Simplicity in Modeling – Use of Analytical Models with PEST

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ABSTRACT

Analytical models can be powerful tools in the analysis of hydrogeologic data. The application of these models can be facilitated by simple geometric transformations. To illustrate their utility, two example applications of the analytical model ATRANS are presented. ATRANS is a three-dimensional chemical transport model program that uses an analytical solution to the advection-dispersion equation. The model allows for the consideration of a time-varying source emanating from a rectangular area at the origin of coordinates. In the first example, ATRANS was used to compute the historical evolution of a contaminant plume within a single hydrogeologic unit. ATRANS parameters were estimated using PEST where the orientation of the ATRANS coordinate system was one of the estimated parameters. The results were compared with results obtained using an elaborate three-dimensional MT3D model. The results show that application of ATRANS was able to explain the data variation as well or better than the more elaborate model. In a second example, ATRANS was applied to the analysis of a large elongate contaminant plume. In this case, a segmented pathline was used to define the general orientation of the plume that was evaluated using the ATRANS model. Again, PEST was used to assist in the estimation ATRANS parameters. However, because of the nature of the sampling data, an envelope approach was used to evaluate the computed concentrations within the principal zone of migration. These examples demonstrate the both the utility and the effectiveness of analytical models for understanding and evaluating hydrogeologic data.

INTRODUCTION

Simple analytical models can be powerful tools for analyzing and evaluating groundwater data and they have certain advantages over numerical models. The input data necessary to use an analytical model is typically less complex and less extensive than that of numerical models. Analytical models also typically require much less computer time to obtain results and, as a result, are easily and effectively incorporated into parameter estimation programs such as PEST (Doherty, 2002). Analytical models also do not suffer from problems such as discretization error or numerical dispersion which can plague some numerical models.

The obvious limitations associated with analytical models are that problem geometries, boundary conditions, and initial conditions often must be simple and uniform. In spite of such limitations, analytical models often can be used to evaluate complex field data and provide useful results and knowledge about the problem at hand. This paper describes the application of the analytical model, ATRANS (Neville, 1998), to two contaminant transport problems.

THE PROBLEM

The problem was a need to evaluate the timing and amount of contaminant release and growth of two contaminant plumes. The first case involved a multi-aquifer groundwater system in southern California. Chlorobenzene and other contaminants had penetrated into the aquifer system and were migrating laterally within several of the aquifer units. A complex three-dimensional groundwater flow and transport model had been developed using the MT3D model program to evaluate the evolution of the contaminant plume. However, calibration of the MT3D model using PEST was computationally intensive and a very idealized source term (constant concentration) had been used in each of upper aquifer units. The question was whether a more variable source term could better explain the contamination and, if so, what impact would that have on other model parameters.

The second case involved an extensive plume of perchlorate contamination. The plume extended over a distance of about 10 miles and appeared to be migrating preferentially through thin, more permeable zones. The question to be addressed was what was the timing and amount of perchlorate released to the groundwater to create the extended plume.

In each of these cases, the analytical model program ATRANS was applied to evaluate the evolution of the contaminant plumes.

THE ANALYTICAL MODEL

ATRANS is a three-dimensional analytical chemical transport model program (Neville, 1998). The model program assumes a time-varying contaminant source emanating from a vertically rectangular area at the origin. This rectangular area is referred to as a patch source. The time sequence of source concentration is applied as a set of varying concentrations applied at specified points in time. The analytical solution is obtained by applying the principle of convolution to the time sequence. Other model parameters such as velocity, retardation, dispersivity, and degradation are assumed to be uniform over the domain. The program will calculate the concentration at any coordinate location x, y, and z, and time, t.

To facilitate the application of ATRANS with chemical sampling data, a driver program was developed that utilized the ATRANS model as a core. The purpose of the driver program was to orient the ATRANS coordinate system into the coordinate system of the sampling data. In the first example, this was accomplished simply by an origin offset and rotation of the sampling data coordinates. In other words, the sampling data were referenced to the ATRANS model origin and the coordinate system was rotated to align the x-coordinate along the direction of groundwater flow and chemical transport.

In the second example, the extended plume followed a slightly curved path from the source area. A segmented line was constructed from the contaminant source location (ATRANS model origin) along the central axis of the contaminant plume. This approximate curvilinear path was assumed to represent the x-axis in the ATRANS coordinate system. Y-coordinates in the ATRANS coordinate system were calculated as the perpendicular offset from the segmented line.

THE DATA AND ANALYSIS

Multi-Aquifer Chlorobenzene Problem

The first example is associated with cholorbenzene contamination of a multi-aquifer groundwater system in southern California. The problem was being analyzed using the MT3D groundwater transport program. A fairly complex model had been constructed and was being calibrated using the PEST parameter estimation program. Because of the size and complexity of the MT3D model, the parameter estimation process was very computationally intensive. During a review of the MT3D modeling process, questions arose regarding some of the MT3D model parameters, in particular assumptions regarding source conditions and the impact of those assumptions on other model parameters.

To address these questions, the ATRANS model program was used to evaluate the lateral contaminant transport within some of the individual aquifer units. Because the MT3D model used a constant concentration source in each of several aquifer units, most of the contaminant mass in each aquifer unit was derived from the constant concentration source.

Sampling data from monitoring wells over time was assembled to define the spatial and temporal contaminant distributions in each aquifer unit. These data were used to formulate a set of observations that could be used in a parameter estimation exercise using PEST with ATRANS as the core model. PEST was applied to estimate the ATRANS model parameters. The estimation process was focused on the timing and amount of contaminant release at the source and on the groundwater velocity. The rotation angle used to align the ATRANS coordinate system with the sampling data was also estimated using PEST.

Extended Perchlorate Plume Problem

In the second example, extensive sampling data were available that defined the spatial and temporal patterns of perchlorate contamination. Over 1,800 samples had been collected over an approximately 10-mile long area downgradient from the contaminant source location. The sampling data indicated that concentrations in wells were very dependent upon the degree to which individual wells penetrated and/or were open to the more permeable zones that were transporting the contaminants. Wells that were not open to these zones would indicate low or non-detectable concentrations while wells that were open to these zones would show higher concentrations.

The primary question being addressed was what was the timing and amount of contaminant release at the source area and how did the plume evolve over time. Because the sampling data showed a wide variation in concentration depending on well depth and open interval, the ATRANS program was applied to estimate concentrations within the primary zone or zones of transport. The sampling data were considered to represent a distribution of values that would generally fall below an enveloping distribution of concentrations associated with the primary zone or zones of transport. As such, parameter estimation programs such as PEST could not be applied directly using the concentration data because only some of the measurements reflected conditions within the primary zone or zones of transport.

PEST was used to develop some initial estimates of the ATRANS model parameters using selected subsets of data from the overall sampling data. The ATRANS parameters were adjusted manually to developing spatial distributions that, for the most part, enveloped the overall sampling data.

RESULTS AND CONCLUSIONS

For the first example, the results of the analysis using the ATRANS model were compared to the results obtained from the more complex MT3D model. Figure 1 shows the scatter diagram for sampling data from one of the shallower aquifer units compared to the concentrations computed using the MT3D model and computed using the ATRANS model. Logarithmic scales are used to allow for comparisons at both high and low concentration values. Although there is a fairly wide scatter at lower concentrations, the ATRANS model was able to explain as much or more of the data variability than the MT3D model. In fact, statistical summaries show an improved mean error, standard error and correlation using the ATRANS model versus the MT3D model. While part of the improvement is undoubtedly related to the time-varying source term in the ATRANS model as opposed to a constant concentration source term in the MT3D model, it may also relate to better estimates of transport parameters (velocity and dispersivity).

Similar results were obtained for analysis of a deeper aquifer unit. In that case, the improvement in calibration statistics using the ATRANS model was somewhat mixed. However, the timing of the source term in the ATRANS model was significantly different from the assumption used in the MT3D model. This led to significantly different conclusions regarding values for other transport parameters such as velocity, retardation and dispersivity. These differences could have important impacts on conclusions drawn from applications of the MT3D model.

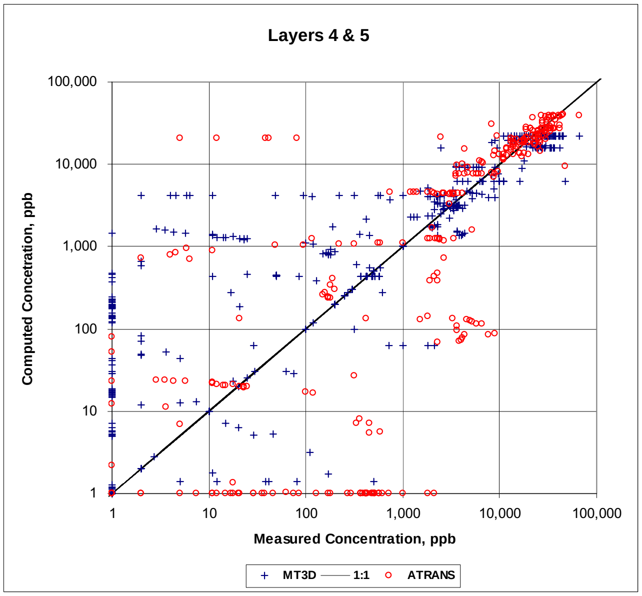

Figure 1. Scatter Diagram of Measured and Computed Concentrations.

In the second example, parameter estimation using PEST was applied to a subset of the sampling data to obtain initial estimates of ATRANS model parameters. However, it was recognized that contaminant transport was likely occurring predominately through more permeable zones. As a result, ATRANS model parameters were subsequently adjusted manually and model results were examined by comparison of sampling data along longitudinal and transverse transects to model results along the transects.

Some example graphics used to compare the sampling data with model results are shown in Figures 2 and 3. Figure 2 shows a graph of the sampling data plotted against the longitudinal distance from the source location. This distance was computed along the segmented plume centerline from the source location to the location where a perpendicular from the sampling point intersected the segmented line.

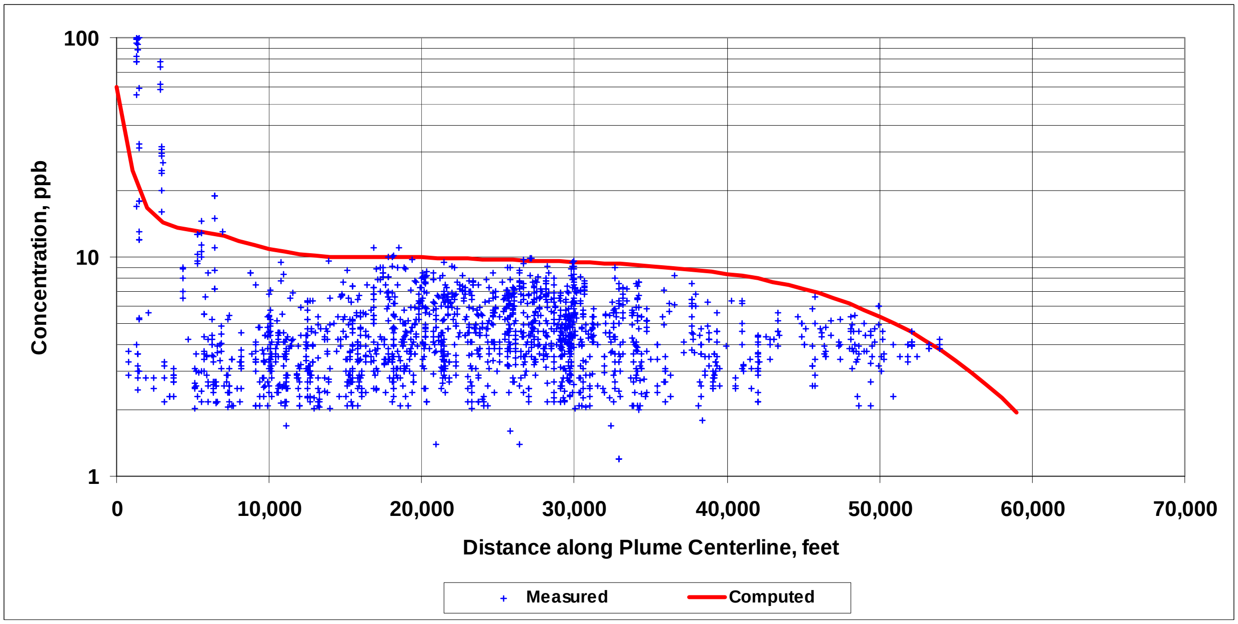

Figure 2. Sampling Data and Model Results versus Distance along Plume Centerline.

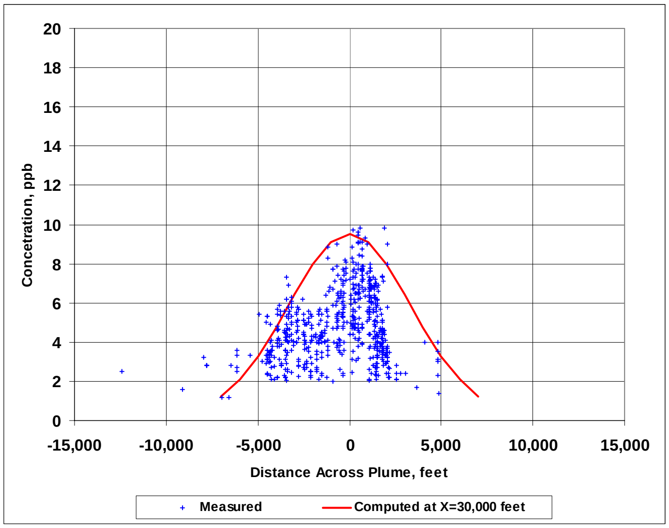

Figure 3. Sampling Data and Model Results versus Distance Across Plume Centerline.

Figure 3 illustrates model performance perpendicular to the plume centerline. Similar graphs were prepared at 10,000-foot increments along the centerline. Sampling data were plotted if the longitudinal distance of the sampling point was within 5,000 feet of a specific transect, in this case the 30,000-foot transect.

These results show that the ATRANS model was able to reasonably estimate an enveloping concentration distribution. The results also show that the resulting distribution provides a reasonable explanation of the sampling data when it is recognized that the degree to which wells might have been open to the principal zone of transport was likely quite variable.

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