SOLUTE TRANSPORT MODELING AND 3-D VISUALIZATION AS THE BASIS FOR LONG-TERM GROUNDWATER MONITORING RECOMMENDATIONS AT MURDOCK, NEBRASKA

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INTRODUCTION

With the results of QuickSite® expedited site characterization, three-dimensional numerical groundwater flow and transport models were developed to evaluate the fate and transport of carbon tetrachloride (CCl_4) contamination in the shallow groundwater surrounding a former grain storage facility at Murdock, Nebraska. Integration of quality-assured geologic, hydrogeologic, and geochemical data obtained from extensive field sampling through the QuickSite® program provided the conceptual basis for the modeling and the parametric constraints on the groundwater model attributes. The flow and transport models based on QuickSite® characterization closely adhere to site properties, thus providing a high level of reliability in their predictions.

BACKGROUND

A calibrated MODFLOW-99 (McDonald and Harbaugh 1988) model was constructed on the basis of conceptualization of shallow groundwater flow at Murdock. The shallow groundwater system at Murdock is localized with natural control by recharge from precipitation and discharge to the springs, seeps, and creeks that flank Murdock (Figure 1). The model grid contains 107 southwest-northeast (x-direction) cells and 80 northwest-southeast (y-direction) cells. The model grid extends well beyond the immediate area of interest in Murdock to use natural flow boundaries where possible and to reduce the artificial influence of the model boundaries on the simulated flow regime near Murdock. A variable spacing grid was employed to accurately simulate groundwater flow and solute transport in and near Murdock and to provide the highest model resolution in areas of known groundwater contamination. The minimum x-direction spacing is 50 ft.

The Murdock finite-difference groundwater flow and transport models employ a non-horizontal layering approach in which the model layering conforms to the geologic geometry of the site better than with strict horizontal layering. The three important geologic/lithologic surfaces upon which the vertical layering of the Murdock groundwater model is based are (1) the elevation of land surface, (2) the elevation of the top of the shallow aquifer, and (3) the elevation of the bottom of the shallow aquifer. To achieve sufficient vertical resolution of groundwater flow, and subsequently CCl_4 transport, the Murdock groundwater flow model was divided into 12 layers, with individual layers 2-12 representing the aquifer materials, ranging between 3 ft and 6 ft in thickness depending on location. Layer 1 represents silt and clay.

FIGURE 1 Plan View of Area of Murdock, Nebraska, Covered by Groundwater Flow and Transport Models

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MURDOCK CCL_4 TRANSPORT MODEL

The purpose of the solute transport modeling was to predict the spatial and temporal evolution of the dissolved CCl_4 plume, beginning with the configuration observed in late 1996-early 1997 (Figure 2).

Transport Model Calibration

The Murdock CCl_4 solute transport model includes relevant physical and chemical processes (i.e., advection, dispersion, sorption, and natural decay) by incorporating reasonable values for all transport parameters controlling these processes. The computer code used for the CCl_4 solute transport modeling was MT3D-99 (S.S. Papadopulos and Associates, Inc., 1992). MT3D-99 is a modular three-dimensional, finite-difference model that is fully compatible and interfaced with MODFLOW-99 and uses the same model configuration as MODFLOW-99. MT3D-99 is capable of simulating advective dispersive transport and chemical reactions (e.g., sorption and degradation). The required transport parameters were adjusted until an acceptable match to concentrations observed in late 1999 could be achieved (Figure 3), starting with the concentrations observed in 1996-1997.

Figure 4 shows the final results of the Murdock transport model calibration process. The simulated concentrations for each observation location are the concentrations in the model cell (row, column, layer) associated with the midpoint of the screen interval. Agreement between observed concentrations and simulated concentrations is extremely good at the three critical locations associated with the center of mass of the plume. This is important, considering that initial concentrations (December 12, 1996) were in excess of 7,000 µg/L. Remaining calibration concentrations cluster around low values, as shown in Figure 4.

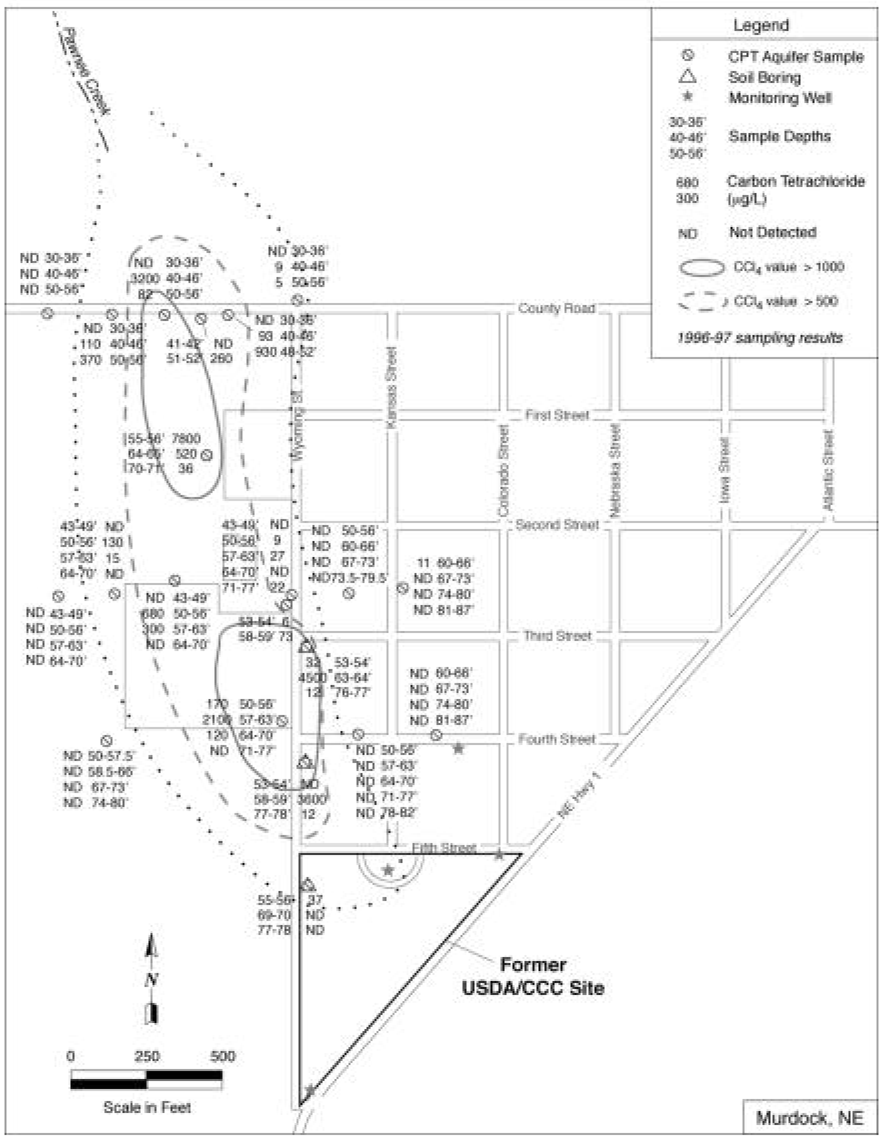

FIGURE 2 CCl_4 Concentrations as of 1996-1997

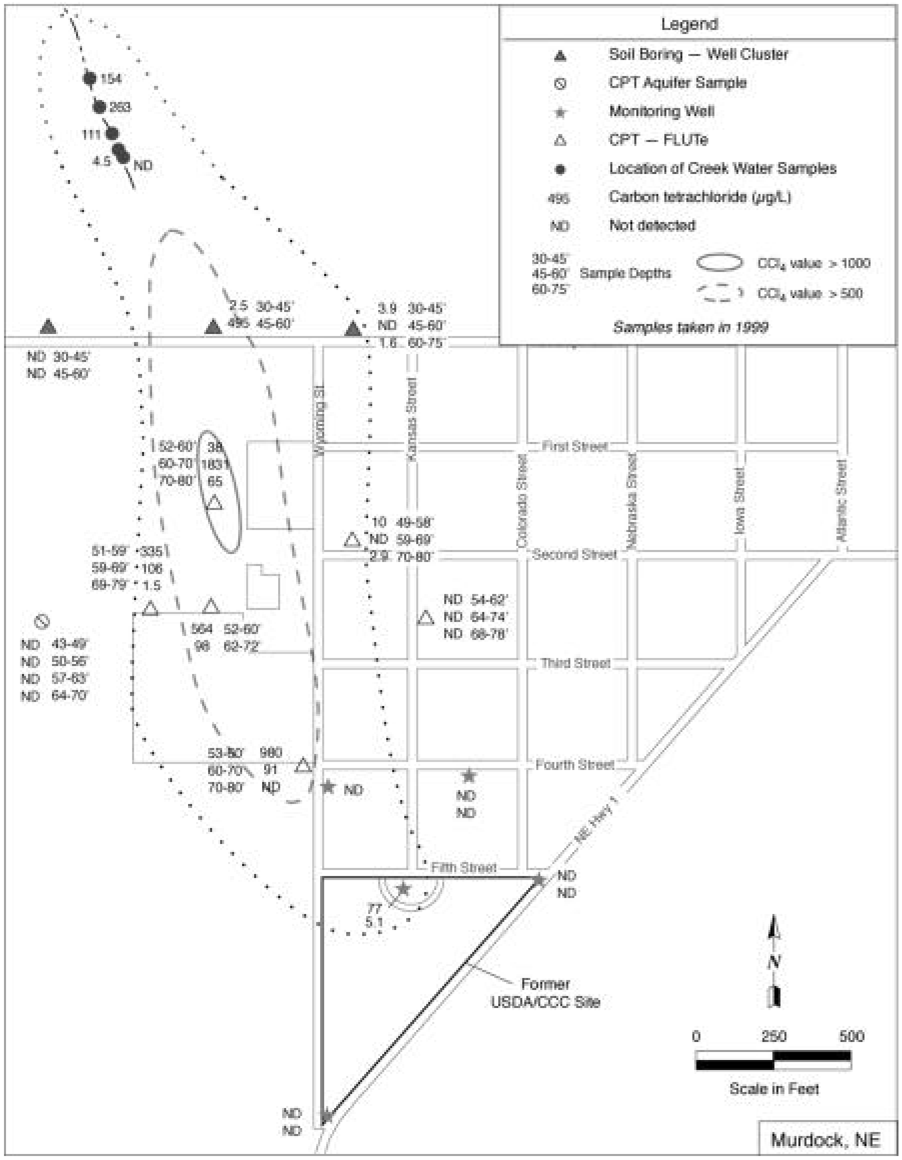

FIGURE 3 CCl_4 Concentrations as of Late 1999

All transport parameters are reasonable for the type of geologic environment and solute at Murdock. The longitudinal dispersivity is 32.7 ft; horizontal dispersivity is 3.3 ft; and vertical dispersivity is 0.0 ft. The calibrated retardation factor of 2.65 is only slightly above the initial estimate of 2.2 and well within published guidelines. The calibrated natural decay coefficient is 1.9×10^{-5} (d^{-1}), which equates to a conservative 100-year half-life for dissolved CCl_4 in the Murdock groundwater system.

Transport Model Predictions and Monitoring Recommendations

All indications from the QuickSite® characterization, groundwater flow modeling, and CCl_4 transport modeling conducted at Murdock are that the CCl_4 plume and plume dynamics are well understood and predictable. Thus, an effective and efficient groundwater monitoring plan can be devised and implemented at Murdock to track the CCl_4 plume throughout the remainder of its migration history and eventual final discharge, dilution, and dissipation in Pawnee Creek, which originates just northwest of Murdock.

A set of strategically selected sampling locations was developed, designed to track the three-dimensional main body of the CCl_4 plume and ensure its lateral confinement to predicted pathways. The monitoring strategy is based on both the concentrations observed in wells during site characterization at Murdock and long-term (through 2010) simulations of the transport of CCl_4 at Murdock.

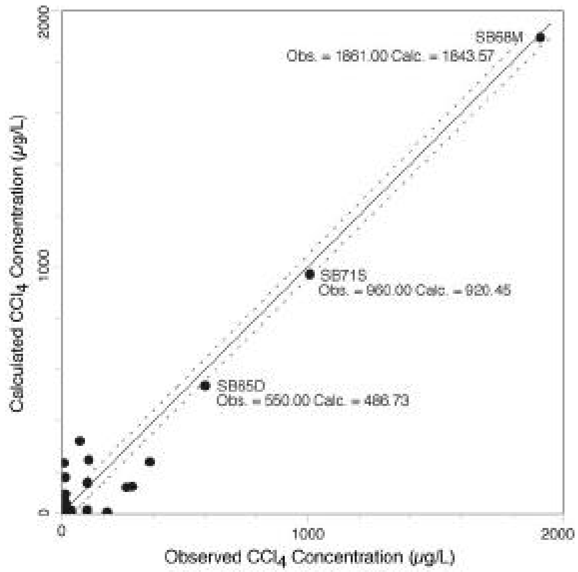

FIGURE 4 Results of Murdock Solute Transport Model Calibration

As of early 2000, the bulk of the CCl_4 plume at Murdock was confined to a rather narrow vertical segment of the aquifer. By using the calibrated CCl_4 transport model and beginning with concentrations observed in late 1996, concentrations were simulated for each monitoring well through 2010. The results of this exercise were plotted for each well along with concentrations observed through April 2000.

The trend in CCl_4 concentration reduction at Murdock is important. For example, as previously indicated, field data and simulation data show a significant reduction in the highest plume concentrations from over 7,000 µg/L in late 1996 to around 2,000 µg/L in early 2000. However, there are natural short-term fluctuations in observed concentrations. The trigger action levels established for each monitoring well represent an upper bound to the long-term expected concentrations. Figure 5 shows an example of the results for the monitoring location with the highest CCl_4 concentrations.

Beginning with the initiation of quarterly sampling at Murdock, no action is being recommended until two successive quarterly samplings exceed the trigger action level for the well. Sampling is recommended quarterly for two years and semi-annually for eight years thereafter, if no unexpected behavior in concentrations occurs.

CONCLUSIONS

Following successful model calibration, the Murdock solute transport model was used in a second phase of modeling to predict longer-term CCl_4 migration at Murdock in support of the design of an effective and efficient monitoring program. The calibrated CCl_4 transport model was used to predict the CCl_4 concentration regime, over time, at Murdock until the end of 2010. These results form the basis of a long-term monitoring program with trigger action concentrations determined from model-predicted breakthrough curves at strategic locations within the plume and along its flanks. Three-dimensional visualization techniques were used to display the results of the modeling effort.

ACKNOWLEDGMENT

This work was supported by the Commodity Credit Corporation of the U.S. Department of Agriculture under interagency agreement through U.S. Department of Energy contract W-31-109-Eng-38.

REFERENCES

McDonald, M.G., and A.W. Harbaugh, 1988, *A Modular Three-Dimensional Finite-Difference Ground-Water Flow Model*, Chapter A1, Open-File Report 83-875, U.S. Geological Survey, Denver, Colorado.

S.S. Papadopulos and Associates, Inc., 1992, *MT3D: A Modular Three-Dimensional Transport Model —Documentation and User's Guide*, S.S. Papadopulos and Associates, Inc., Bethesda, Maryland.

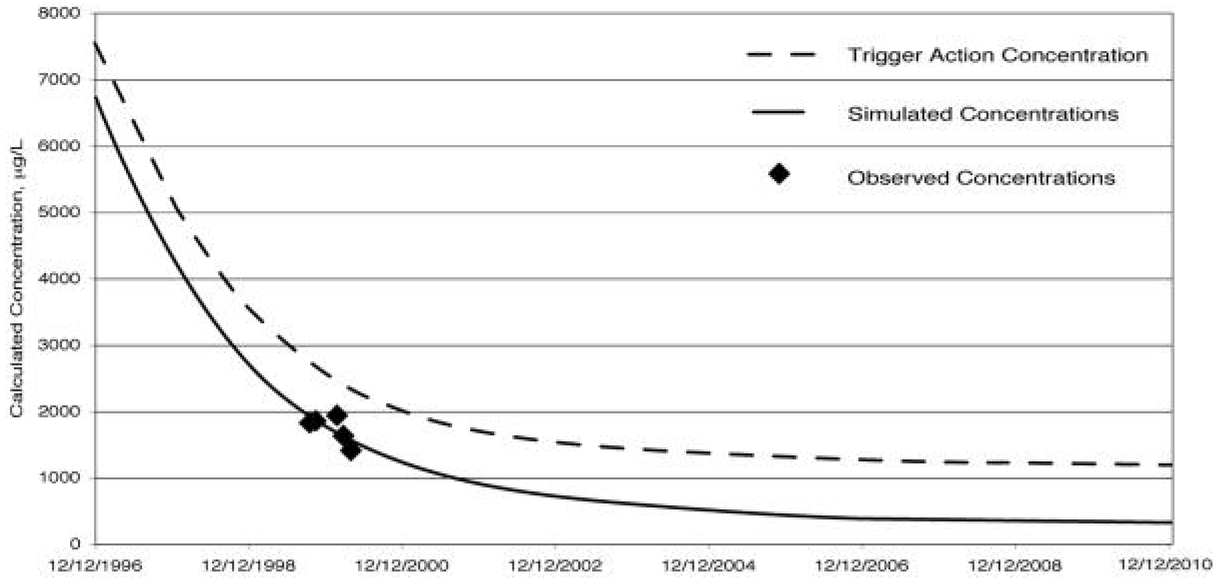

FIGURE 5 Example Long-Term Simulation and Associated Trigger Action Concentration