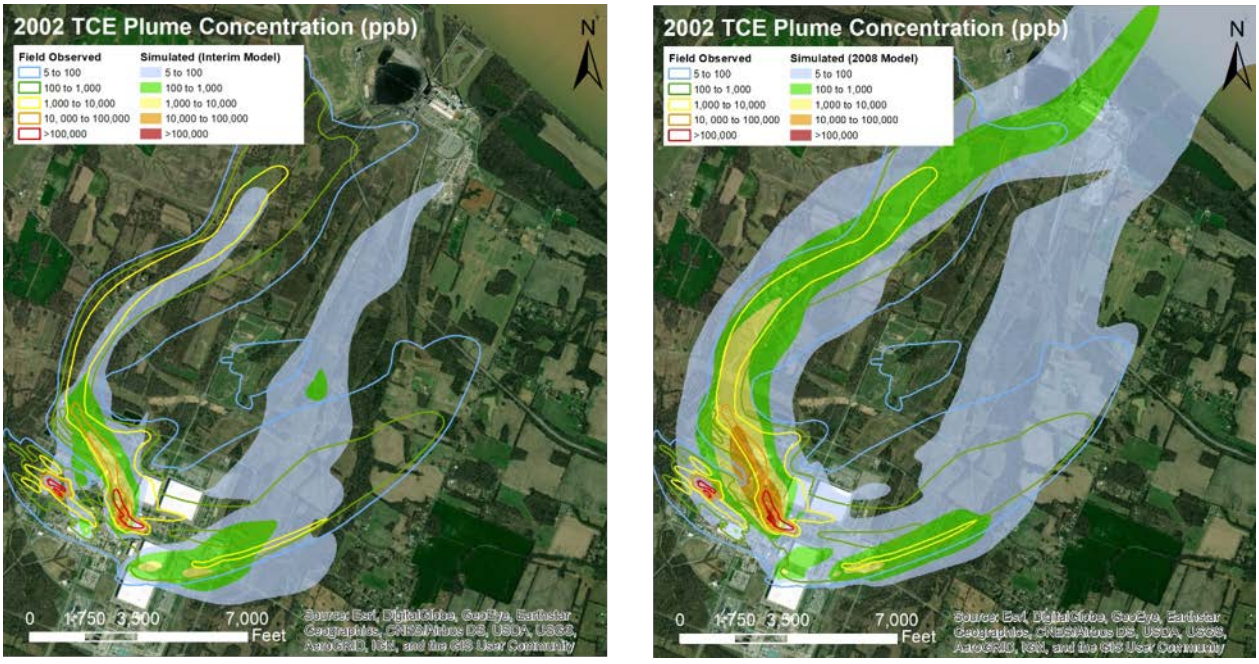

Figure 2. Comparison of TCE Plume Simulation Results for 2002 Between the Interim Model (left) and the 2008 Model (right). Color Floods Illustrate Simulation Results and Solid Lines Show Field Observed Plumes.

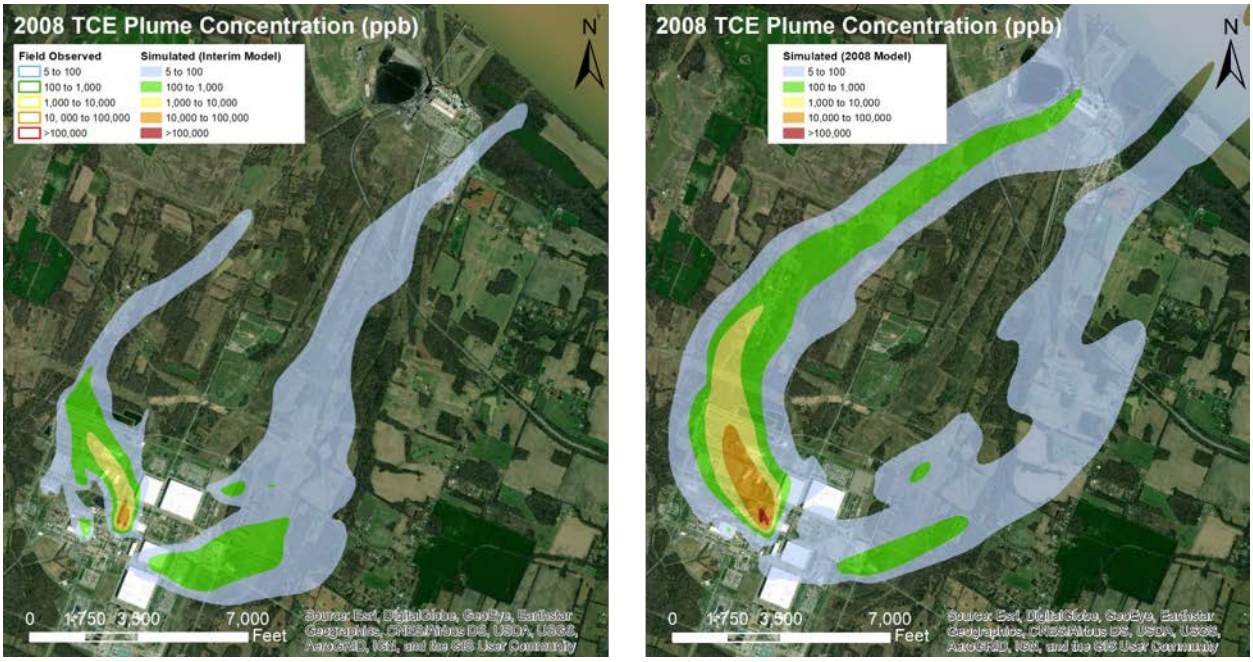

Figure 3. Comparison of TCE Plume Simulation Results for 2008 Between the Interim Model (left) and the 2008 Model (right). Color Floods Illustrate Simulation Results.

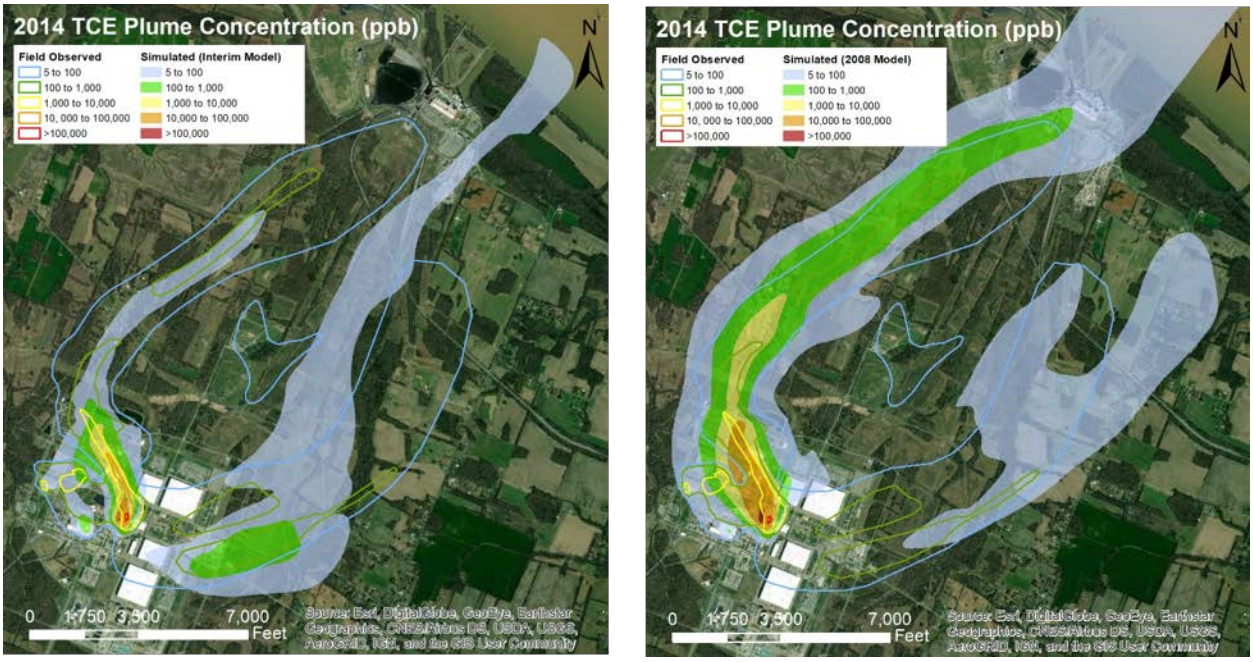

Figure 4. Comparison of TCE Plume Simulation Results for 2014 Between the Interim Model (left) and the 2008 Model (right). Color Floods Illustrate Simulation Results and Solid Lines Show Field Observed Plumes.

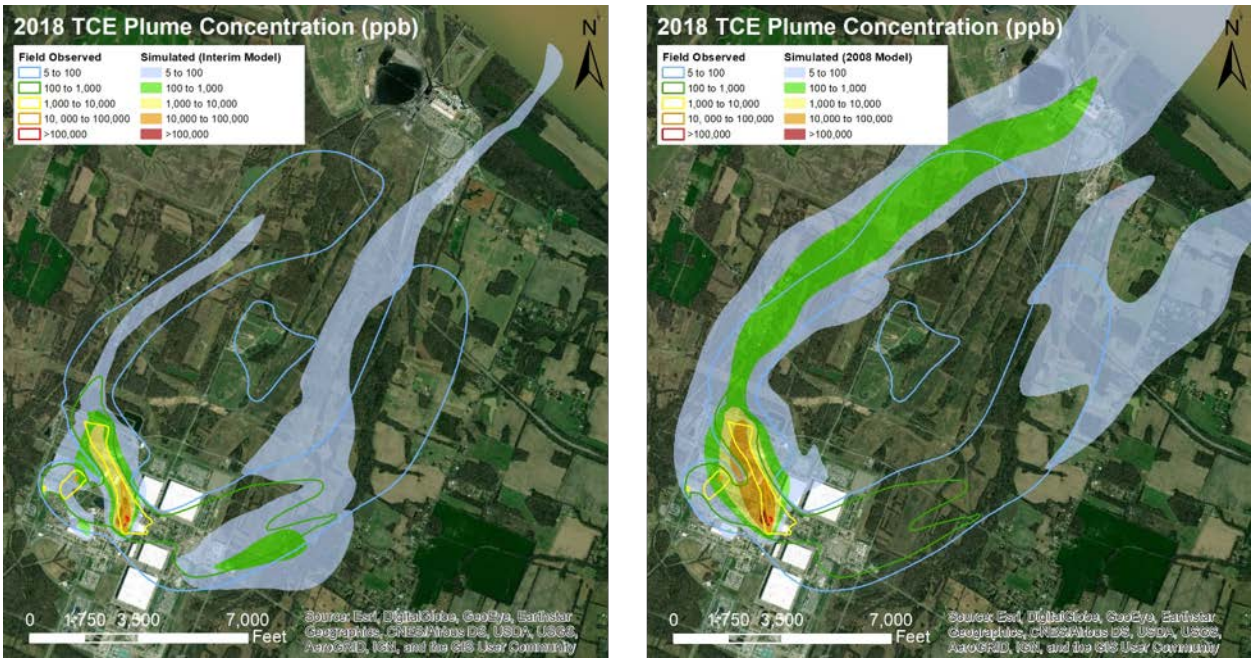

Figure 5. Comparison of TCE Plume Simulation Results for 2018 Between the Interim Model (left) and the 2008 Model (right). Color Floods Illustrate Simulation Results and Solid Lines Show Field Observed Plumes.

6. Conclusions

In this study, an interim TCE transport model was established to incorporate transport parameters of the 2008 TCE model into the 2016 flow model to assess the impacts of the changed flow field on simulating contaminant transport at the PGDP site. The simulated plumes from the interim model were compared with the results from the 2008 TCE model and field observed plumes. The study concludes:

1. The interim model underestimates the plume size and migration distance. If the 2016 flow model is used to build an updated TCE transport model, porosity and dispersivity will need be adjusted to increase plume travel velocity and spreading to better match field observed plumes.

2. The interim model matches Northwest plume trajectory well but deviates westward for the Northeast plume. A re-calibration of the 2016 flow model may be needed if it is used to build a transport model to simulate the Northeast plume.

7. Recommendations

Even though it incorporates more field data than the 2008 model, the 2016 flow model does not represent an improvement in flow simulation at the site, especially for the area associated with the Northeast plume. Running the 2008 TCE transport model through 2018, on the other hand, suggests that the 2008 model reasonably matches field plume trajectory for both the Northwest and Northeast plumes although plume shapes and extents need improvement. Consequently, we consider the 2008 model as a more cost-conscious choice for further contaminant transport modeling for the site.

If the 2008 model is used for future transport modeling, we recommend the following steps:

1. Re-calibrate the Northeast plume using field TCE source characterization data.

2. Adjust transport parameters to better match field plume shapes and extents.

Alternatively, if the 2016 flow model is selected for future transport modeling effort, we recommend the following steps:

1. Re-calibrate the flow model to better capture field flow direction in the Northeast plume area.

2. Incorporate transport parameters and sources for the Northwest and Southwest plumes from the 2008 transport model.

3. Calibrate the Northeast plume by adjusting TCE sources based on field TCE source characterization data.

4. Adjust transport parameters to better match field plume shapes and extents.

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