APPENDIX E

MODEL DEVELOPMENT AND CALIBRATION DOCUMENTATION

Introduction

A series of two-dimensional (2D) and three-dimensional (3D) models were calibrated to the results of the Steam Injection Treatability Study in the Regional Gravel Aquifer (RGA) at the C-400 Area at the Paducah Gaseous Diffusion Plant site in Kentucky. The RGA at Paducah is highly permeable, and it is bounded above by the low permeability Upper Continental Recharge System (UCRS) and below by the low permeability McNairy unit. The RGA is contaminated with trichloroethylene (TCE), and TCE is potentially present at the base of the RGA, at the RGA/McNairy contact.

A previous effort to heat the RGA using electrical resistance heating (ERH) resulted in substantial heating of the top part of the RGA, but poor heating of the lower part of the RGA (LATA, 2011). Consequently, a more aggressive steam injection approach is under consideration. In a high permeability formation that is below the water table, injected steam is subject to strong buoyancy forces that tend to cause the steam to rise. The upward buoyancy forces are countered by horizontal viscous forces that are caused by the relatively high pressure gradient that exists in the steam zone. The tendency for injected steam to rise and override parts of the formation (steam override) is proportional to the ratio of permeability to steam mass flux (van Lookeren, 1983; Basel and Udell, 1989; Falta, 1990; Falta, 2001). High permeability systems with low steam injection rates may be subject to strong steam override, while lower permeability systems with high steam injection rates will exhibit less steam override. The horizontal and vertical permeabilities of the RGA in the C-400 area have not been measured, although pumping tests in the RGA at other locations on the Paducah site have indicated that the permeabilities are high, with horizontal hydraulic conductivities of hundreds to thousands of ft/d (DOE, 2014b).

Falta (2013) performed a series of multiphase flow numerical simulations of possible steam injection behavior in the RGA at the C-400 area. The numerical simulations reported in Falta (2013) bounded the range of hydrogeologic and operational conditions that reasonably could be expected during steam injection in the RGA at Paducah. A total of twenty-five 2D and 3D simulations were performed using steam injection rates of 1000 to 5000 lbs/hr per well, with either one or two injection screen intervals per well location. The horizontal hydraulic

conductivity varied from a minimum of 100 ft/d, to a maximum of 1000 ft/d, and the horizontal to vertical hydraulic conductivity anisotropy ratio varied from a high of 18:1 to a low of 3:1. The simulations were performed using the Department of Energy TOUGH2-TMVOC model, developed at the Lawrence Berkeley National Laboratory (Pruess et al., 1999; Pruess and Battistelli, 2002). TOUGH2 has been applied to numerous multiphase flow heat transfer problems over the past 30 years, including applications in geothermal reservoir engineering and high-level nuclear waste isolation. The TMVOC module is designed specifically for simulating the steam injection remediation process.

The Falta (2013) simulations suggested that steam injection with injection rates of 1000 lbs/hr per well could be effective in treating the RGA provided that the horizontal hydraulic conductivity was moderate (less than a few hundred ft/day) and the anisotropy ratio was high (10:1 or more). That report also concluded that effective steam remediation performance will likely require injection well spacing on the order of 40 ft, with simultaneous operation of the injection and extraction wells.

The Steam Injection Treatability Study was performed between April 9, 2015 and June 30, 2015. The study consisted of four stages: a Phase 1 steam injection from April 9 through April 29, where steam was injected at a rate of 500 lbs/hr into the upper and lower screen, a Phase 2 cooldown period that lasted from April 29 through May 12, a Phase 3 steam injection from May 12 through May 31, where steam was injected into the lower screen at a rate of 1000 lbs/hr, and a Phase 4 cooldown period that lasted from May 31 through June 30, 2015.

The purpose of the numerical model calibration simulations described here is to develop better estimates of the horizontal and vertical permeability structure in the RGA at the C-400 area, to assess the effects of regional groundwater flow on the steam injection and cooldown behavior, and to provide insights into the movement of steam in the RGA during the Treatability Study.

The calibrated horizontal and vertical permeability structure from this modeling effort is used in a series of 3D simulations that are designed to evaluate full-scale steam remediation configurations.

TOUGH2 Numerical Simulator

The simulations were performed using the TMVOC (Pruess and Battistelli, 2002) version of TOUGH2 (Pruess et al., 1999). TOUGH2 is a 3D multiphase flow heat and mass transport code that was developed at the Department of Energy Lawrence Berkeley National Laboratory over the past 30 years. The code originated in the 1980's as a geothermal reservoir simulator, and was later adapted for use in a variety of fields including high level nuclear waste isolation, enhanced oil recovery, environmental remediation of volatile organic contaminants (VOCs), and carbon dioxide sequestration. The models are written in FORTRAN, and the source code is publicly available from the DOE. TOUGH2 is currently in use at more than 350 research laboratories, private companies, and universities in 40 countries. The results of scientific and engineering studies using the TOUGH2 codes have appeared in more than 500 refereed journal papers (http://esd1.lbl.gov/research/projects/tough/documentation/publications.html). A graphical user interface called PetraSim (http://www.thunderheadeng.com/petrasim/) was used to develop the input files for TMVOC, and to process the output files for the work reported here.

The TMVOC module of TOUGH2 has a capability for simulating 1D, 2D, or 3D geometries using cylindrical, Cartesian, or unstructured grids, with the integral finite difference method. The model domain may be fractured or porous, heterogeneous and anisotropic, with various types of boundary conditions. The model simulates full multiphase (gas, aqueous, NAPL) flow with relative permeability and capillary pressure effects. Each phase moves in response to pressure and gravitational forces, including buoyancy driven flows. Heat transfer occurs by multiphase convection of sensible and latent heat with thermal conduction. Multiphase thermodynamics include evaporation and condensation of water and multiple VOCs that may form a NAPL. Multiphase contaminant transport occurs by advection and diffusion with retardation and first order decay in the aqueous phase. The calibration simulations reported here did not include any contaminants, so only air and water were included as mass components.

The TMVOC code, and its predecessors, M2NOTS (Adenekan et al., 1993) and T2VOC (Falta et al., 1995; 1992a,) have been used to simulate a variety of steam injection operations, ranging from the lab scale (Falta, 1990; Falta et al., 1992b; Falta, 2001; Gudbjerg et al., 2004a,b; Hodges

et al., 2004; and Chen et al., 2012) to the field scale (Adenekan and Patzek, 1994; Ochs et al., 2003; and Gudbjerg et al., 2005).

During a previous study, Falta (2013) found that the numerical performance (speed) was relatively poor compared to past experience on other problems. It was later determined that this was due to a numerical phenomenon identified and described by Gudbjerg et al. (2004b). During steam injection into cold water with high permeability, small numerical pressure fluctuations can sometimes occur at the steam/water interface. While these fluctuations do not affect the overall accuracy of the simulations, they can dramatically reduce the rate of numerical convergence, leading to very small time-steps, and poor numerical performance (Gudbjerg et al., 2004b; 2005). To alleviate this problem, the TOUGH2 code modification proposed by Gudbjerg et al. (2004b) was made to the TMVOC source code. This eliminates the numerical pressure fluctuations, and it improved the speed of the simulations by a factor of 20 or more for some cases. The FORTRAN code modification is shown in Figure 1.

The TMVOC version of TOUGH2 has been subjected to a comprehensive quality assurance/quality control (QA/QC) process by the Department of Energy. Complete details of the program structure, mathematical and physical assumptions, input and output formats, and test problems are given in the two DOE model user's guides (Pruess et al., 1999; Pruess and Battistelli, 2002). The TOUGH2 codes (including TMVOC) have been used in scientific and engineering studies that have been published in more than 500 referenced journal papers and reports. A comprehensive listing of these publications can be found at the Lawrence Berkeley National Laboratory TOUGH website:
(http://esd1.lbl.gov/research/projects/tough/documentation/publications.html).

```
C-----FLUX IN PHASE NP.
      FNPM=DMOBI*RHOX*DR*AX
c
c-----add Gudbjerg et al 2004 modification for steam flooding; limit spurious
c     cold water flow into steam element at steam front  Falta 11/26/12
c
c     Only for NP=2, aqueous
      if(np.ne.2) go to 665
c     get gas saturations, water mole fractions in gas phase
      sg1=par(n1l2np+1-nbk)
      sg2=par(n2l2np+1-nbk)
      xmwg1=par(n1l2np+nb+1-nbk)
      xmwg2=par(n2l2np+nb+1-nbk)
      xma1=1.-xmwg1
      xma2=1.-xmwg2
c     case #1, element 1 is in steam zone, element 2 is not
      if((sg1.gt.0.).and.(xma1.lt.0.01)) then
        if((sg2.eq.0.).or.(xma2.gt.0.01))  then
c     check for flow from 2 to 1 and large temp grad
          if((DR.gt.0.0).and.((t1-t2).gt.15.0)) then
            fnpm=0.0
      else if((dr.gt.0.0).and.((t1-t2).lt.15.0)) then
            fnpm=fnpm*(1.-(t1-t2)/15.)
      endif
      endif
      endif
c
case #2, element 2 is in steam zone, element 1 is not
        if((sg2.gt.0.).and.(xma2.lt.0.01)) then
        if((sg1.eq.0.).or.(xma1.gt.0.01))  then
c     check for flow from 1 to 2 and large temp grad
          if((DR.lt.0.0).and.((t2-t1).gt.15.0)) then
            fnpm=0.0
      else if((dr.lt.0.0).and.((t2-t1).lt.15.0)) then
            fnpm=fnpm*(1.-(t2-t1)/15.)
      endif
      endif
      endif
c
c
  665 continue
C
```

Figure 1. This FORTRAN code fragment was added to TMVOC in subroutine MULTI in the location where the phase mass fluxes are computed. This modification was based on the method developed by Gudbjerg et al. (2004b), designed to reduce numerical pressure fluctuations that occur as cold water flows into the steam zone at the condensation front.

2D RZ Simulations

Model design

The 2D rz calibration simulations use a cylindrical model that is centered around a steam injection well with 2 screens. In the vertical direction, the model extends from the ground surface, to a depth of 115 ft and it includes the UCRS, the RGA, and the uppermost part of the McNairy unit. The ground surface is maintained at atmospheric temperature (20 C) and pressure (1 atm; 101.3 kPa). In the radial direction, the model starts at the center of the steam injection well borehole. The first gridblock has radius of 6 inches (corresponding to the borehole) and the grid extends to an outer radius of 328 ft. The outer lateral boundary, and the model initial condition have a constant temperature of 20 C, and a water table at a depth of 57 ft, with the fluid pressures and saturations determined from gravity-capillary equilibrium. During the calibration process, the water table was raised several feet in order to match the observed hydrostatic pressure in the steam zone as reflected in the steam temperatures. The bottom boundary is a no-flow boundary. Figure 2 shows a scale cross-section of the rz grid. The 2D model has a total of 2451 gridblocks, and simulations of the Phase 1 steam injection run in about 15 minutes. Simulations of all four Phases require close to one hour of computer time.

In the model, the UCRS extends from the ground surface to a depth of about 57 feet. The base of the UCRS/top of the RGA is slightly variable across the different TMP locations. The RGA extends from about 57 feet to about 93 feet below ground surface. The base elevation of the RGA is also slightly variable across the TMP locations. Figure 3 shows the TMP locations in the grid. Due to the assumption of radial symmetry, all of the TMP locations appear in one rz plane in this model. In Figures 2 and 3, the RGA has been divided into two layers: an upper zone, and a lower zone.

Initial simulations of the Phase 1 steam injection were performed as the steam injection was taking place in April, 2015. It quickly became apparent that at least a two-layer configuration was needed to approximately match the field measured temperatures at the TMP locations. The properties of these layers is described in the 2D calibration section.

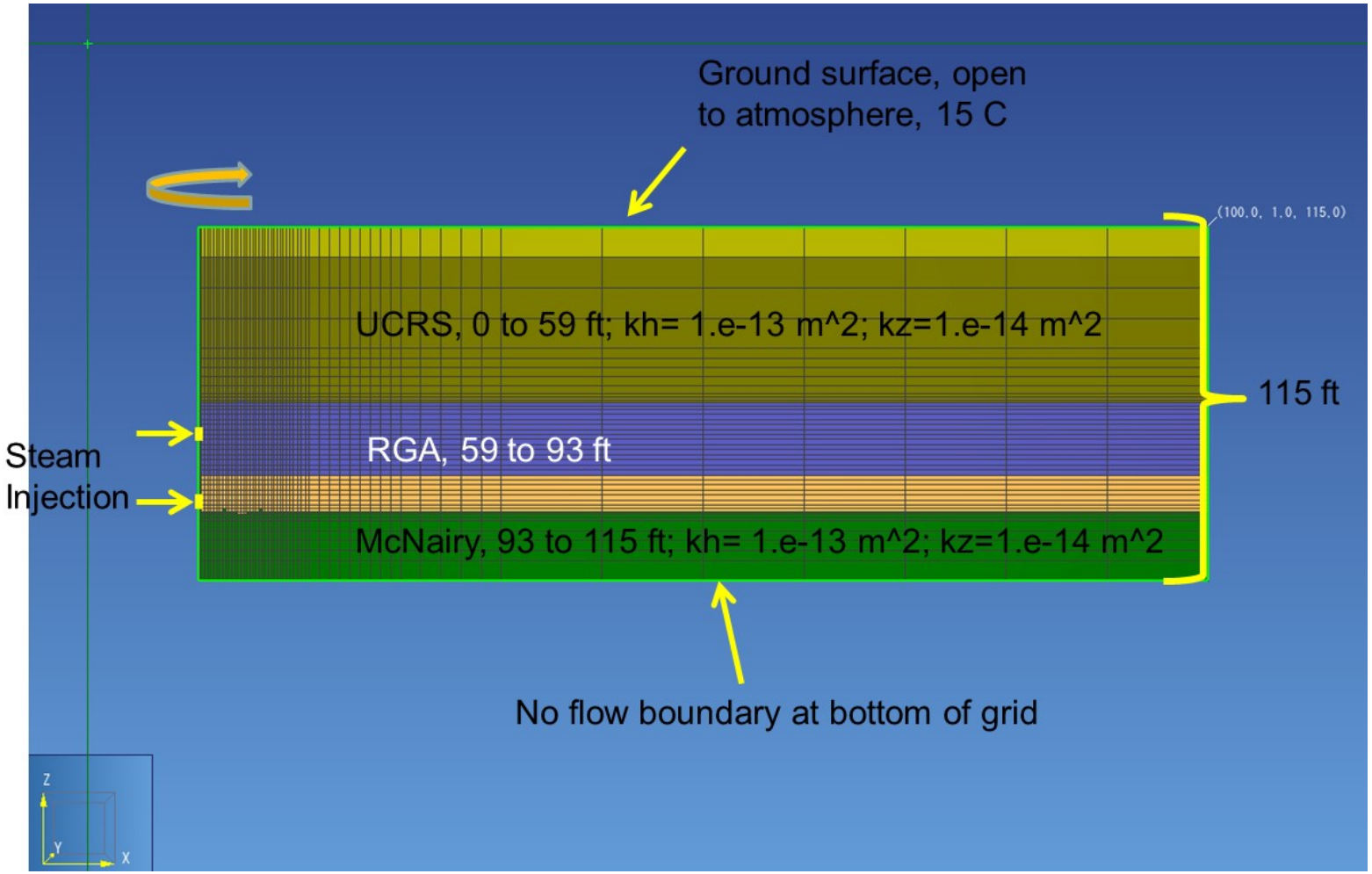

Figure 2. Cross-section of rz grid used in the TMVOC simulations. The grid is rotated around the left hand side to form a cylinder, and steam is injected into one or two locations at the radial center of the model.

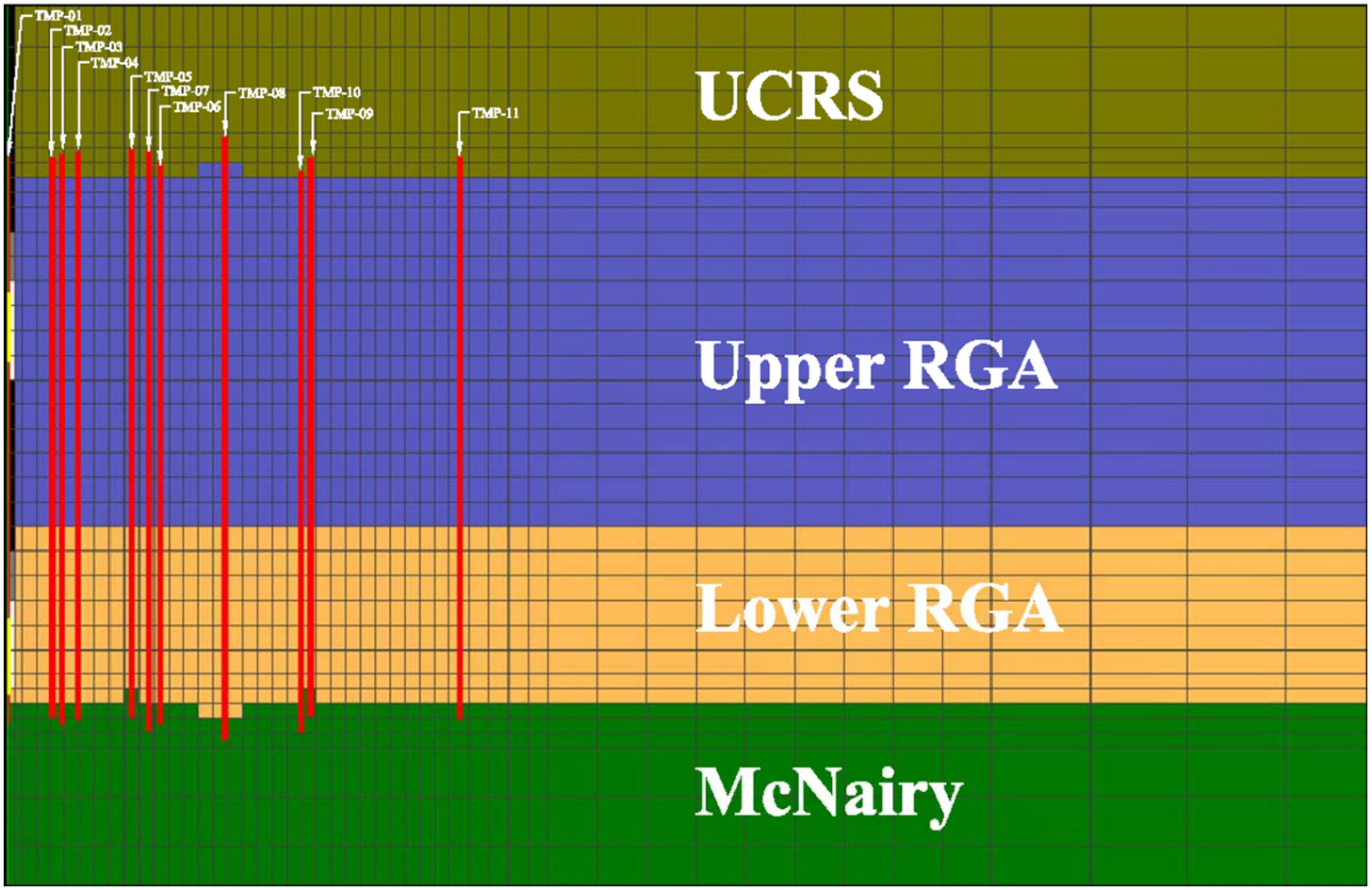

Figure 3. Cross-section of rz grid used in the TMVOC simulations showing the TMP locations.

The TOUGH2 codes use intrinsic permeability (*k*) instead of hydraulic conductivity (*K*). The relationship between quantities is:

$$k = \frac{K\mu}{\rho g}$$

where μ is the viscosity of water at groundwater temperatures, ρ is the water density, and g is gravitational acceleration. Using these quantities, a hydraulic conductivity of 100 ft/d is equivalent to an intrinsic permeability of about 4×10^{-11} m^2.

Throughout the simulations, the properties of the UCRS and the McNairy were held constant, with a horizontal permeability of 1×10^{-13} m^2, and an anisotropy ratio of 10:1. The layered permeability structure in the RGA was the primary calibration variable used to generate a best match of the field data from the Treatability Study. Thermal properties, soil grain heat capacity and thermal conductivity, were varied within the narrow range of expected values but they had little effect on the simulation results.

Capillary pressures were calculated using the van Genuchten (1980) model. In the UCRS and McNairy, the vG α was 1 m^{-1}, the vG n was 2.0, and the water residual saturation was 0.3. In the RGA, the capillary pressure is much lower, and was calculated using a vG α of 10 m^{-1}, a vG n of 2.2, and a residual water saturation of 0.2. Gas and water phase relative permeabilities were calculated using scaled cubic functions of saturation (Pruess and Battistelli, 2002; Falta et al., 1995).

The thermal properties of the three formations were uniform, with a rock grain density of 2650 kg/m^3, a porosity of 0.35, a rock grain heat capacity of 800 J/kgC, a water saturated bulk thermal conductivity of 3 W/mC, and a dry bulk thermal conductivity of 0.6 W/mC. These values are consistent with those reported in Lake (1989) for unconsolidated sands. The thermodynamic properties of water are computed inside the code using international steam table equations. In most simulations, the specific enthalpy of injected steam was 2,265,000 J/kg, which corresponds to a 120 C saturated steam with a quality of 0.8. This value of specific enthalpy assumes that conductive heat losses in the piping and borehole above the injection screen cause some of the steam vapor to condense. During the review of the calibration

modeling, there was some discussion about the magnitude of these heat losses in the piping. Based on the properties of the steam boiler, the pressure reducing valves, and the piping, it is likely that an injected specific enthalpy of 2,265,000 J/kg represents more or less a lower bound for the actual injected specific enthalpy. If the heat losses downstream of the pressure reducing valves are small, then the injected steam would have a quality close to one, and the specific enthalpy would be about 2,700,000 J/kg. Simulations performed using this higher value were similar to ones with the lower value, except that the predicted temperature in some parts of the subsurface were slightly higher. Overall, the use of this larger enthalpy value only changed the error in the model predictions of the TMP temperatures by about 1%. The uncertainty in the actual steam enthalpy leaving the screens is similar to the uncertainty in the soil grain specific heat capacity. The simulations reported here assumed a value of 800 J/kgC, but the likely range is about 750-1000 J/kgC. If the larger heat capacity is used with the larger steam specific enthalpy in the model, the results are practically the same as when the lower heat capacity is used with the lower steam specific enthalpy.

The steam injection rate during Phase 1 was 500 lbs/hr into both screens. During Phase 3, steam was injected into the bottom screen at a rate of 1000 lbs/hr. Both screens are 5 feet in length. The upper screen extends from a depth of 67 to a depth of 72 feet, while the lower screen extends from to a depth of 88 feet to the base of the RGA at a depth of 93 feet.

Phase 1 rz model calibration

The 2D rz Phase 1 model calibration was performed during, and immediately following the Phase 1 steam injection. Interestingly, a model that was calibrated to the Day 4 steam injection temperatures provided a match to the 20 day Phase 1 steam injection temperatures that was practically as good as any produced during the later 2D calibration runs.

Initial calibration efforts used both the temperature profiles from the TMP locations and the steam arrival times at the TMPs. It soon became apparent that the use of steam arrival times as the main calibration target was inferior to the use of temperature profiles as a calibration target. There are several reasons why steam arrival time was found to be a relatively poor choice as the calibration target.

First, there are a total of 186 different temperature monitoring points in the 11 TMP arrays. During the Phase 1 steam injection, steam temperatures were only observed in about 70 of the TMPs, or about 1/3 of the total. By using steam arrival times as the calibration objective, the valuable experimental data from nearly 2/3 of the measuring points are not used.

Second, the model error determined by summing the square of differences in the observed and simulated steam arrival times was relatively insensitive to poor model performance. This is due to the fact that only locations where both the model and the field data show steam arrival are used in this calculation. Therefore if the model fails to predict steam arrival at a location where it is observed, or if steam is not observed at a location where the model predicts it, that data point is removed from the calculation, and there is no penalty for the inaccuracy of the model.

Third, in some locations it can be difficult and ambiguous to determine exactly when the steam front reaches a given location from temperature measurements alone. This is due to the fact that the water boiling point is a function of depth, distance from the injection well, and time, as the subsurface pressure changes. At several locations, the field measured temperature climbed slowly past 100 C (212 F), and gradually approached 124 C (255 F). It is not clear from these data when to pick the steam arrival time.

Fourth, the steam arrival time is irrelevant during the Phase 2 and Phase 4 cool downs, so there is no way to compare model performance during these periods using steam arrival times.

Finally, it is very time-consuming to extract the steam arrival time (if any) from each of the 186 TMP locations in the model. For each simulation, it requires generating a time series plot of temperature and gas saturation for each temperature monitoring point to find the model steam arrival time.

Based on these considerations a decision was made to use the temperature data from the 186 TMPs at the end of the Phase 1 steam injection as the Phase 1 calibration target. The model calibration is based on a minimization of the residual sum of squares (RSS) between the observed and simulated TMP temperatures at the end of Phase 1 using a trial and error

method. From the RSS, the root mean square error (RMSE) and the normalized root mean square error (NRMSE) in the predicted temperatures can be computed.

After performing more than 20 simulations, it was found that the best matches with the 2D rz model had a NRMSE of around 20%, which is somewhat larger than the NRMSE goal of 10% stated in the Treatability Study Design document (DOE, 2014b). The criterion of 10% NRMSE was considered a goal, because this criterion is based on groundwater modeling studies where the simulation variable is the hydraulic head, not on studies of SEE results, where the simulation variable is temperature. Figure 4 shows a comparison of the simulated and observed temperatures at the end of Phase 1 for a simulation with a NRMSE of 21%. This model run will be referred to as the "base rz model"; it was the one that was originally calibrated during the fourth day of steam injection. Subsequent rz modeling efforts for Phase 1 did not improve on this model substantially.

This model uses a 2 layer structure for the RGA as shown in Figures 2 and 3. The upper part of the RGA has a horizontal hydraulic conductivity of 100 ft/d, and an anisotropy ratio of 20:1. The lower part of the RGA has a horizontal hydraulic conductivity of 300 ft/d, and an anisotropy ratio of 30:1.

The base rz model does a good job of matching several of the TMP locations such as TMP 3, 4, and 7, and a fair job of matching TMP locations 1, 2, and 8. This model, however, produces a relatively weak match with locations 5, 6, 9, 10, and 11 due to the effects of lateral heterogeneities that cannot be accounted for in the radially symmetric 2D model.

These field data indicate that the steam flow is not radially symmetric. For example, TMP 6 and TMP 7 are both located 10 feet from the steam injection well, but they show different temperature responses. Similarly, TMP 9 and TMP 10 are both located 20 feet from the injection well, but they also show different temperature responses. Due to the asymmetry of steam flow, a 3D model was used for the final model calibration and model validation. This second calibration effort will be described in a later section (see 3D Simulations).

Deleted: 10

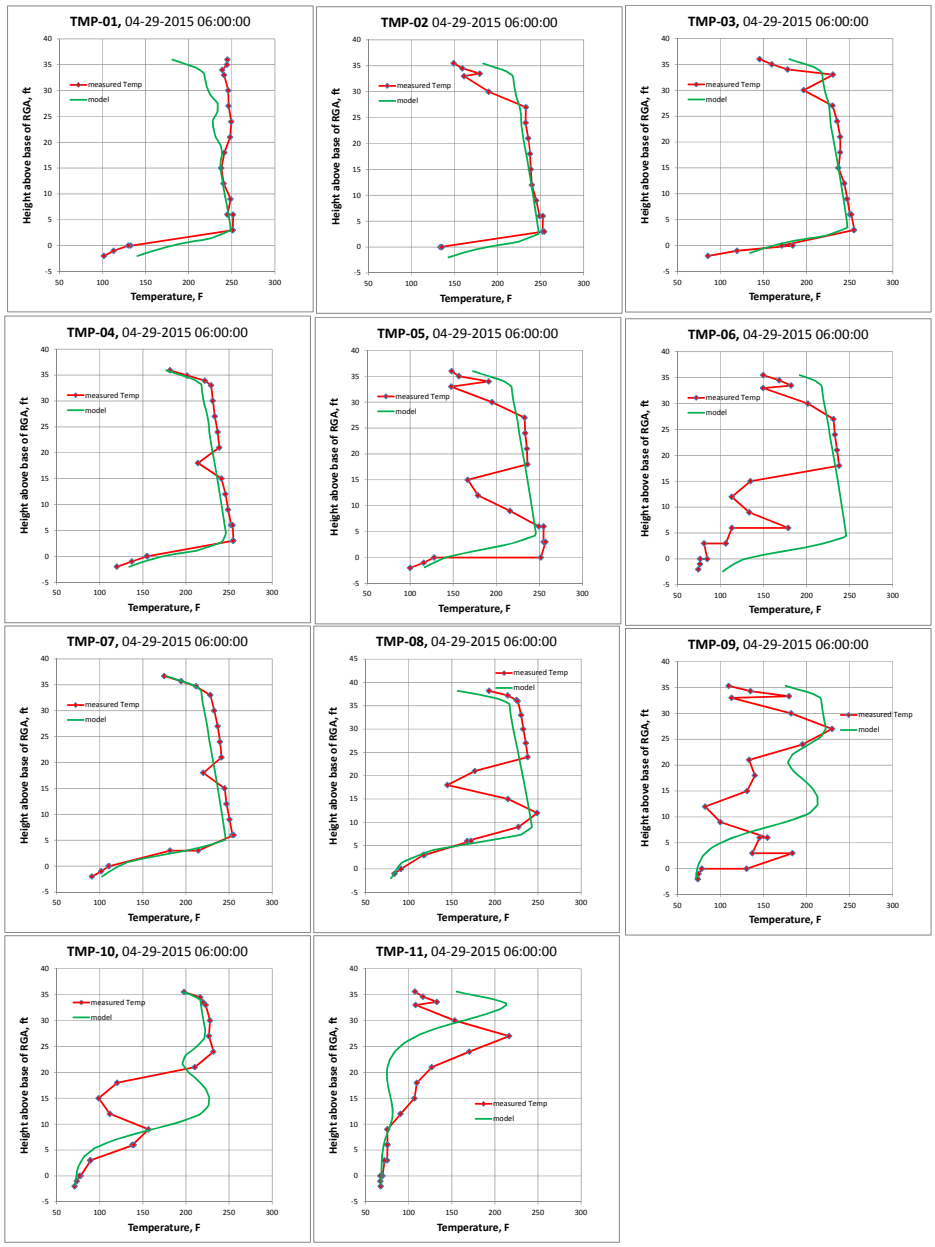

Figure 4. Comparison of simulated and observed temperatures at the end of Phase 1. Simulation performed using a model that will be referred to as the "base rz model".

Phase 1 rz model sensitivity

The 2D rz Phase 1 model sensitivity was evaluated by systematically varying the key parameters (horizontal hydraulic conductivity and the anisotropy ratio) and comparing the model fit to the data using the residual sum of squares (RSS). Table 1 shows the rz phase 1 model sensitivity.

Table 1. Phase 1 rz model sensitivity showing the residual sum of squares (RSS)

Kh/anisotropy	**5:1 (u) 7.5:1 (l)**	**10:1 (u) 15:1 (l)**	**20:1 (u) 30:1 (l)**	**40:1 (u) 60:1 (l)**
50 upper 150 lower		289k	382k	
100 upper 300 lower	383k	238k	295k (base rz model)	364k
200 upper 600 lower		383k	243k	
400 upper 1200 lower			391k	

The horizontal hydraulic conductivity (ft/d) is plotted along the vertical axis, and the anisotropy ratio is plotted along the horizontal axis. Several model parameter combinations (shown in green) produced RSS values that were as good, or better than the rz base case. However, the two cases with the lowest RSS failed to match the temperature profiles near the base of the RGA as accurately as the base rz model. Overall, the results of this sensitivity study show that the horizontal hydraulic conductivity is likely to be in the range of 50 to 200 ft/d in the upper part of the RGA and in the range of 150 to 600 ft/d in the lower part of the RGA. The anisotropy ratio is high, likely ranging from 10:1 to 20:1 in the upper RGA and 15:1 to 30:1 in the lower RGA. It should be noted that the lower end of the anisotropy range (10:1; 15:1) only produces good results when the lower hydraulic conductivity values are used. Similarly, the

higher anisotropy values produce the best results when the larger hydraulic conductivity values are used.

Phase 1, 2, and 3 rz model calibration

The base rz model (which was developed on day 4 of Phase 1) was used during the Treatability Study to predict the future performance of the Phase 1 steam injection, the Phase 2 cooldown, and the Phase 3 steam injection. This model did a reasonably good job of predicting all of Phase 1, the Phase 2 cooldown, and the early part of the Phase 3 lower steam injection. However, as the Phase 3 injection continued, it became apparent that the original base rz model was starting to overpredict the amount of vertical steam migration from the lower zones.

Based on these observations, the model was rebuilt in an effort to match the temperature profiles during all 3 phases. A total of 15 parameter combinations were tested. The key feature that was required in order to match the Phase 3 temperature data was the inclusion of a thin layer of lower permeability material at the top of the lower RGA high permeability zone. In the model, this layer is 1.6 ft. thick, and it has a horizontal hydraulic conductivity of 1.5 ft/d, with an anisotropy ratio of 10:1. The addition of this lower permeability layer is consistent with geologic well logs from the site (see, for example, DOE, 2014a, Figures 4 and 6) that show isolated lenses of finer grained materials within the RGA.

The water table was raised by 3 feet in this model to a depth of 54 feet from the ground surface. The increase in the water table elevation increases the hydrostatic pressure and thus the temperature in the steam zone. The slightly increased temperatures from this revised model better match the field data.

The calibrated model, which will be called the “rz Phase 3” model has an accuracy during Phase 1 that is similar to the base rz model, but it does a much better job of matching the Phase 3 temperature results. Figures 5, 6, and 7 show the model comparison with the field temperature data at the end of Phase 1, the end of Phase 2, and near the end of Phase 3. With the exception of TMP 5, 6, and 11, this model does a reasonable job of reproducing the Phase 3

temperatures. As before, the effects of lateral heterogeneity prevent a better match of the field data with the rz model.

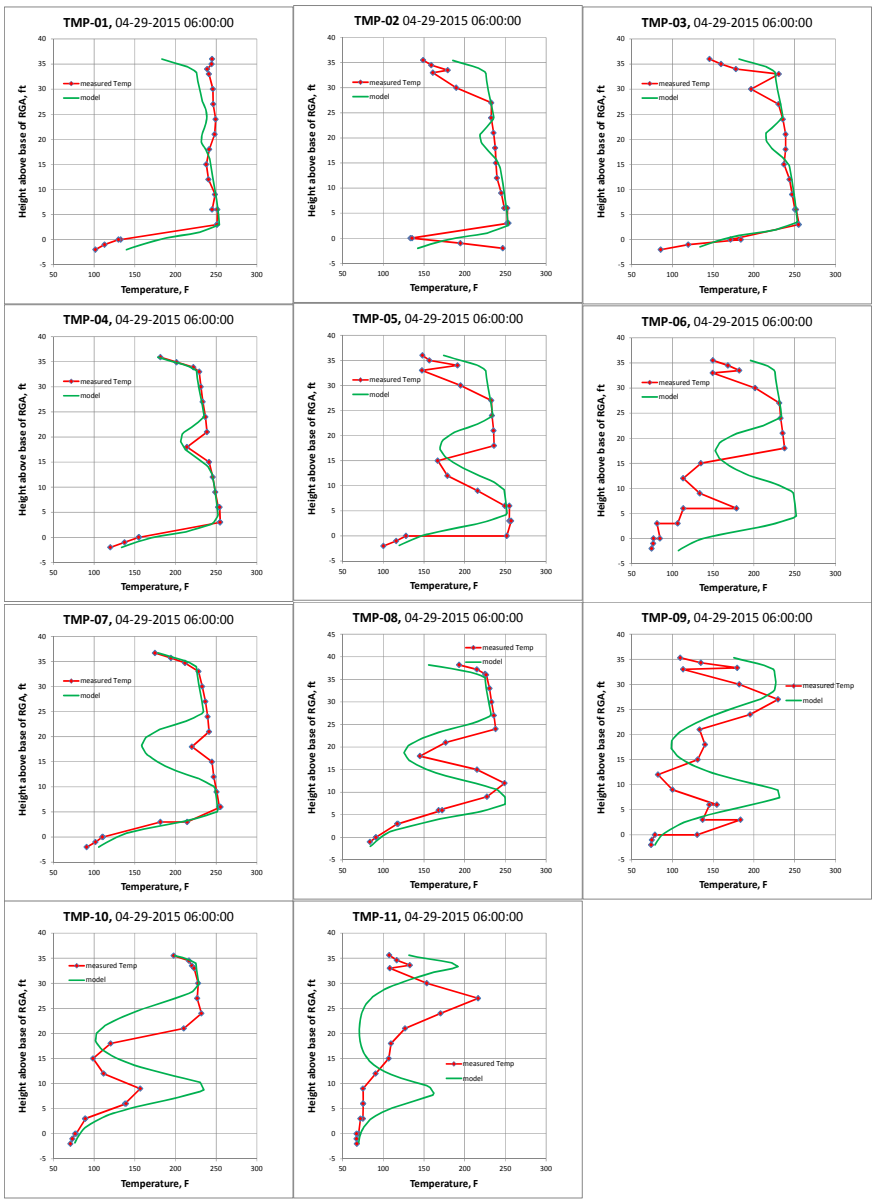

Figure 5. Comparison of simulated and observed temperatures at the end of Phase 1. Simulation performed using a model that will be referred to as the "rz Phase 3" model.

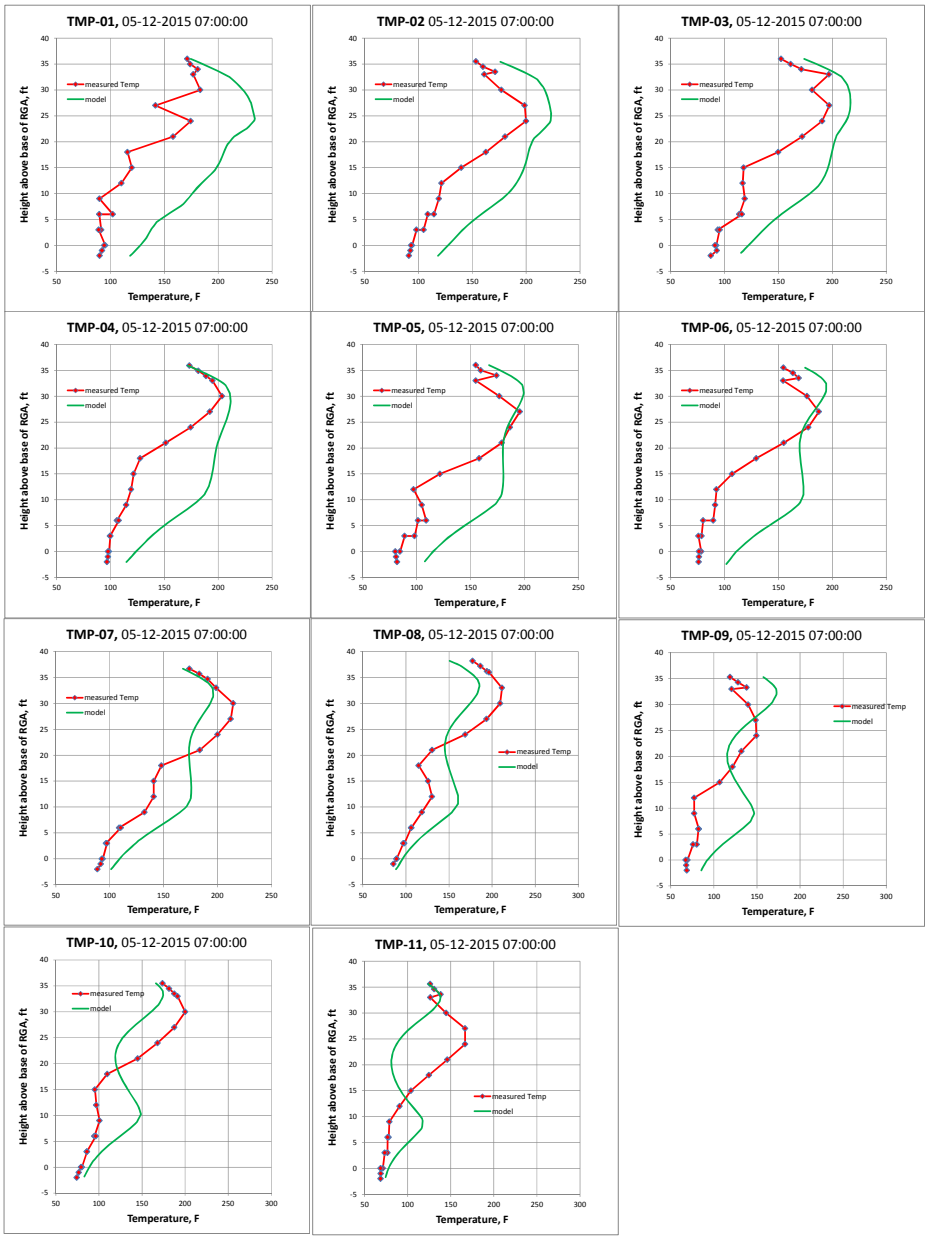

Figure 6. Comparison of simulated and observed temperatures at the end of Phase 2. Simulation performed using a model that will be referred to as the "rz Phase 3" model

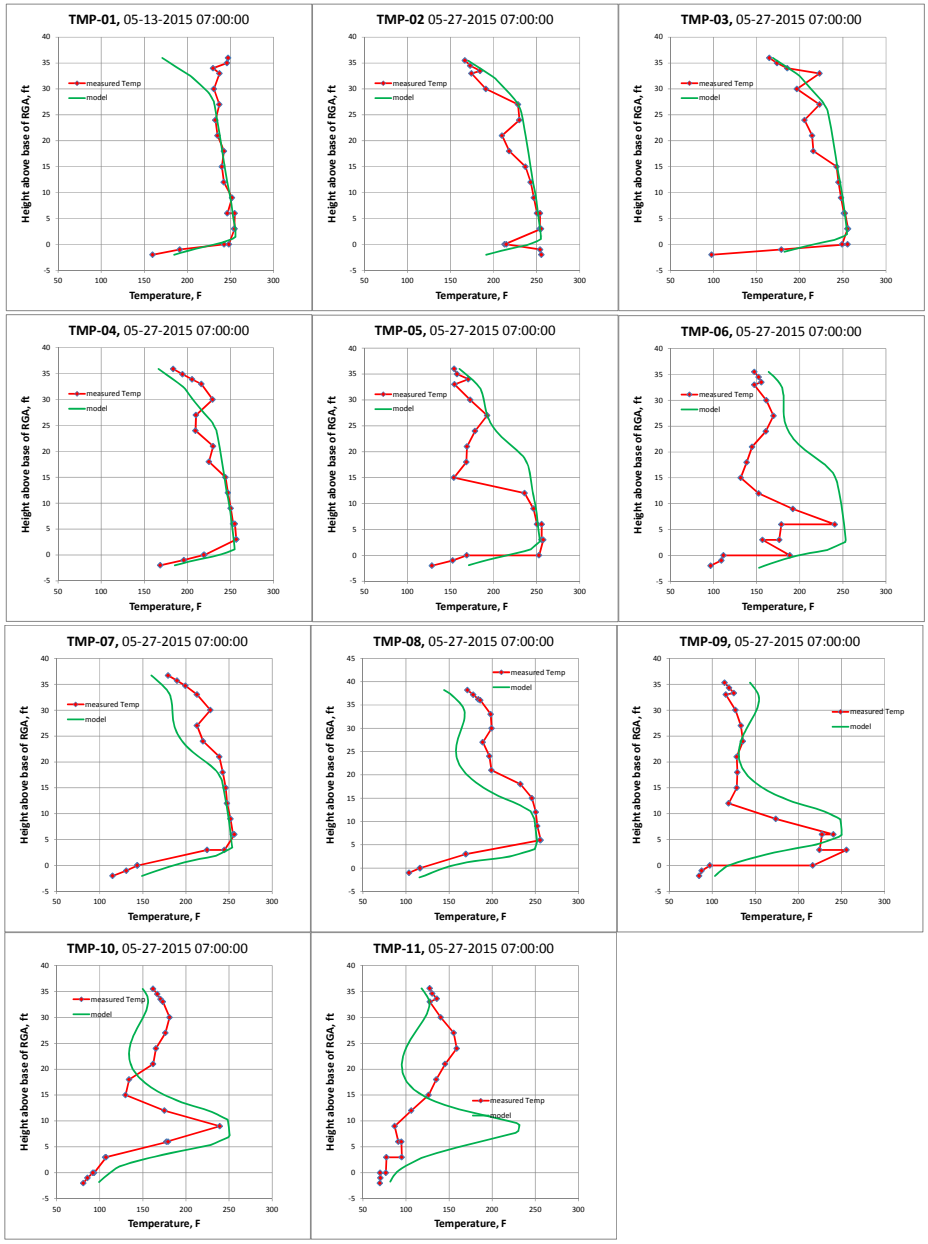

Figure 7. Comparison of simulated and observed temperatures near the end of Phase 3. Simulation performed using a model that will be referred to as the "rz Phase 3" model.

3D Simulations[1]

Model design

A 3D model of the Treatability Study was built in order to account for the effects of lateral heterogeneity and regional groundwater flow on the steam flow and cooldown patterns. The initial model was based on the layered structure of the 2D model described above. The model grid, shown in Figures 8 and 9 extends from the ground surface to a depth of 115 feet, and it has horizontal dimensions of 120 feet on a side. The rectangular model volume is oriented so that it is parallel to the regional groundwater flow direction (DOE, 2014b).

The 3D model was developed by building geologic layers that correspond to the UCRS, the RGA, and the uppermost part of the McNairy. The ground surface was assumed to be flat, but the top and bottom surfaces of the RGA were interpolated and extrapolated using the well logs from each of the 11 TMP locations. Both surfaces undulate slightly, with elevation changes of about 1.5 feet across the TMP array. The model is centered around the steam injection wells (Figure 10), and it extends well beyond the steam zone in the test.

[1] The 3D figures presented in these sections are screenshots from the modeling software simulations. These screenshots are provided as visual aids to assist the reader with interpretation of the theoretical model(s).

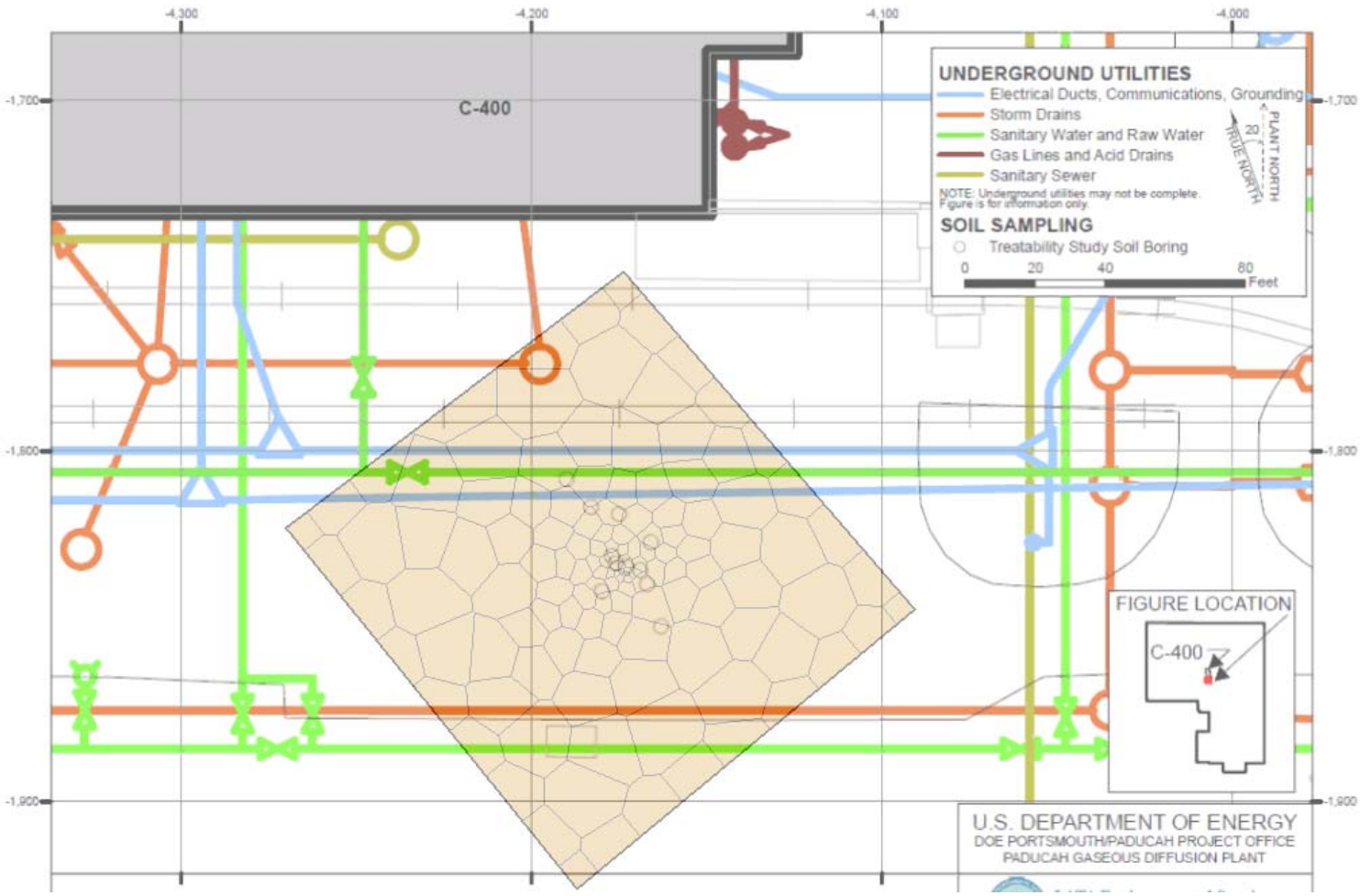

Figure 8. Top view of the 3D model used to simulate the Treatability Study.

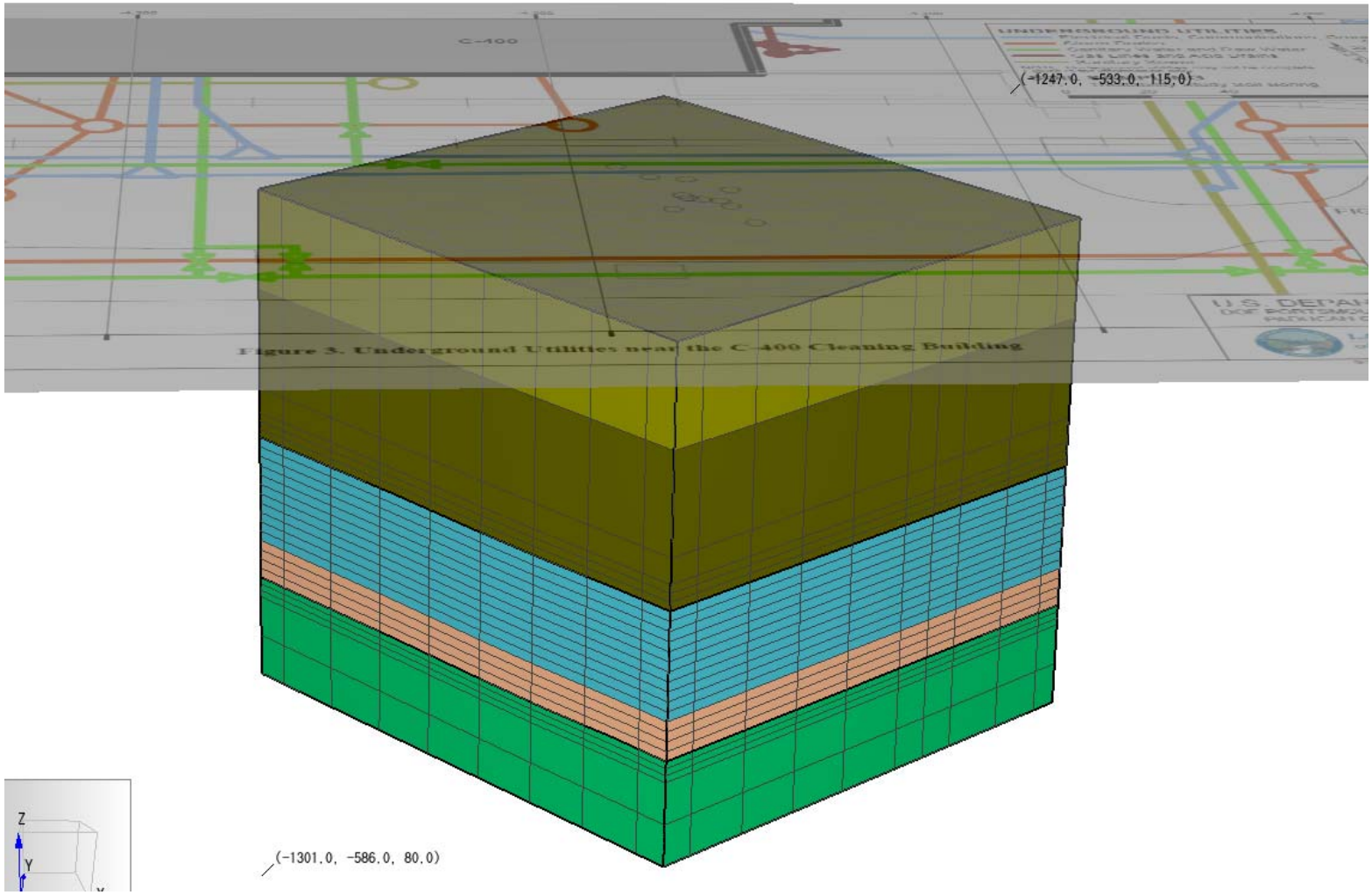

Figure 9. Perspective view of the 3D model from Plant South.

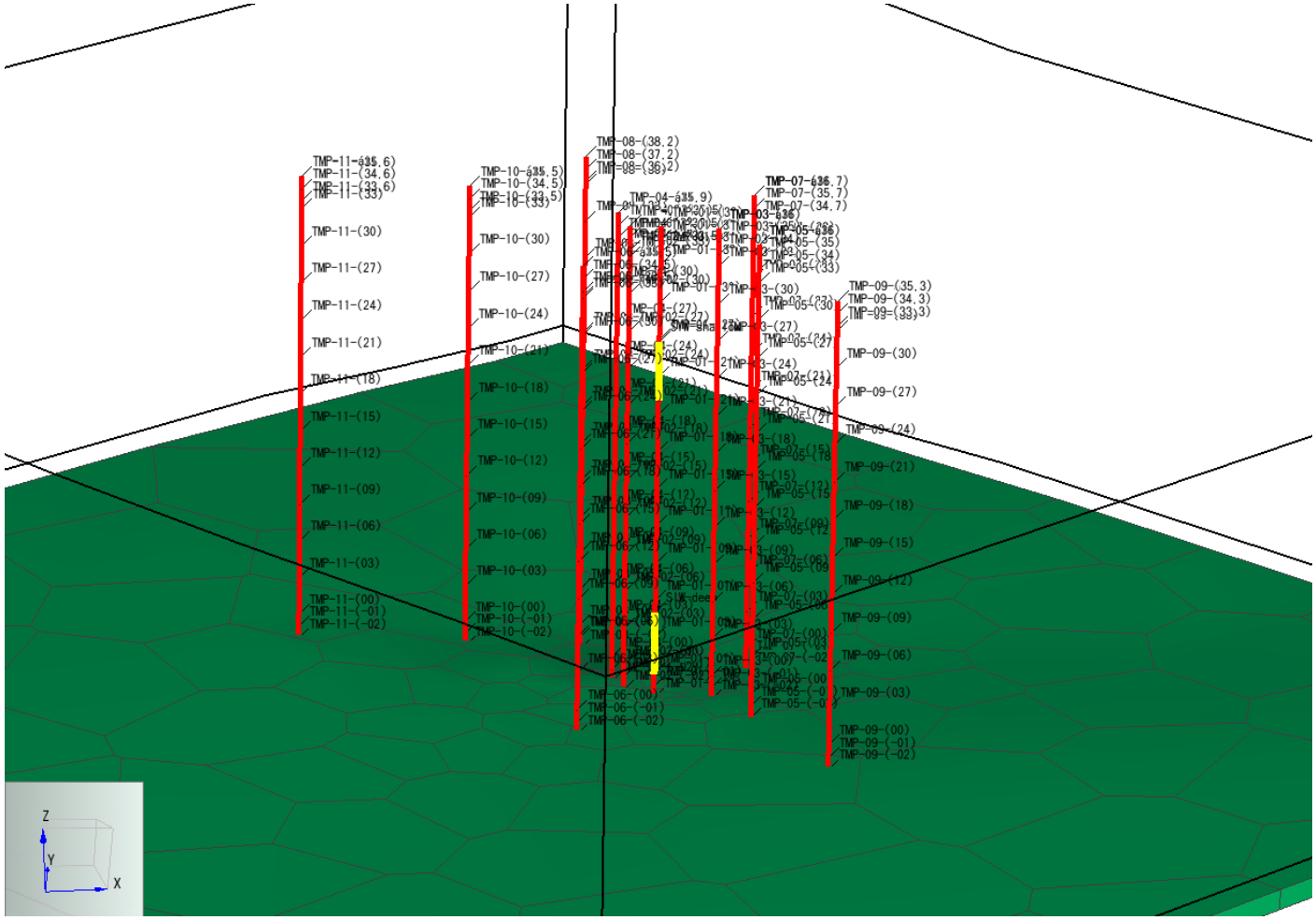

Figure 10. Perspective cutaway view of the 3D model from Plant South showing the 188 temperature monitoring point locations. The steam injection well screens are shown in yellow.

The model contains 26 layers, with a vertical spacing that is slightly coarser than the 2D rz model. In the horizontal dimensions, the model is discretized using Voronoi polygons (Thunderhead Engineering, 2015). The Voronoi polygons allow for a fine model discretization near the steam injection wells, with coarser discretization as the model boundaries are approached. The overall model contains 3432 gridblocks, and typical simulations of the entire Treatability study require about 30 minutes of computer time.

The initial and boundary conditions for this model are similar to the 2D rz model, except that this model includes a regional hydraulic gradient from the southeast to the northwest. The top of the model is maintained at atmospheric temperature and pressure (20 C, 1 atm), while the bottom is a no-flow boundary. The regional hydraulic gradient in this area has been observed to range from a minimum of 1.79×10^{-5} to a maximum of 6.10×10^{-4} (DOE, 2014a). The gradient is largely controlled by the stage of the nearby Ohio River. During the early part of the Treatability Study, the river was in near flood stage, so gradients would have been minimal at C-400. During the latter part of the Treatability Study, the river stage was low, and hydraulic gradients would have been near the higher part of the range (http://waterdata.usgs.gov/nwis/uv?site_no=03611000).

The hydraulic gradient was implemented in the model by fixing the water table at the appropriate elevations at either end of the model (assuming gravity-capillary equilibrium for the water pressure and saturation above the water table). Then a steady-state groundwater flow simulation was performed with no-flow boundaries on the sides of the model parallel to flow. The results of this steady-state groundwater flow model were then used for the model initial conditions. The outer lateral boundary conditions are fixed in time, and consist of the fluid pressures and saturations determined from the steady state flow simulation, with gravity-capillary equilibrium.

3D model calibration and validation for Phase 1

The data used for the 3D model calibration consisted of 80% of the 186 temperature monitoring points. These data points were selected by performing a stratified random sampling of the entire data set to remove 20% of the points. The random sampling was done

by taking each horizontal TMP location, and generating a random number for each depth point. Then for each TMP location, the depth locations with the 3 or 4 lowest random numbers were removed from the calibration data set, and placed in the validation data set (DOE, 2014b). Table 2 lists the TMP depth locations that were removed from the calibration data set.

Table 2. Temperature Monitoring Point locations that were used for model validation.

TMP-01	TMP-02	TMP-03	TMP-04	TMP-05	TMP-06	TMP-07	TMP-08	TMP-09	TMP-10	TMP-11
27	33	33	33	36	33.5	36.7	27	24	35.5	33
18	9	26	15	33	33	33	21	21	15	30
-1	3	6	9	12	12	24	18	-1	-1	3
			-1	-2	-2		0		-2	

The numbers in Table 2 correspond to the monitoring point elevation above the base of the RGA (ft), and are used in the individual TMP naming convention.

The model calibration was performed by trial and error, adjusting the 3D distribution of permeability to minimize the RSS of difference between the simulated and measured TMP temperatures at the end of the Phase 1 steam injection. As would be expected, it was necessary to include substantial volumes of lower permeability material around the TMP locations that showed reduced heating (e.g. TMP 6 and some locations around TMP 5, 9, 10, and 11). The Phase 1 simulations were performed using the minimum observed hydraulic gradient due to the fact that the Ohio River was near flood stage during this time.

Sixteen 3D calibration simulations were performed to minimize the RSS. The best simulation, which will be called “3D phase 1” had a RSS of 79,000, and a NRMSE of 12.1% (using 80% of the temperature data points).

The 3D model validation was performed by computing the NRMSE for the 37 TMP locations (Table 2) that were randomly removed from the calibration data set. The NRMSE for the 37 temperature points was 9.6%.

If all of the data points from the study are grouped together, the 3D phase 1 model had an RSS of 91,000, and a NRMSE of 11.6%. By comparison, the 2D rz model of Phase 1 had a RSS of

around 300,000, and a NRMSE of 21% (using all of the data). Comparisons of the simulated and observed temperature profiles at the end of Phase 1 are shown in Figure 11.

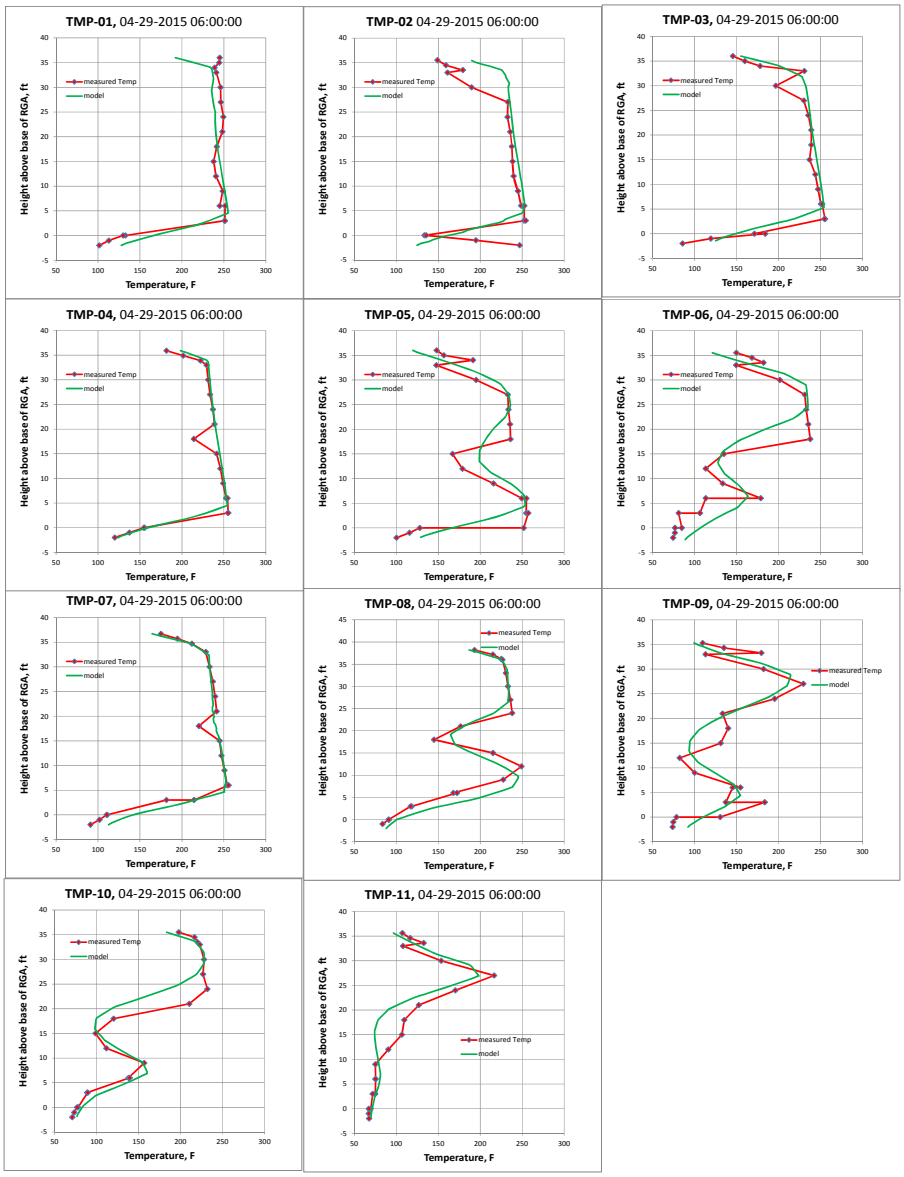

Figure 11. Comparison of 3D phase 1 model results with field temperature data for the end of Phase 1 steam injection.

Calibrating the 3D model required adding substantial zones of lower hydraulic conductivity material in some areas of the model. The basic hydrogeologic structure from the 2D rz model was modified mainly through the addition of these localized, discontinuous zones of lower conductivity. Figures 12 and 13 show southeast-northwest and southwest-northeast cross sections through the calibrated model. The grey material in these figures represents a lower conductivity sand or silty sand, with a horizontal conductivity of 1.5 ft/d. The tan material and the light blue material represent the main lower and upper RGA gravels, with horizontal hydraulic conductivities of 300 ft/d and 100 ft/d, respectively. The anisotropy ratio for the fine sand is 10:1, while the anisotropy ratios for the lower and upper RGA gravels are 30:1 and 20:1 as before.

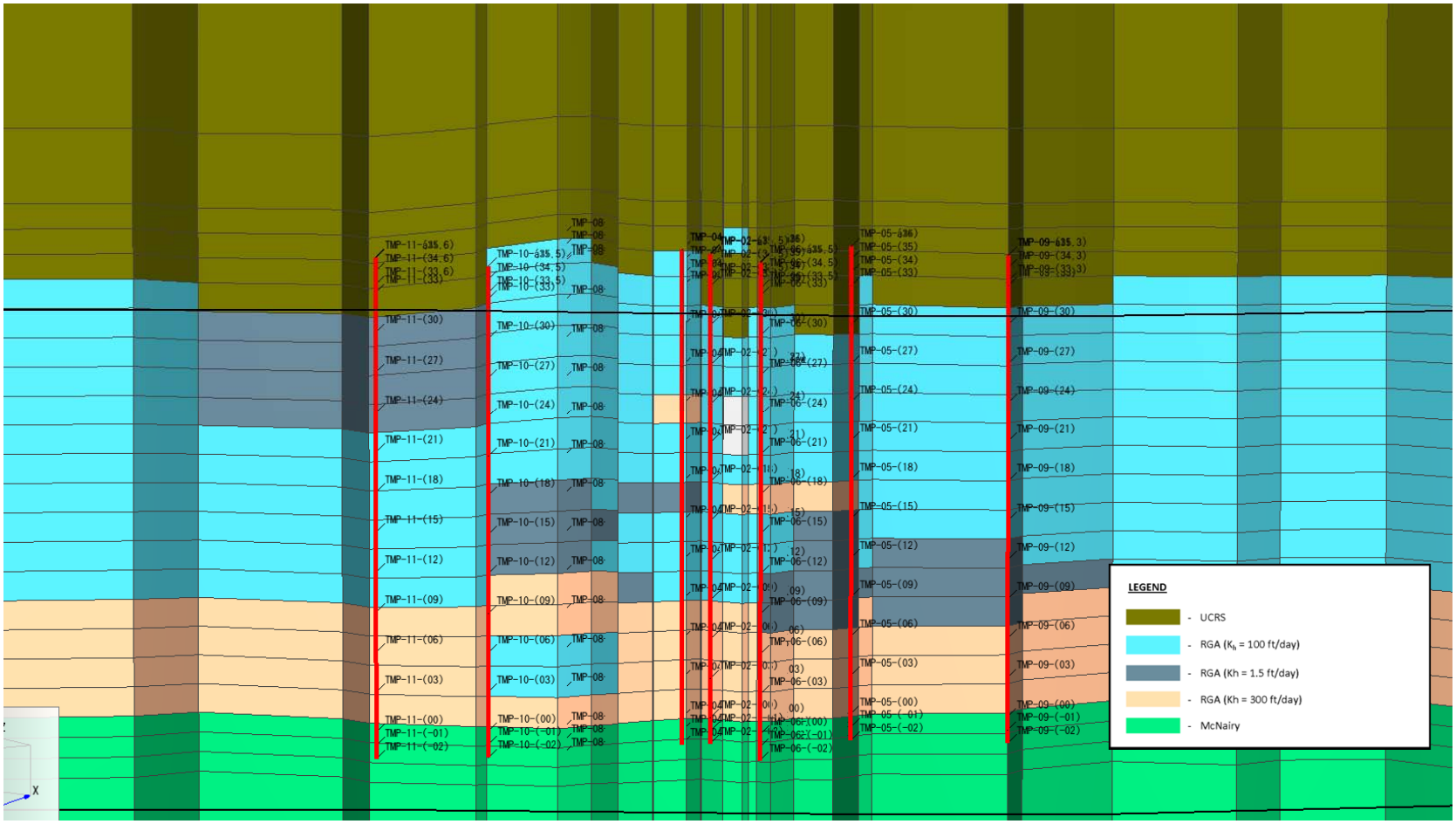

Figure 12. Southeast-northwest cross section through model. The grey material represents a fine sand or silty sand with a horizontal hydraulic conductivity of 1.5 ft/d.

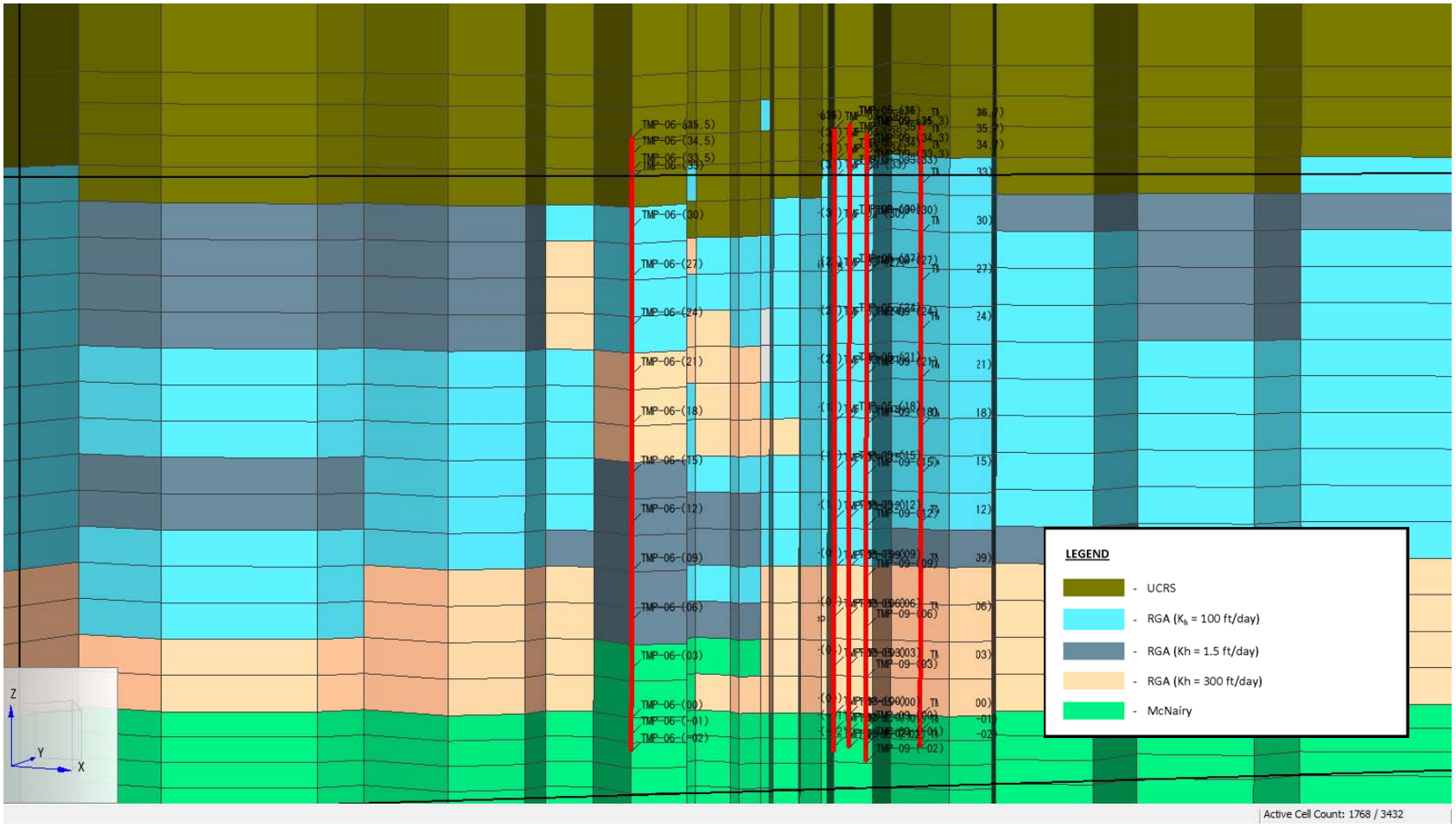

Figure 13. Southwest-northeast cross section through model. The grey material represents a fine sand or silty sand with a horizontal hydraulic conductivity of 1.5 ft/d.

3D model of Phases 1, 2, 3, and 4

The calibrated model described above was used to simulate the entire Treatability Study. The matches the Phase 3 temperature profiles (NRMSE=13.6%), but the match with the temperature profiles at the end of the two cooldown periods (Phases 2, and 4) is not as good with NRMSE values of 17.9% and 21.2%, respectively. Because this simulation used the minimum observed hydraulic gradient of 1.79×10^{-5}, a second simulation was performed with the same model, but using the maximum observed hydraulic gradient of 6.10×10^{-4}. This second 3D model matches the Phase 1 and Phase 3 temperatures with an accuracy similar to the low gradient model (NRMSE = 12.2 and 13.5%, respectively), but it does a significantly better job of matching the Phase 2 and Phase 4 cooldown periods with NRMSE values of 16.5% and 18.1%, respectively. Model comparisons with the measured temperature profiles for the end of Phase 2, near the end of Phase 3, and the end of Phase 4 are shown in Figures 14, 15, and 16.

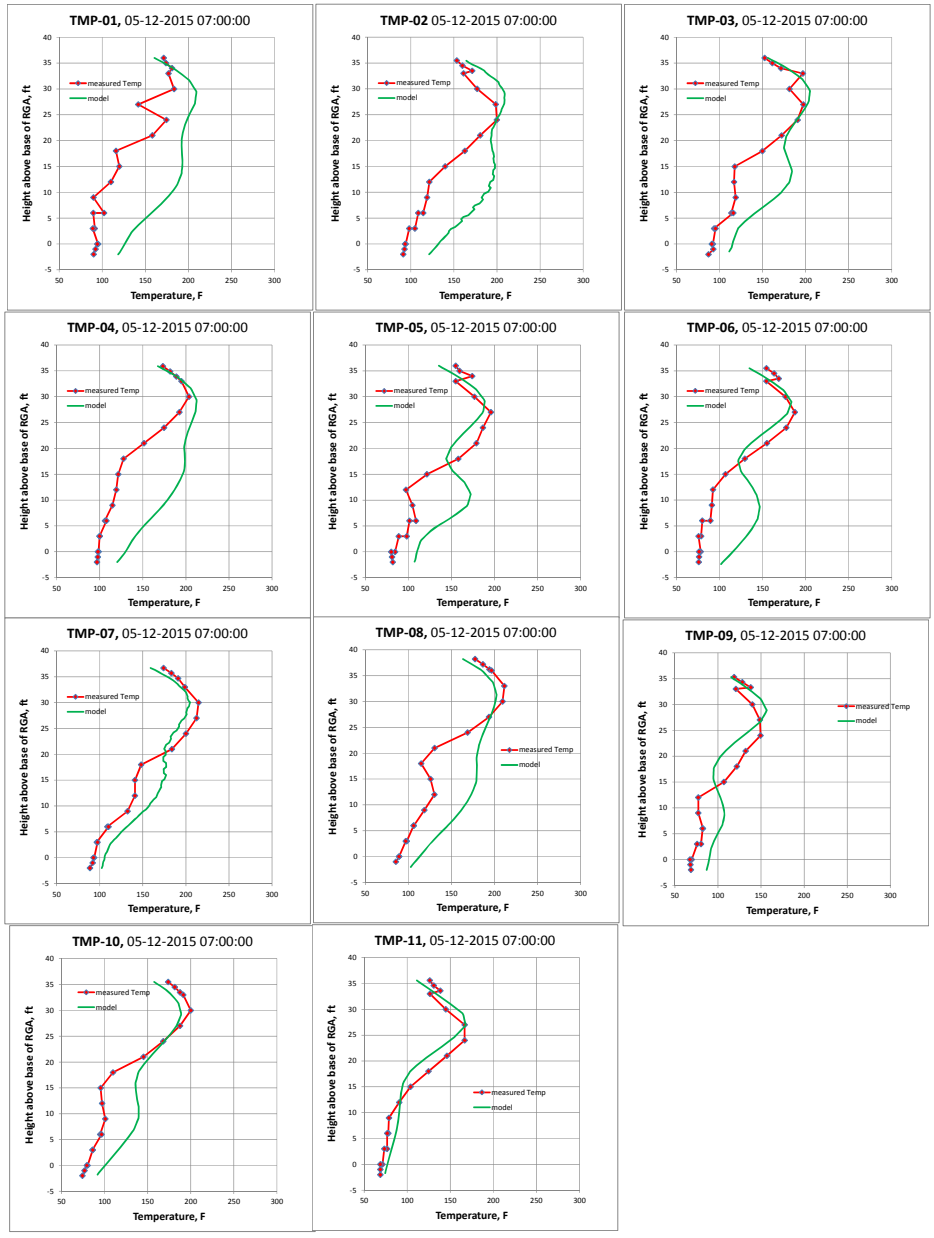

Figure 14. Comparison of 3D phase 1 model results with field temperature data for the end of Phase 2 cooldown.

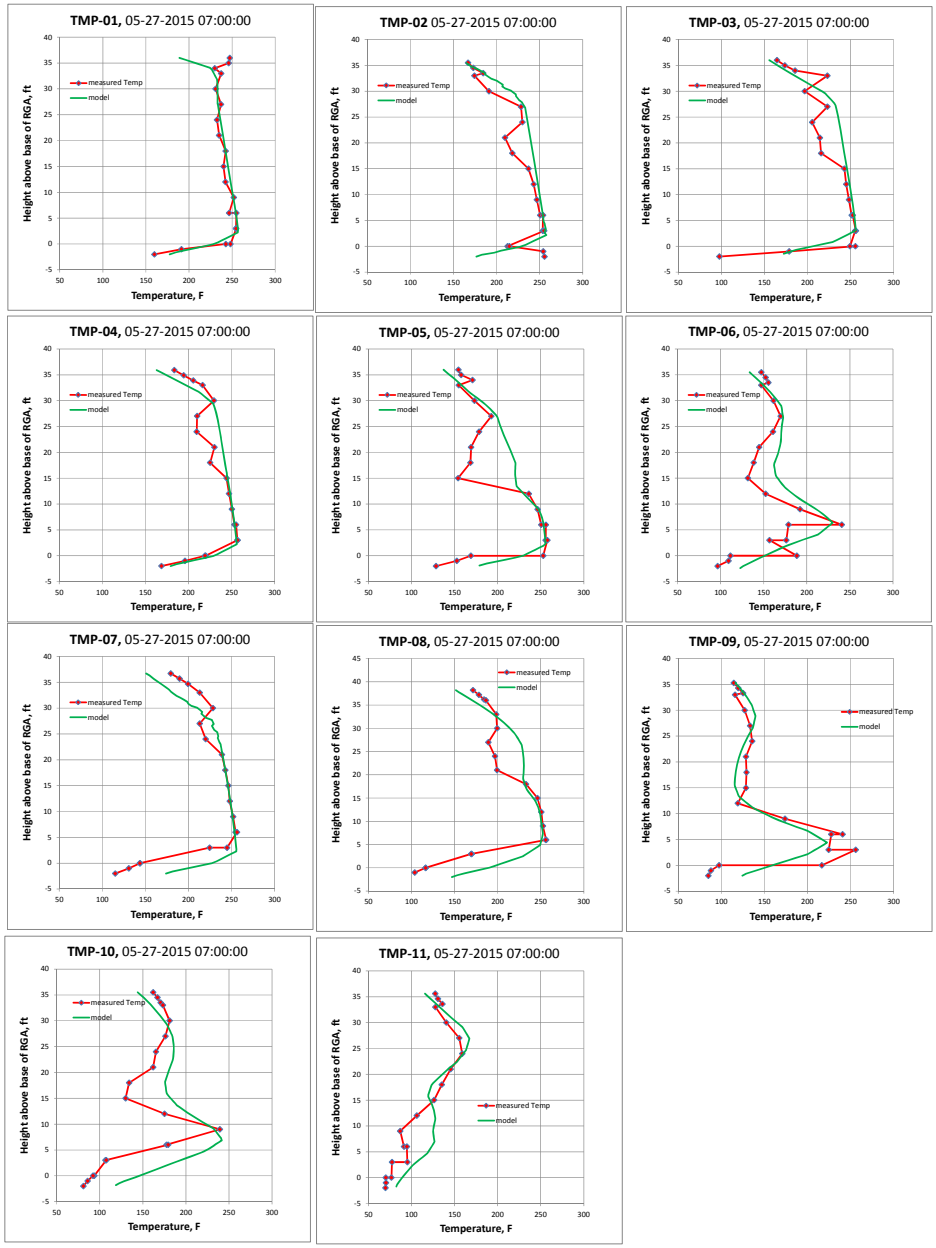

Figure 15. Comparison of 3D phase 1 model results with field temperature data near the end of Phase 3 steam injection.

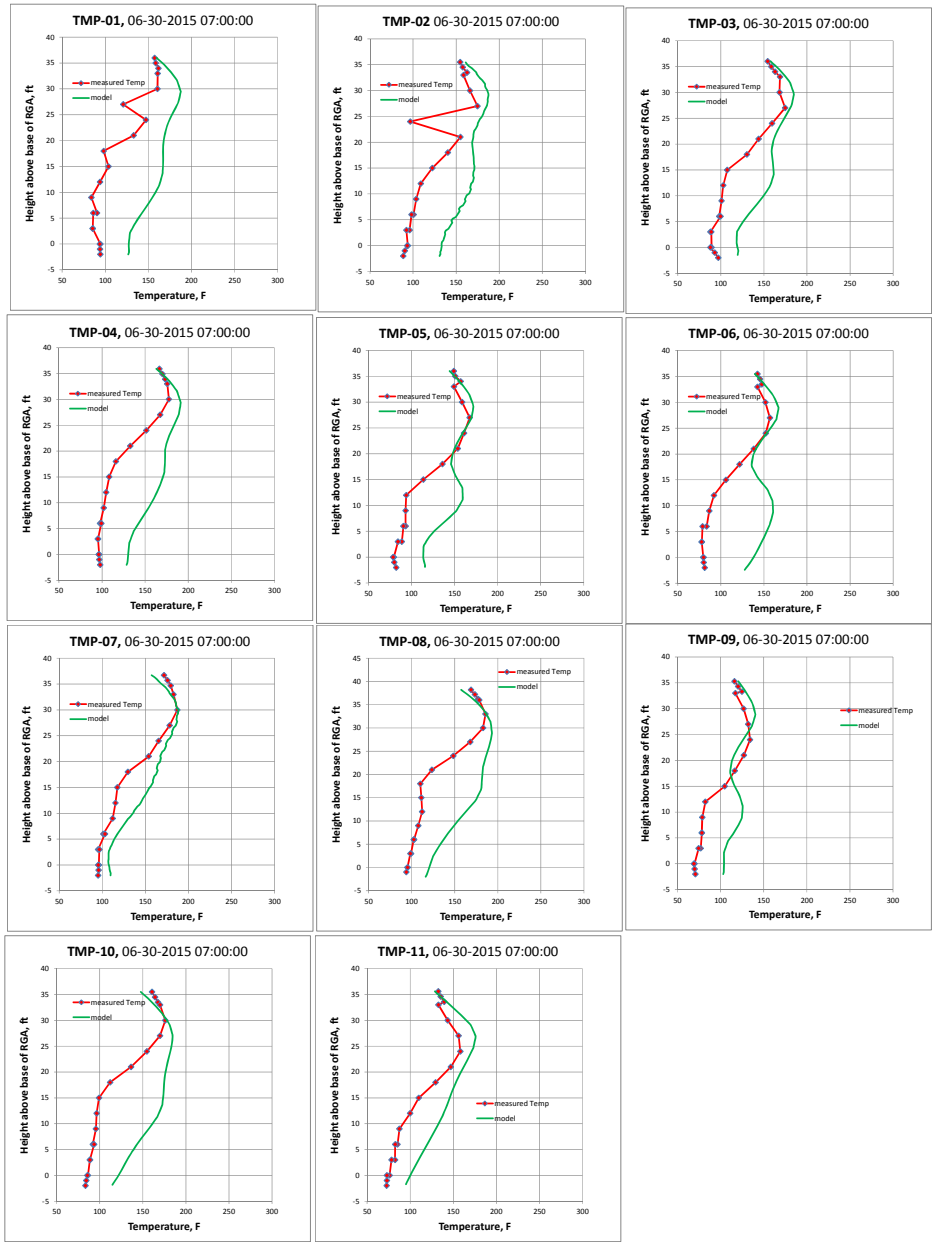

Figure 16. Comparison of 3D phase 1 model results with field temperature data for the end of the Phase 4 cooldown.

The relatively poorer match during the cooldown phases suggests that the assumptions related to water flow past the site may be underestimated and that somewhat more heat might be lost during the cooldown period than predicted. However, although the TMP locations were not optimally located, it is also noted that a laterally displaced plume of hot water was not observed in the TMP data.

Deleted:

The simulation run with the maximum hydraulic gradient shows that the regional groundwater flow has little effect on the development of the steam zone during steam injection. When steam injection stops, the steam zone quickly (over a matter of a couple day) collapses back into liquid water, causing a rapid radial inflow of cold groundwater. The steam zone collapse tends to occur from the bottom of the steam zone towards the top. Once the steam zone has collapsed, the entire system is once again in a single phase liquid water condition. At this point, there are still significant temperature variations within the system (nearly 80 C or 176 F). These temperature variations results in water density differences of up to 40 kg/m^3. It can be shown that the form of Darcy's law that applies to buoyancy flow is driven by the density contrast divided by the magnitude of the density (Falta et al., 1989). During the steam collapse period, the density contrast between the steam and liquid water is equivalent to a hydraulic gradient of one, which is thousands of times larger than the regional hydraulic gradient. Following collapse, the density difference between the hot and cold groundwater is equivalent to hydraulic gradient of 0.04, which is about 100 times larger than the regional hydraulic gradient.

The regional flow does appear to affect the heat plume slightly during the cooldown phases, moving the hot water downgradient by a few feet. Although the general trends of steam collapse and cooling are simulated by the model, the field data show a somewhat more rapid cooldown in the lower RGA than what the model predicts. It is conceivable that the horizontal groundwater flow in the lower RGA could be higher than what is reflected in the average regional gradients.

Figures 17 through 22 show the progression of the steam zone development during Phases 1 and 3 using the 3D model that includes the maximum regional gradient. The isosurface in these figures corresponds to a gas phase saturation of 20%; much higher gas saturations (up to 70%) occur inside the steam zone.

To summarize, the calibrated 3D heterogeneous model provides good matches with the experimental data throughout the Treatability Study. The basic structure of the RGA used in the final model consists of an upper zone of moderate horizontal hydraulic conductivity (100 ft/d) and high anisotropy (20:1), a lower zone of higher horizontal hydraulic conductivity (300 ft/d) and high anisotropy (30:1). The calibration required zones and lenses of lower conductivity materials.

Near the top and bottom of the RGA, it appears that the interface with the overlying UCRS and underlying McNairy formations is irregular. Throughout the RGA there also appear to be discontinuous lenses of a lower conductivity materials that are fine enough to affect steam migration, but are not thick enough to inhibit heating. These finer grained zones and lenses are important to consider for the full scale implementation because they are likely to affect both the steam migration and heating, and the contaminant transport and removal.

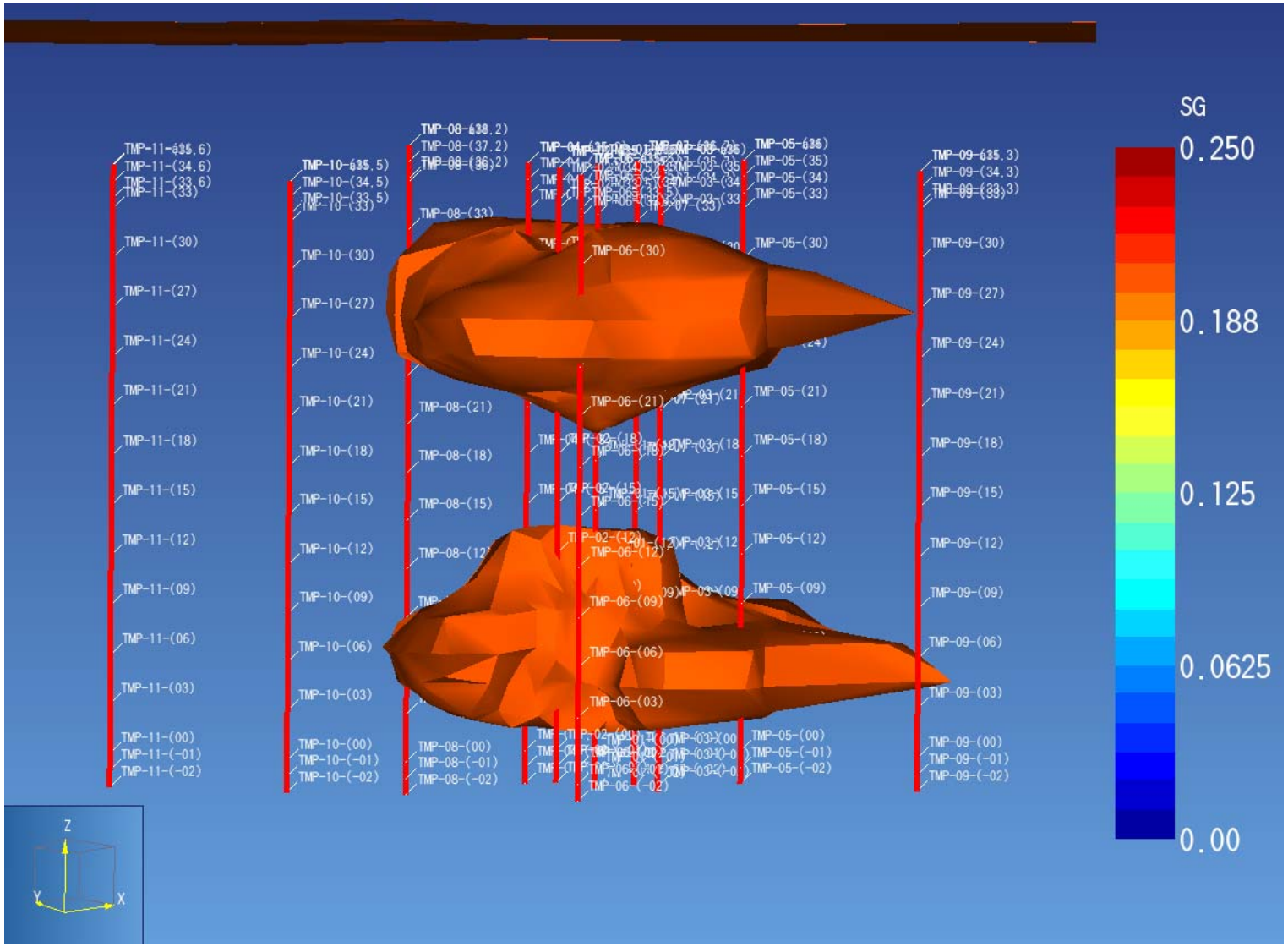

Figure 17. Simulated steam zone after 3.8 days of steam injection in Phase 1.

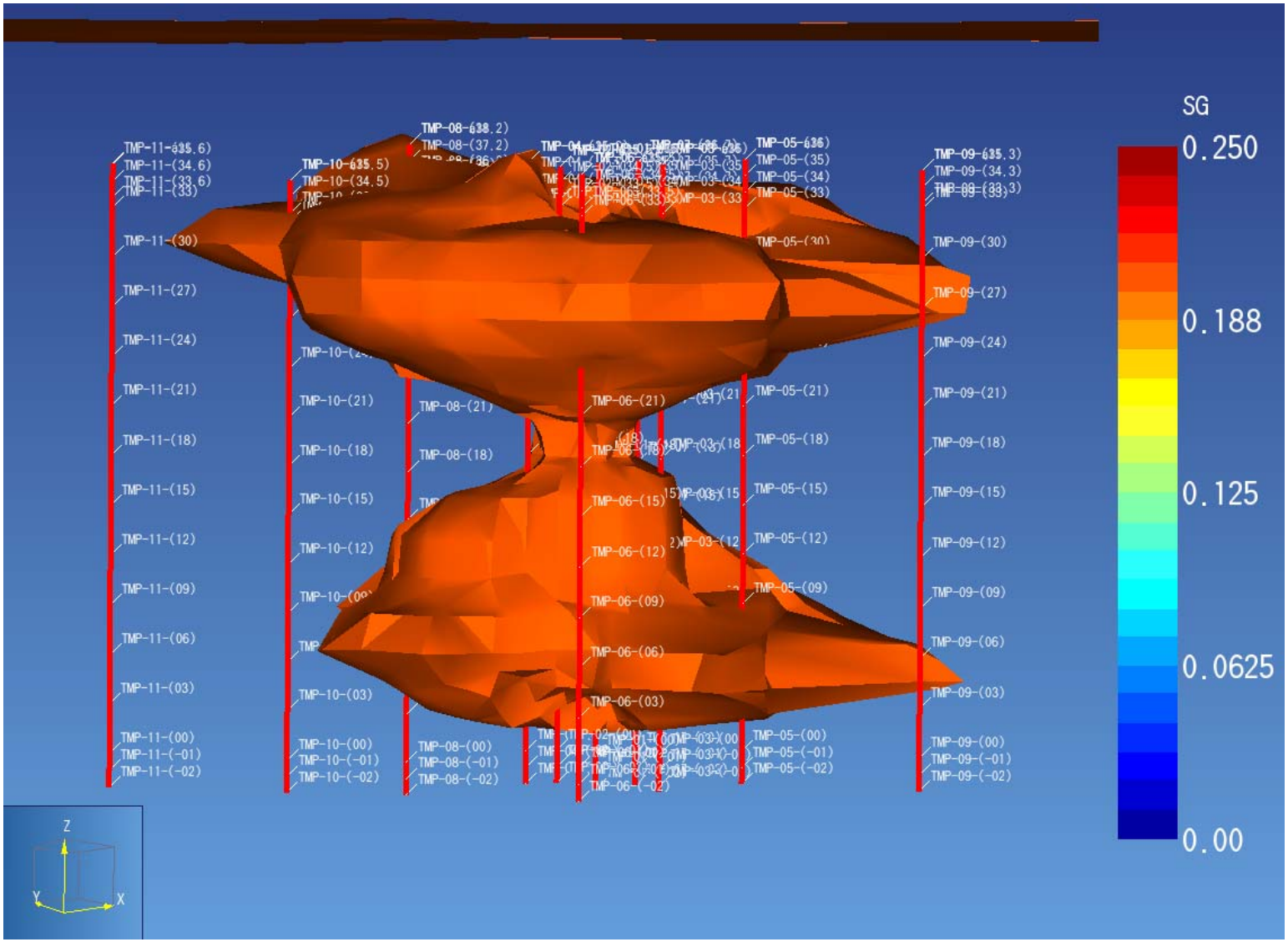

Figure 18. Simulated steam zone after 10.6 days of steam injection in Phase 1.

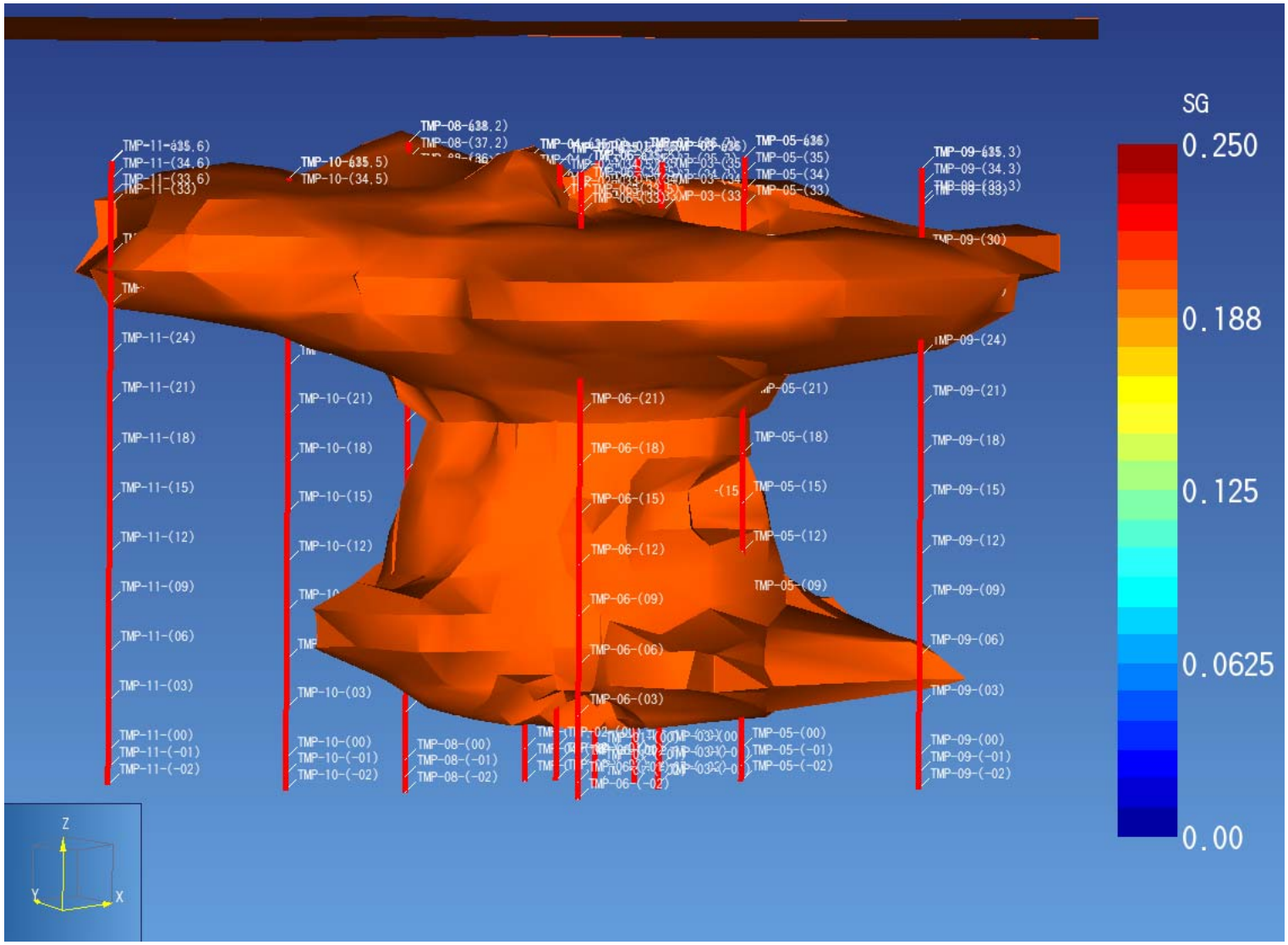

Figure 19. Simulated steam zone at the end of Phase 1 steam injection.

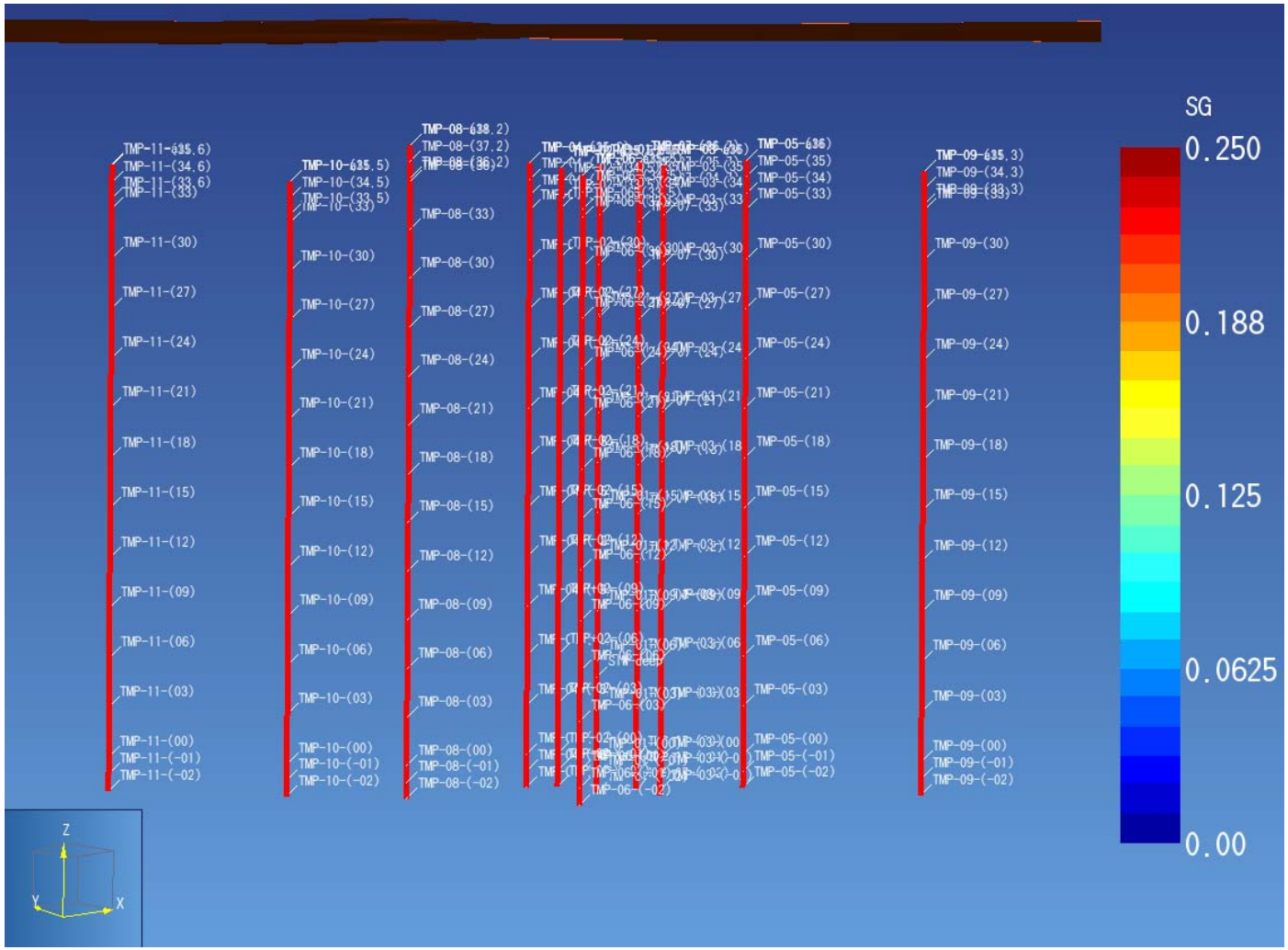

Figure 20. Simulated steam zone after 2 days of cooldown (Phase 2). Steam zone has completely disappeared.

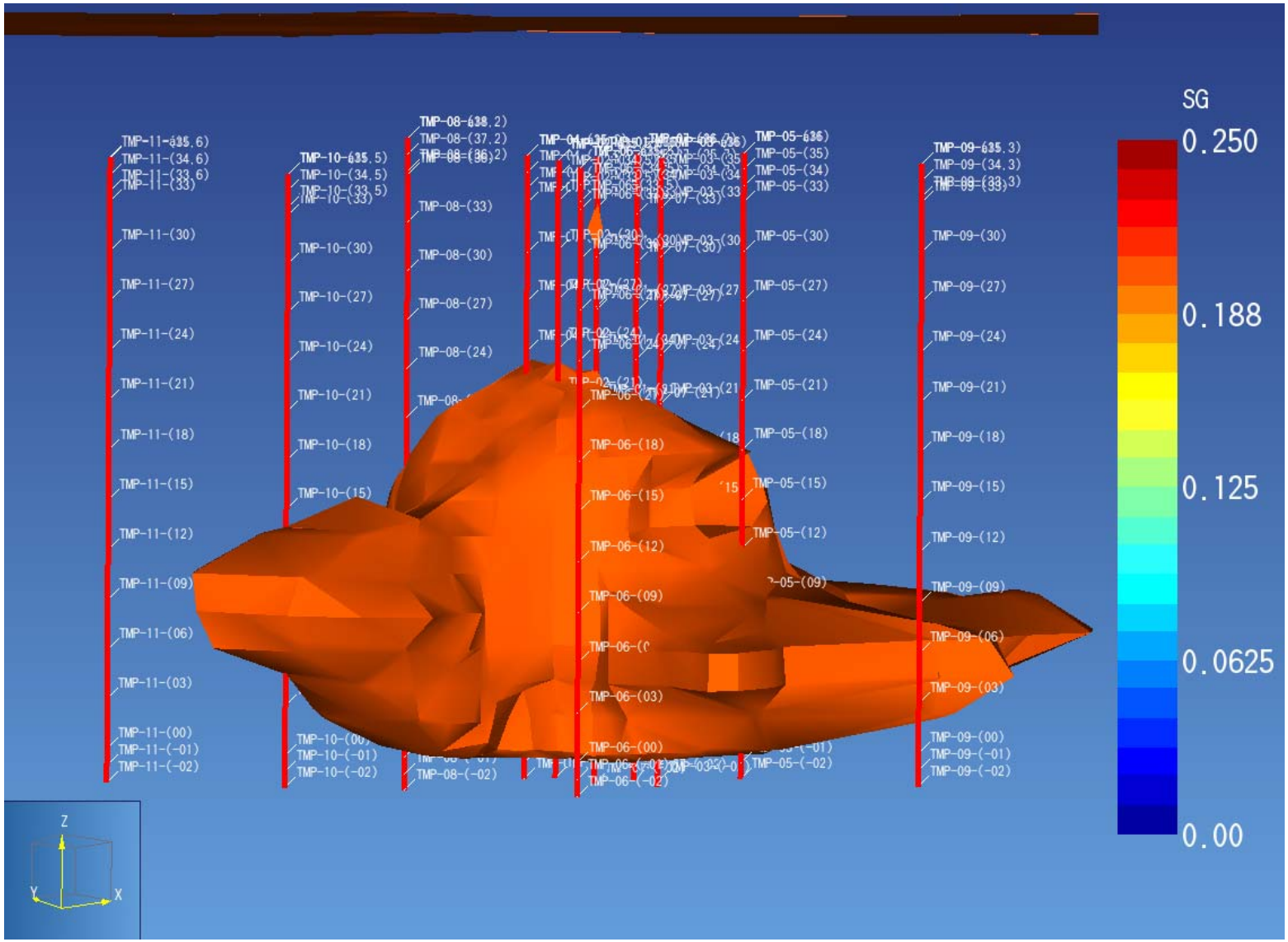

Figure 21. Simulated steam zone after 7.75 days steam injection into the lower screen (Phase 3).

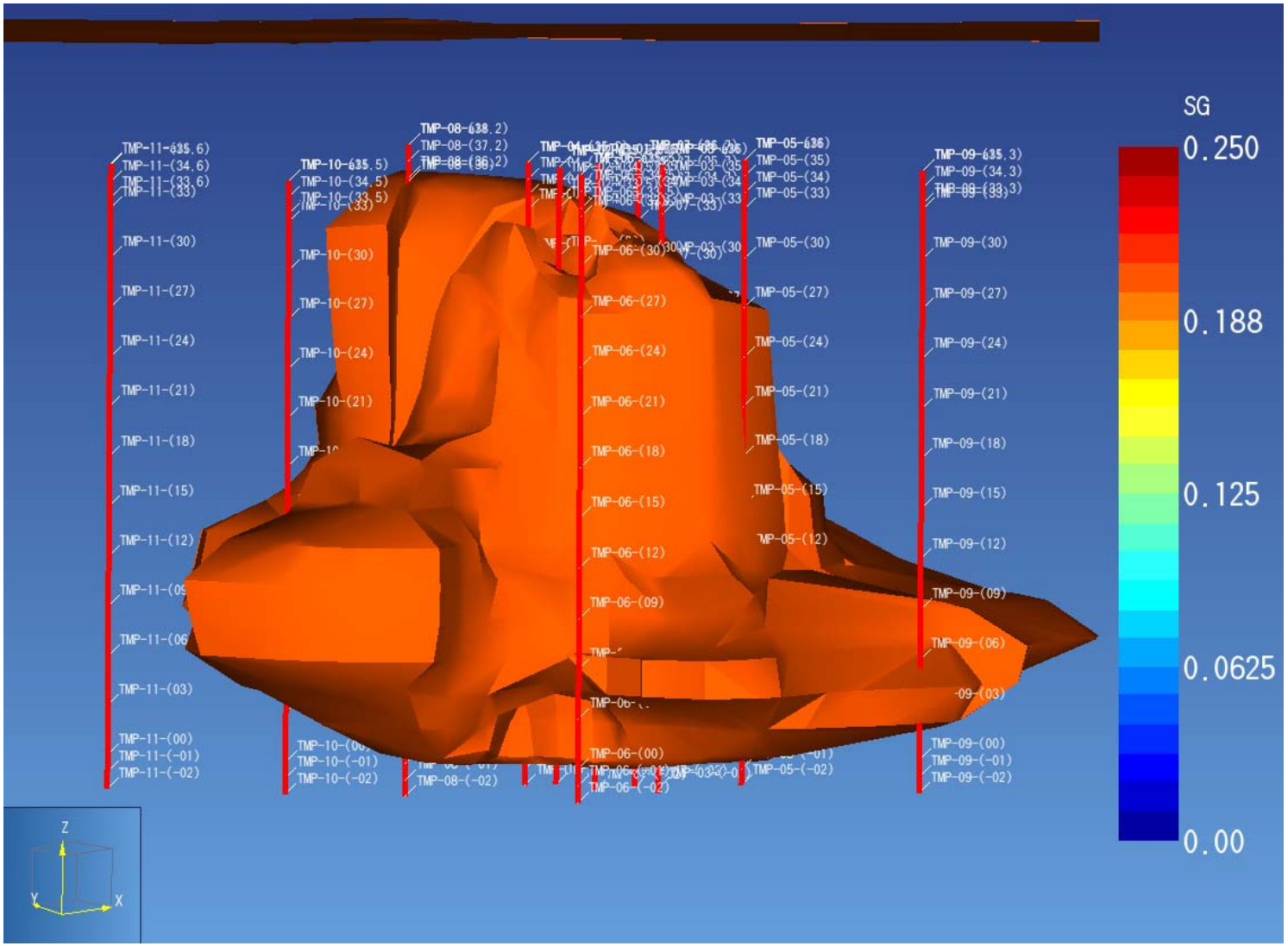

Figure 22. Simulated steam zone steam injection into the lower screen at the end of Phase 3.

References

Adenekan, A.E., and T.W. Patzek, 1994, Cleanup of the gasoline spill area with steam: Compositional simulations. In Dynamic Underground Stripping Project: LLNL Gasoline Spill Demonstration Project, ed. R. Newmark. Lawrence Livermore National Laboratory, UCRL-ID-116964-V-1-4.

Adenekan, A.E., T.W. Patzek, and K. Pruess, 1993, Modeling of multiphase transport of multicomponent organic contaminants and heat in the subsurface: Numerical model formulation, Water Resources Research, 29, no. 11, p. 3727-3740.

Basel, M.D. and K.S. Udell, 1989, Two-dimensional study of steam injection into porous media, Multiphase transport in porous media, ASME-HTD-127, New York: ASME.

Chen, F., R.W. Falta, and L.C. Murdoch, 2012, Numerical analysis of contaminant removal from fractured rock during boiling, Journal of Contaminant Hydrology, 134-135, p. 12-21.

Chen, F., X. Liu, R.W. Falta, and L.C. Murdoch, 2010, Experimental demonstration of contaminant removal from fractured rock by boiling, Environmental Science and Technology, 44, p. 6437-6442.

Coats, K.H., 1977, Geothermal reservoir modeling, paper SPE-6892, presented at the 52nd Annual Fall Technical Conference and Exhibition of the SPE, Denver, Colorado, October, 1977.

DOE, 2014a, Treatability Study Work Plan for Steam Injection, Groundwater Operable Unit, at Paducah Gaseous Diffusion Plant, Paducah, Kentucky, US Department of Energy, DOE/LX/07-1294&D2.

DOE, 2014b, Treatability Study Design, Design Drawings and Technical Specifications Package for the C-400 Interim Remedial Action Phase IIb Steam Injection Treatability Study at Paducah Gaseous Diffusion Plant, Paducah, Kentucky, US Department of Energy, DOE/LX/07-1295&D2/R1.

Falta, R.W., 1990, Multiphase transport of organic chemical contaminants in the subsurface, Ph.D thesis, University of California, Berkeley.

Falta, R.W., 2001, Steam Flooding for Environmental Remediation, in Groundwater Contamination by Organic Pollutants, Analysis and Remediation, , J.J. Kaluarachchi, editor, *ASCE Manuals and Reports on Engineering Practice No. 100*, p. 153-192.

Falta, R. W., I. Javandel, K. Pruess, and P. A. Witherspoon. 1989. Density-driven flow of gas in the unsaturated zone due to the evaporation of volatile organic compounds, *Water Resources Research*, V. 25, No. 10, p 2159-2169.

Falta, R.W., K. Pruess, S. Finsterle, and A. Battistelli, 1995, T2VOC User's Guide, *Lawrence Berkeley Laboratory Report LBL-36400,* March, (copyright through University of California, Lawrence Berkeley National Laboratory).

Falta, R.W., K. Pruess, I. Javandel, and P.A. Witherspoon, 1992a, Numerical Modeling of Steam Injection for the Removal of Nonaqueous Phase Liquids from the Subsurface, 1. Numerical Formulation, *Water Resources Research, Vol. 28, No. 2*, February.

Falta, R.W., K. Pruess, I. Javandel, and P.A. Witherspoon, 1992b, Numerical Modeling of Steam Injection for the Removal of Nonaqueous Phase Liquids from the Subsurface, 2. Code Validation and Application, *Water Resources Research*, *Vol. 28, No. 2,* February

Gudbjerg, J., T.O. Sonnenborg, and K.H. Jensen, 2004a, Remediation of NAPL below the water table by steam-induced heat conduction, Journal of Contaminant Hydrology, 72, p. 207-225.

Gudbjerg, J., O. Trotschler, A. Farber, T.O. Sonnenborg, and K.H. Jensen, 2004b, On spurious water flow during numerical simulation of steam injection into water-saturated soil, Journal of Contaminant Hydrology, 75, p. 297-318.

Gudbjerg, J., T. Heron, T.O. Sonnenborg, and K.H. Jensen, 2005, Three-dimensional numerical modeling of steam override observed at a full-scale remediation of an unconfined aquifer, Ground Water Monitoring and Remediation, 25, no. 3, p. 116-127.

Hodges, R.A., and R.W. Falta, 2008, Vertical Confinement of Injected Steam in the Vadose Zone Using Cold Air Injection, *Vadose Zone Journal*, Vol. 7, No. 2, 732-740.

Hodges, R.A., R. Falta, and L. Stewart, 2004, Controlling steam flood migration using air injection wells, *Environmental Geosciences*, Vol. 11, No. 4, p. 221-238.

Lake, L.W., 1989, Enhanced Oil Recovery, Prentice FHall, Englewood Cliffs, New Jersey.

LATA Environmental Services of Kentucky, LLC, 2011, Technical Performance Evaluation for Phase I of the C-400 Interim Remedial Action at the Paducah Gaseous Diffusion Plant, Paducah, Kentucky, prepared for the US Department of Energy, DOE/LX/07-1260&D1.

Ochs, S.O., R.A. Hodges, R.W. Falta, T.F. Kmetz, J.J. Kupar, N.N. Brown, and D.L. Parkinson, 2003, Predicted Heating Patterns During Steam Flooding of Coastal Plain Sediments at the Savannah River Site, *Environmental and Engineering Geoscience, Vol. 9, No. 1, 51-69*.

Pruess, K., and A. Battistelli, 2002, TMVOC, A Numerical Simulator for Three-Phase Non-Isothermal Flows of Multicomponent Hydrocarbon Mixtures in Saturated-Unsaturated Heterogeneous Media, Lawrence Berkeley National Laboratory Report LBNL-49375.

Pruess, K., C. Oldenburg, and G. Moridis, 1999, TOUGH2 User's Guide, Version 2.0, Lawrence Berkelely National Laboratory Report LBNL-43134.

Thomas, G.W., 1982, Principles of Hydrocarbon Reservoir Simulation, International Human Resources Development Corporation, Boston, MA.

Thunderhead Engineering, 2015, PetraSim 2015 User Manual, https://www.thunderheadeng.com/wp-content/uploads/dlm_uploads/2015/04/PetraSimManual.pdf

Van Genuchten, M.Th., 1980 A closed form equation for predicting the hydraulic conductivity of unsaturated soils, Soil Sci. Soc., Vol 44, p. 892-898.

THIS PAGE INTENTIONALLY LEFT BLANK