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§194.23 - DENSITY EFFECTS ON RADIONULCIDE

TRANSPORT IN THE CULEBRA AT THE WIPP SITE

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Executive Summary

In the 1992 PA, the DOE did not simulate the potential effects that variable fluid densities could have on ground-water flow and radionuclide transport in the Culebra. To ensure that this assumption would be acceptable to support DOE's final application, a series of model simulations were performed using the computer code STAFF3D (Huyakorn, et. al. 1992). These analyses were focused on evaluating the importance of groundwater density variations on radionuclide transport in the Culebra. Other modeling studies conducted by for the WIPP site (TSD,V-B-7) and modeling conducted for the 1992 PA assumed that density effects would not be an important factor; however, there are significant variations in groundwater density currently within the Culebra. Furthermore, potential releases of radionuclides form the repository through boreholes would likely result in an even denser brine being injected into the Culebra. Thus, it is important to verify that the assumption of negligible density effects is correct.

The STAFF3D simulations incorporated observed density variations in the Culebra. The model assumed a dual-porosity, homogeneous system with a single fracture. Simulations were performed with and without matrix diffusion. In both cases, the velocities computed by STAFF3D were 30 to 80 percent higher for the density simulations when compared to simulations neglecting density variations. However, these velocity differences were localized over relatively small areas and were not sufficient to produce significant changes in radionuclide concentration or mass loading at the downgradient boundary of the land withdrawal area. Furthermore, the single fracture assumption would be conservative in that the differences between the velocities would be accentuated. Therefore, EPA has determined that density effects do not need to be included in the CCA modeling.

1. Introduction

1.1 BACKGROUND

EPA's investigation of the effects that the presence of variable density brine may have on groundwater flow and radionuclide transport stemmed from the Agency's review of work performed by Dr. Davies while at the U.S. Geological Survey. While working for the USGS, Dr. Davies (now at SNL) published a paper entitled "*Modeling Areal, Variable-Density, Ground-Water Flow using Equivalent Freshwater Head— Analysis of Potentially Significant Errors*." (A-93-02, Ref# 158). The issues related to density dependent ground-water flow and transport are best summarized *via* the abstract of Dr. Davies's paper which states:

> " The concept of equivalent freshwater head is widely used in modeling ground-water flow systems that contain water with substantial spatial variation in fluid density. The use of equivalent freshwater head implicitly assumes that ground-water flow is approximately horizontal, and, therefore, density-related gravity effects are small and can be ignored. The relative importance of density-related gravity effects can be examined by expanding the gravity term in Darcy's Law and separating an equivalent freshwater-head term, which represents the pressure-driven component of flow, from a density-related error term, which represents the gravity-driven component of flow. The resulting expression illustrates that it is not the absolute magnitude of the density-related error term but rather the relative magnitude of this term versus the magnitude of the equivalent freshwater-head term that determines whether density-related gravity effects will be significant in a given situation. A useful measure of the relative importance of density-related gravity effects is the dimensionless ratio of the magnitude of the density-related error term to the magnitude of the equivalent freshwater head term. An analysis of the relative magnitude of the density-related gravity effects has been made as part of a regional study of the ground-water flow system in a gently dipping dolomite aquifer in the vicinity of the Waste Isolation Pilot Plant in southeastern New Mexico. A comparison of equivalent freshwater-head simulations with variable-density simulations reveals an area along the flow path leaving the site where equivalent freshwater-head simulations produce errors in the predicted flow direction of as much as 170 degrees and underestimate predicted velocity magnitudes by as much as a factor of 10."

It should be kept in mind that this conclusion drawn by Dr. Davies, that density-dependence could have a significant effect on flow and transport, was made prior to the designation of the WIPP Land Withdrawal boundary as the accessible environment. The large errors that were calculated are associated with areas south of the WIPP land withdrawal boundary and have less relevance to the current problem, now that the accessible environment has been redefined.

EPA, however, was still intent on ensuring that density differences within the Culebra would not significantly affect ground-water flow and radionuclide transport within the land withdrawal area. As presented in the sections below, model simulations were performed that incorporated observed density variations in the Culebra. Although differences in the density *vs*. non density simulations were observed, these velocity differences were localized over relatively small areas and were not sufficient to produce significant changes in radionuclide concentration or mass loading at the downgradient boundary of the land withdrawal area. Furthermore, the only significant difference between DOE's 1992 PA modeling and that in the CCA, with respect to flow and transport in the Culebra, is that the effective thickness of the Culebra was reduced from 7.7 m to 4 m. This change, however, does not present a concern with respect to the applicability of the EPA modeling results, because the modeling analyses were robust in the sense that a single fracture was assumed in making comparisons of relative changes to the velocity fields. Therefore, EPA is confident that density effects do not need to be included in the CCA modeling.

1.2 OBJECTIVES

A series of model simulations are performed using STAFF3D (Huyakorn et.al., 1992) to evaluate the importance of groundwater density variations on radionuclide transport in the Culebra. Other modeling studies conducted for the WIPP site (TSD,V-B-7) and modeling conducted by DOE for the 1992 PA assumed that density effects would not be an important factor; however, there are significant variations in groundwater density currently within the Culebra. Furthermore, potential releases of radionuclides from the repository through boreholes would likely result in an even denser brine being injected into the Culebra. Thus, it is important to verify that the assumption of negligible density effects is correct.

1.3 PROBLEM CONCEPTUALIZATION

Groundwater in the Culebra varies in density from about 1.02 to 1.09 g/cm^3, as shown in Figure 1.1. By contrast, seawater has a density of about 1.025 g/cm^3. Thus, it would appear that flow within the Culebra may be influenced by these density variations since the variation in density is quite extreme. In addition, the density of brine in the vicinity of the repository is about

1.20 g/cm^3, which is much higher that ambient groundwater density within the Culebra. If these deep brines were to migrate up a borehole that penetrates the repository, the variation in brine density at the injection point in the Culebra would be quite large.

The variation in groundwater density within the Culebra is roughly correlated with the base elevation of the Culebra, shown in Figure 1.2. The base of the Culebra slopes to the east-northeast from a high of 2874 feet above sea level to a low of 2551 ft, a relief of 323 ft over about 21,000 ft (slope of 0.015 ft/ft). The areas of lowest Culebra elevation coincide with the highest brine density, as shown in Figure 1.1.

Other STAFF3D modeling (TSD V-B-7) relied on symmetry to reduce the size of the model domain to one-half of the Culebra flow system. Half of the system could be modeled because a uniform gradient was simulated in the Culebra and the source of contaminants to the Culebra was a single borehole intrusion. Thus, contaminant concentrations on either side of the axis of symmetry (a line through the borehole and parallel with the regional groundwater flow gradient) would be identical.

In order to evaluate density effects, the new simulations must more closely approximate the existing Culebra flow system, including the variability in gradient, ground-water density, aquifer bottom elevation, and unit thickness. Given the variation in ground-water density and Culebra elevation described previously, an axis of symmetry cannot be defined and the use of symmetry is not appropriate for these density-dependent flow simulations.

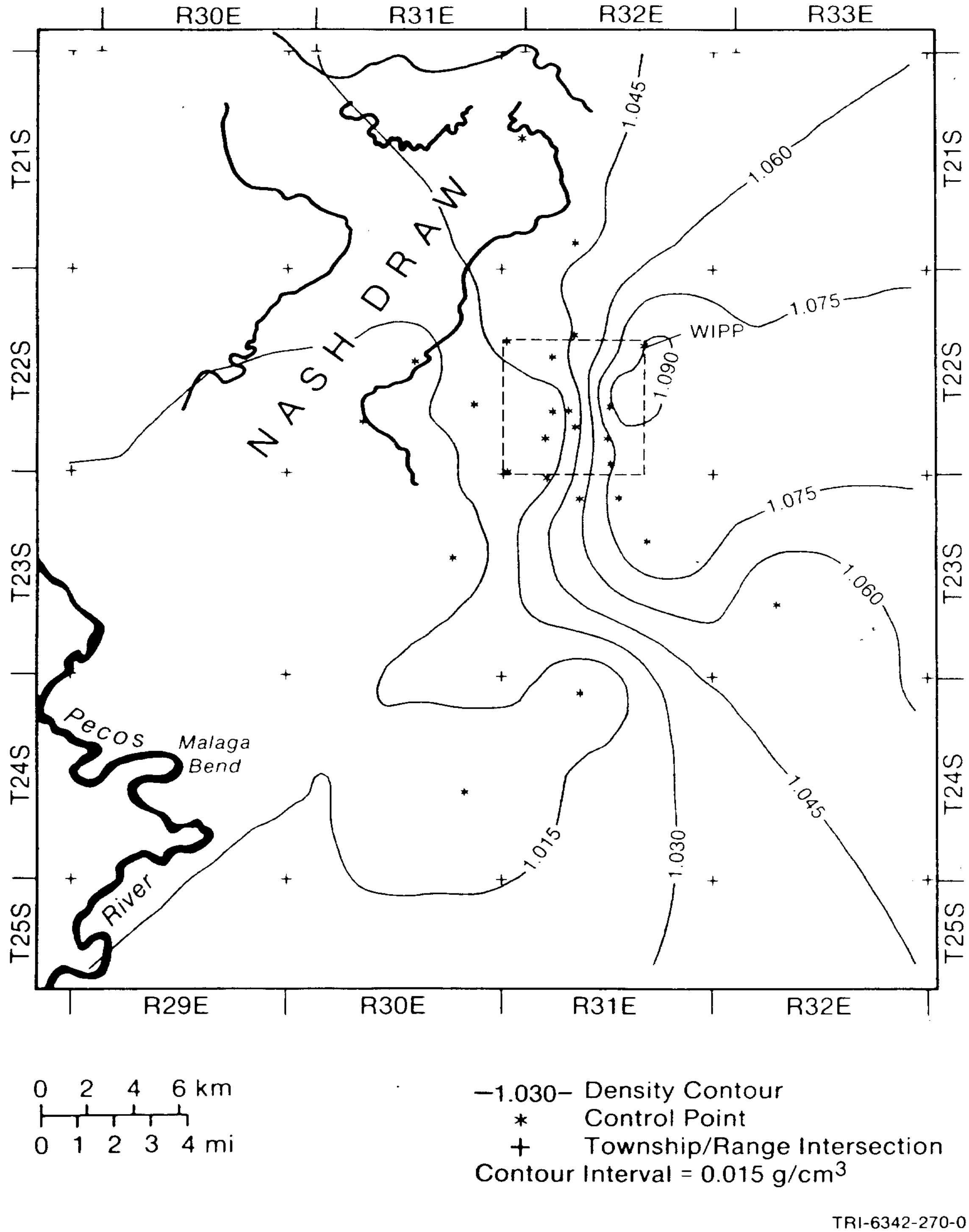

Figure 1.1 Groundwater density within the Culebra in the vicinity of WIPP.

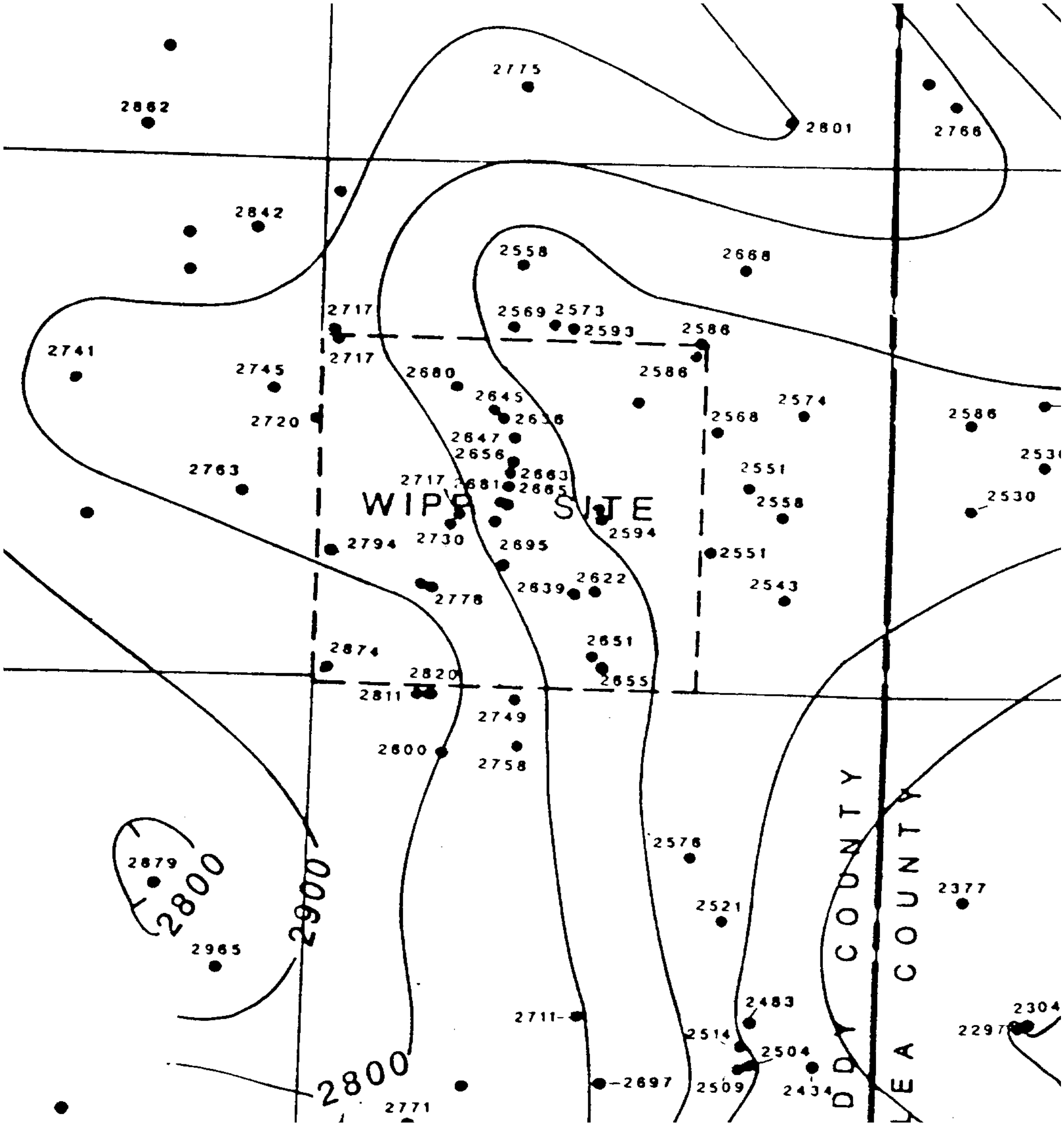

Figure 1.2 Elevation of the base of the Culebra in the vicinity of WIPP.

2. STAFF3D Modeling

2.1 MODEL CONSTRUCTION

The conceptual model for the density-dependent modeling consists of horizontal two-dimensional steady-state flow within the Culebra as is the case for both the 1992 PA and the CCA. The repository is decoupled from the Culebra; meaning that the repository is a source of contaminant mass in the Culebra but fluid flow from the repository is considered negligible. In this manner, the flow of water from the repository into the Culebra does not effect groundwater velocities in the Culebra. A constant concentration source term is used in the model to introduce radionuclides into the Culebra. The model domain covers the WIPP Land Withdrawal Boundary which is four miles on each side.

The flow system is assumed to be two-dimensional with groundwater gradients taken from a potentiometric surface map of the Culebra presented in the 1992 PA that was also used for the CCA (Figure 2.1). Flow is primarily from north to south; however, there is significant variation in gradient across the site and there is a slight eastward component of the regional gradient. The variation in gradient is simulated in the model by setting constant head boundary conditions around the finite-element mesh. The heads are interpolated from the regional potentiometric data (Figure 2.1). These interpolated heads are shown in Figure 2.2 for the model domain (WIPP Land Withdrawal Boundary).

Density variations in the Culebra are preserved by setting constant concentration boundary conditions around the perimeter of the model domain. The concentration values prescribed along the edge of the mesh are computed based upon the groundwater density at the node. The calculation assumes that the brine concentration in the Culebra is a maximum of 1.0 at the highest density value of 1.09 g/cm^3. Concentrations at nodes with density values less than 1.09 are scaled linearly. The density values assigned to each node are interpolated from the regional groundwater density data and are shown in Figure 2.3 for the model domain.

Even though a three-dimensional model is used in these analyses, there are no vertical hydraulic gradients in the system, except for vertical gradients caused by density variations. As in the 1992 PA, recharge to the Culebra is assumed to be zero.

The STAFF3D model for the density-dependent simulations consists of 30,000 nodes and 19,602 elements in 3 planes. The grid spacing was a constant 63 meters in both the X- and Y-directions. The vertical dimension was a constant 7.7 m. Data from the 1992 PA indicate that the Culebra does not vary in thickness significantly across the WIPP Site, even though the base elevation slopes at a rate of 0.015 from west to east. Although thickness is assumed to be constant in the model, the base of the model varies to match the regional Culebra base elevation data. The elevation of the model base is presented in Figure 2.4 for the model domain.

Aquifer properties are assumed to be homogeneous within the Culebra. Only dual-porosity simulations are performed. All simulations assume a single fracture within the Culebra. The equivalent porous medium hydraulic conductivity is assumed to be 7 m/y. For a single fracture, the fracture hydraulic conductivity was 421,240 m/y and the fracture porosity was 1.66×10^{-5}.

Transport parameters are also assumed to be homogeneous and are summarized in Table 2.1. The contaminant was assumed to be a conservative tracer with no retardation and no radioactive decay. The median value of matrix diffusion reported in the 1992 PA (9.46×10^{-3} m^2/y) was used for both simulations.

Table 2.1 Model parameters for the STAFF3D simulations

Parameter	Value
Matrix Hydraulic Conductivity (m/y)	7.0
Fracture Hydraulic Conductivity (m/y)	421,240
Matrix Porosity	0.139
Fracture Porosity	1.66×10^{-5}
Diffusion (m/y^2)	9.46×10^{-3}
Longitudinal Dispersivity (m)	25.0
Transverse Dispersivity (m)	2.5

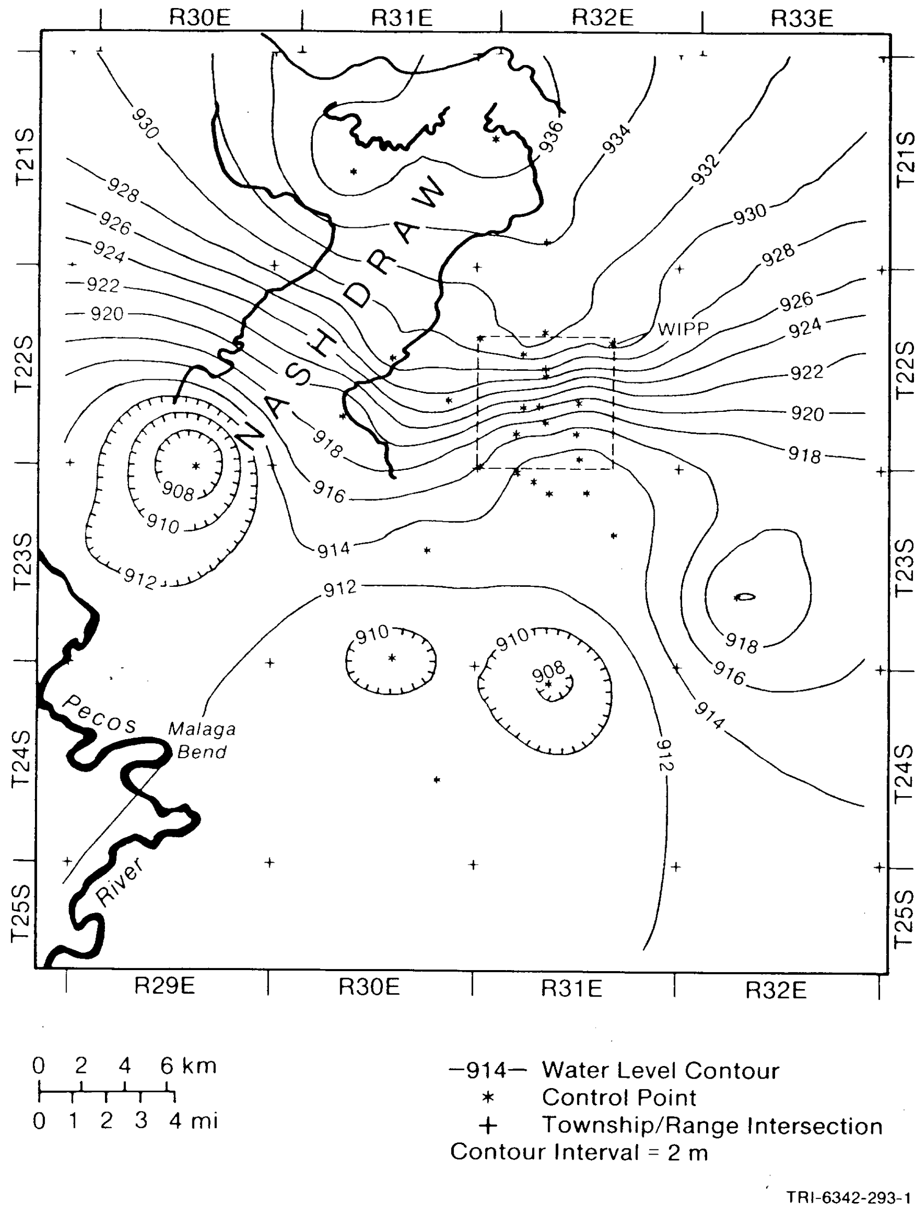

Figure 2.1

Potentiometric surface map for the Culebra from the 1992 PA.

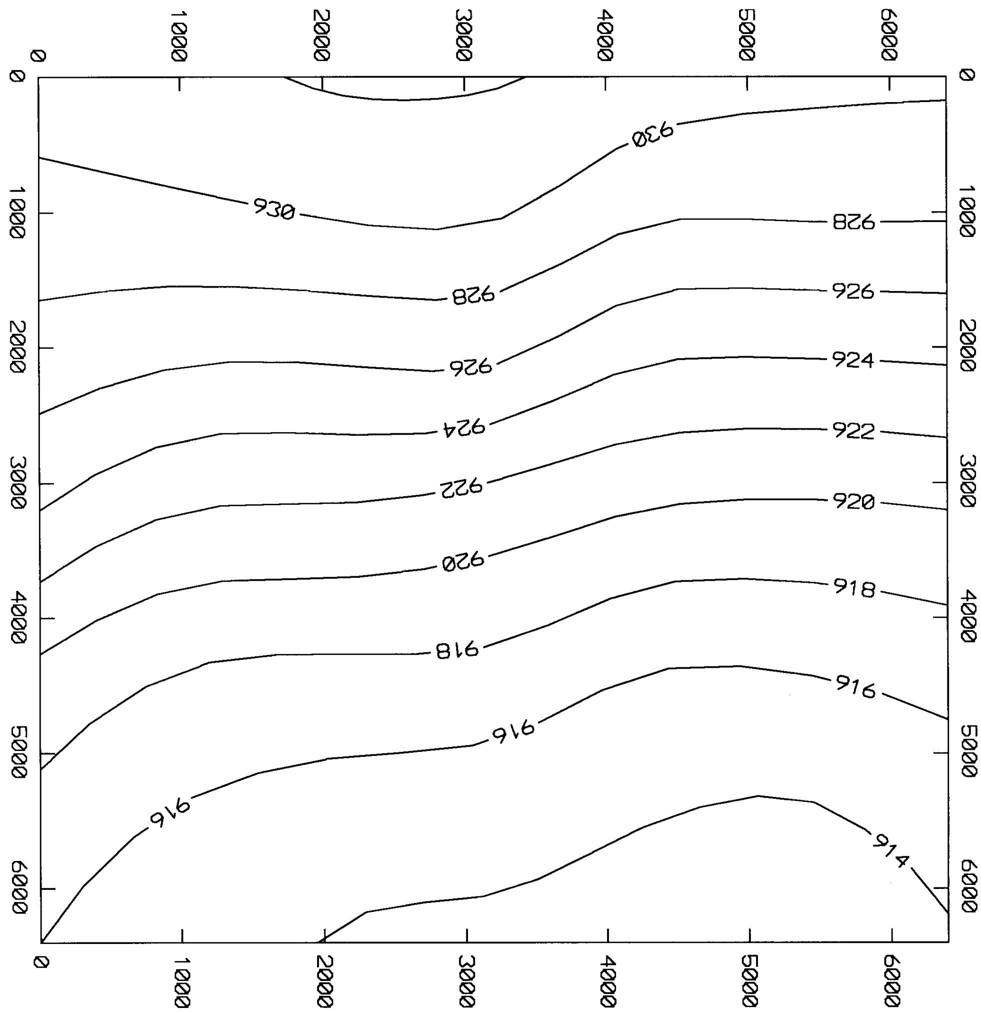

Figure 2.2 Heads in the Culebra interpolated to the STAFF3D model domain.

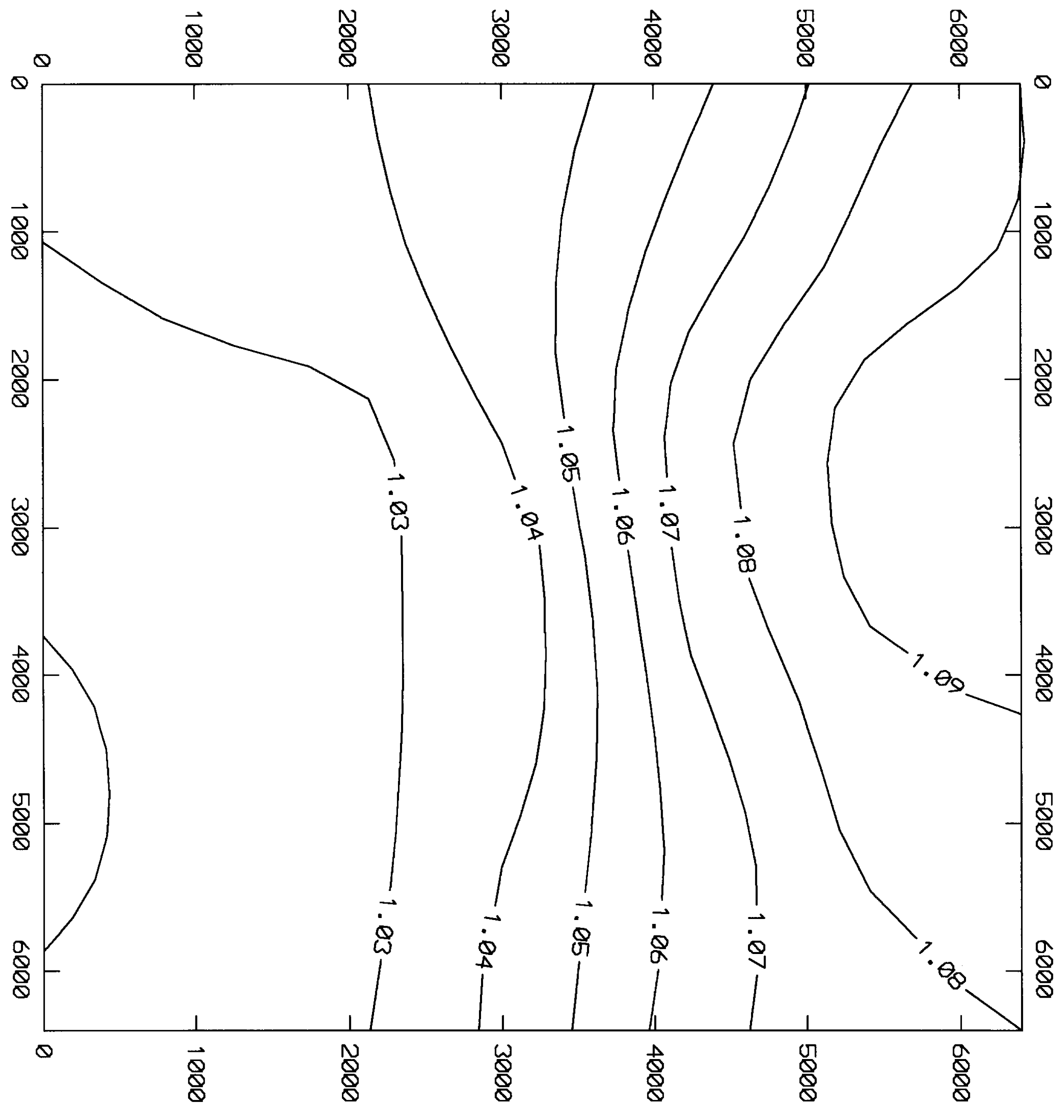

Figure 2.3 Brine density values (g/cm^3) interpolated to the STAFF3D model domain.

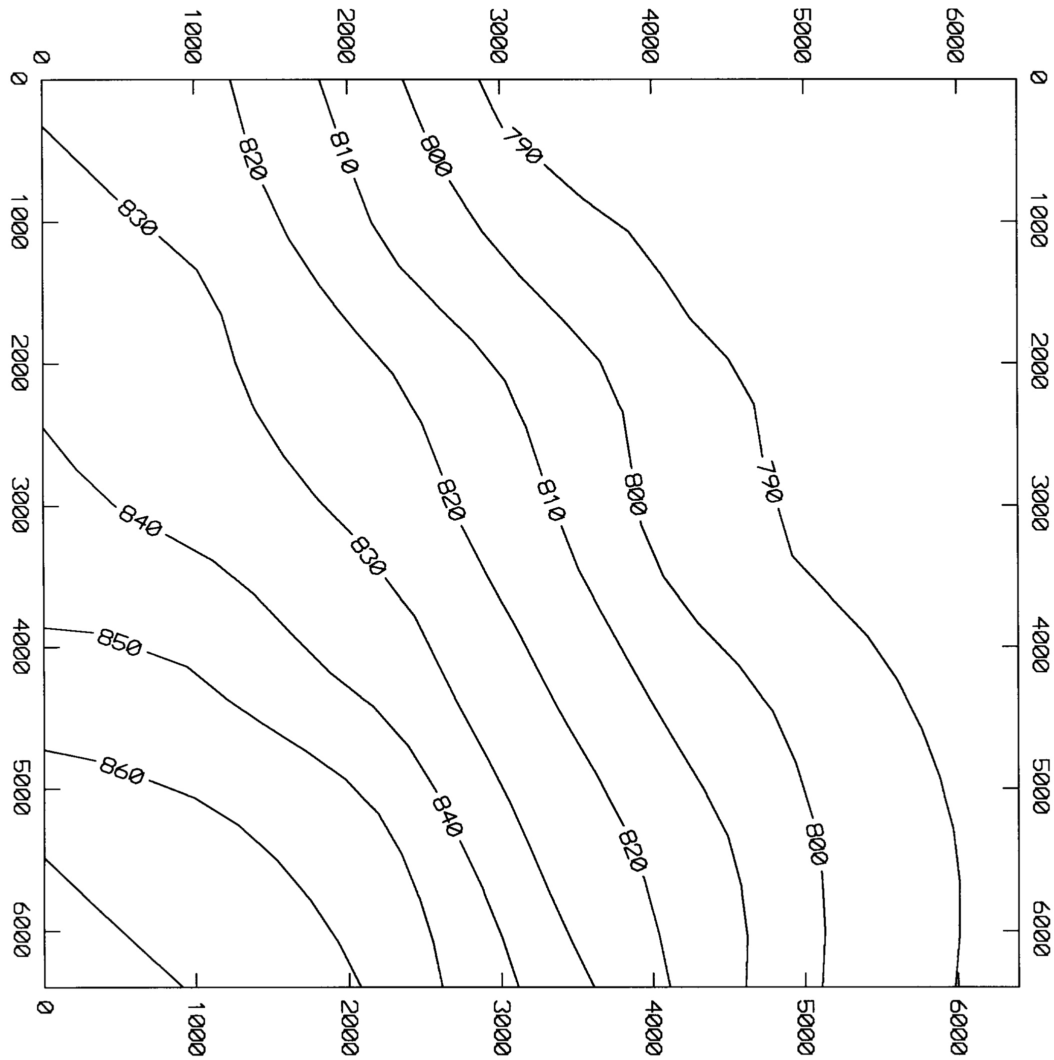

Figure 2.4 Culebra base elevations (m) interpolated to the STAFF3D model domain.

3 Description of Simulations

Two sets of simulations were performed to evaluate the significance of density variation on radionuclide transport in the Culebra. The first set includes the effects of matrix diffusion and the second set neglects diffusion. Both density and non-density simulations are conducted for the diffusion and non-diffusion cases. Thus, a total of four simulations were performed with STAFF3D.

3.1 Matrix Diffusion Case

The first set of STAFF3D simulations includes the effects of matrix diffusion. The diffusion coefficient is 9.46×10^{-3} m/y^2, which is the median value reported in the 1992 PA. In order to evaluate the impact of density variations on radionuclide transport in the Culebra, two runs were performed, with and without density. The runs are compared by (1) contouring radionuclide concentrations at the end of the simulation, (2) contouring the magnitude of groundwater velocity, and (3) plotting contaminant mass accumulation at the downgradient boundary of the model.

The density and non-density simulations produce virtually the same contaminant distribution in the Culebra after 8,817 years (the time selected to present output is based on specified time step intervals), as shown in Figure 3.1a and 3.1b, respectively. The contaminant plume in both cases is skewed slightly to the east in response to head variations along the southern model boundary (Figure 2.2). Both plumes have a maximum relative concentration of about 0.1.

The magnitude of groundwater velocity is plotted in Figures 3.2a and 3.2b for the density and non-density simulations, respectively. Some localized variation can be seen in the shape of the contours and the density run computes groundwater velocities that are up to 80 percent higher than the non-density case (Figure 3.3). This localized increase in velocity, however, is not enough to significantly impact the contaminant distribution, as discussed above.

The cumulative mass of contaminant exiting the downgradient (southern) boundary of the model is almost identical between the density and non-density simulations, as shown in Figure 3.4. The non-density simulation produces approximately 2 percent more mass at the boundary than the density simulation.

3.2 No Matrix Diffusion Case

The second set of STAFF3D simulations neglects the effects of matrix diffusion. The diffusion coefficient in this case is set to 0.0 m/y^2. As with the matrix diffusion simulations, the impact of density variations on radionuclide transport in the Culebra was evaluated by conducting two simulations, with and without density. The runs are compared by (1) contouring radionuclide concentrations at the end of the simulation, and (2) contouring the magnitude of groundwater velocity.

The density and non-density simulations produce virtually the same contaminant distribution (i.e., relative concentrations) in the Culebra after 8,817 years (the time selected to present output is based on specified time step intervals), as shown in Figure 3.5a and 3.5b, respectively. The contaminant plume in both cases is skewed slightly to the east in response to head variations along the southern model boundary (Figure 2.2). Both plumes show substantially greater concentrations exiting the downgradient boundary for the simulations with matrix diffusion because no dilution occurs within the matrix blocks.

The magnitude of the relative groundwater velocities are plotted in Figures 3.6a and 3.6b for the density and non-density simulations, respectively. As in the previous set of simulations that included matrix diffusion, some variation can be seen in the shape of the contours and the density run computes groundwater velocities that are about 30 percent higher than the non-density case (Figure 3.7). This slight increase in velocity, however, is not enough to significantly impact the contaminant distribution, as discussed above.

The cumulative mass of contaminant exiting the downgradient (southern) boundary of the model is also virtually identical between the density and non-density simulations as shown in Figure 3.8. The density simulation produces approximately 1 percent more mass at the boundary than the non-density simulation.

Figure 3.1a Distribution of contaminants with matrix diffusion and density gradients.

Figure 3.1b Distribution of contaminants with matrix diffusion and no density gradients.

Figure 3.2a Magnitude of velocity with matrix diffusion and density gradients.

Figure 3.2b Magnitude of velocity with matrix diffusion and no density gradients.

Figure 3.3 Percent velocity differences between Figures 3.2a and 3.2b.

Figure 3.4 Cumulative mass exiting the boundary.

Figure 3.5a Distribution of contaminants without matrix diffusion and density gradients.

Figure 3.5b Distribution of contaminants without matrix diffusion and no density gradients.

Figure 3.6a Magnitude of velocity without matrix diffusion and density gradients.

Figure 3.6b Magnitude of velocity without matrix diffusion and no density gradients.

Figure 3.7 Percent velocity differences between Figures 3.6a and 3.6b.

Figure 3.8 Cumulative mass exiting the boundary.

4 Conclusions

The STAFF3D simulations incorporated observed density variations in the Culebra. The model assumed a dual-porosity, homogeneous system with a single fracture. Simulations were performed with and without matrix diffusion. In both cases, the velocities computed by STAFF3D were 30 to 80 percent higher for the density simulations when compared to simulations neglecting density variations. However, these velocity differences were localized over relatively small areas and were not sufficient to produce significant changes in radionuclide concentration or mass loading at the downgradient boundary of the land withdrawal area. Furthermore, the single fracture assumption would be conservative in that the differences between the velocities would be accentuated. Therefore, EPA is confident that density effects do not need to be included in the CCA modeling.

5 References

Huyakorn, P.S., Panday, S., Sinha,A., 1992. Users Manual for STAFF3D, *A Three-Dimensional Finite Element Code for Simulating Fluid Flow and Transport of Radionuclides in Fractured Porous Media with Water Table Boundary Conditions*.