The behavior of volatile organic contaminants in the vadose zone with respect to barometric pumping and the estimate of residual mass and mass removal using T2VOC.

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Estimates of residual contaminant mass and removal rates in the zone of influence of a barometric pumping well can be determined by T2VOC analysis of time-series measurements of contaminant concentrations at the well head and flow rate produced by atmospheric pressure changes, under two flow conditions. T2VOC has been augmented by the inclusion of liquid diffusion in addition to gaseous diffusion to more accurately match the conceptual model of mass transfer in the vadose zone.

At the Savannah River Site (SRS), significant fluxes of contaminants out of vadose zone wells have been observed in response to atmospheric pressure drops. The airflow in and out of barometric-pumped wells is a result of the difference in pressure between the formation at the screened zone of the well and the atmosphere at the surface. Earlier work confirmed that atmospheric pressure is transmitted through the subsurface but that this energy is damped and delayed when it encounters zones of lower permeability. The delay and attenuation of the pressure signal in the subsurface with respect to the surface pressure produces a pressure differential between the two zones when they are directly connected as by an open well. Airflow through the well is sustained during the period that the surface pressure is different than the pressure in the subsurface zone accessed by the well. If volatile contaminants are present near the well, gas phase contaminants will be removed during periods of flow out of the well and surface air will be injected during periods of flow into the well.

When concentration and flow are measured under two different conditions: a) simple venting (inflow and outflow) resulting from surface atmospheric pressure fluctuations, and b) controlled venting in which only barometric- produced airflow out of a well is allowed, a significantly different contaminant concentration profile is observed at the well head during outflow periods. This behavior results from both the clean air dilution of soil gas during inflow and mass transfer of the contaminant from liquid or aqueous phases to the gas phase. Using contaminant concentration data collected during these two flow regimes, geology information such as cone penetrometer logs, and T2VOC to model potential contamination scenarios, the amount of contaminant mass in the zone of influence and mass transfer rates can be determined. This simple and inexpensive test strategy may help characterize contaminated sites and determine expected cleanup time.

EXPERIMENTAL

A 2.5 cm diameter well with short screen (approximately 1.5 m) was used in this experiment. The screen zone ranged from a depth of 32.3 m to 33.8 m. A core description from a nearby, conventionally cored well, indicates that all but the top 0.35 m of screen was in a clayey material. The top part of the screen was in a medium sand. The well was monitored for pressure response to atmospheric pressure changes to establish that the formation had sealed adequately and no short-circuiting was occurring through the annulus. A logging station was deployed that monitored surface and well pressure and through the well at ten minute intervals. The system was powered with gel cell batteries charged by solar panels.

Concentration data were monitored and logged separately from the pressure and flow data using a Bruel and Kjaer Model 1302 multigas monitor. The monitor is an infrared photoacoustic system using optical filters selected for specific target analytes. The instrument is capable of effectively discriminating between TCE, PCE, and carbon dioxide in a multigas mixture and has a lower detection limit of around 200 ppbv for both TCE and PCE. The model 1302 was programmed to monitor at ten minute intervals for these experiments.

A one way valve (Baroball®) was used to prevent surface air flow into the formation for part of these experiments. The Baroball is a simple, yet effective check valve that will open in the allowed direction of flow under very low differential pressure (approximately 100 Pa) yet will prevent flow in the opposite direction.

MODEL

The models were developed to simplify the extremely heterogeneous vadose zone system to three major zones with two different materials. This simplification maintains the general integrity of the actual site located in the M area of SRS. The system includes a partially-penetrating well screened in a medium sand which is confined by two relatively wet clayey materials. The models assumed radial symmetry with an infinite lateral extent (for the scope of the simulations that were run). For the more idealized simulation, tetrachloroethylene non aqueous phase liquid (NAPL) was distributed uniformly within the interior of the uppermost clay at a saturation of 0.001. This value was selected based on characterization results obtained from NAPL investigations at several areas of the SRS A/M Area. Although this saturation value appears low when compared with NAPL saturation values assumed in much of the literature, it is quite close to the highest values found in many investigations performed here.

Simulations were also performed with a more accurate depiction of the actual subsurface conditions. In this scenario, a 2.5 cm-diameter well with 0.35 m of effective screen length (the rest of the screen is in the clay) is located in the sandy section just above the lowermost clay. A residual NAPL saturation of 0.05 was used here. Figure 1 depicts the grids for the two scenarios.

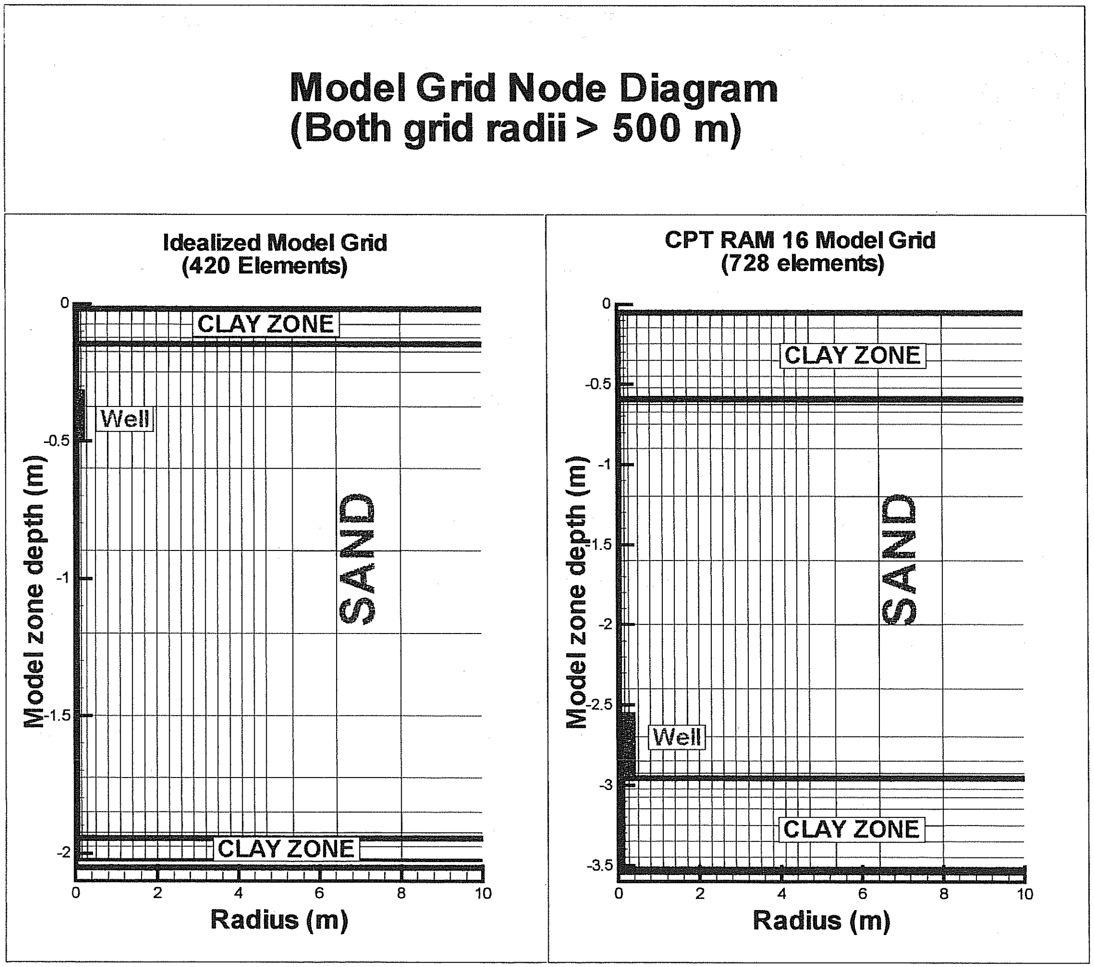

Figure 1. Model grid for simulations.

The subsurface volume was assumed to be at a steady state residual saturation based on porosity, and capillary and relative permeability parameters of the two materials, and the height above the water table with no contaminant present. Once the gas water relations were defined, contaminant in the form of a non-aqueous phase fluid was manually introduced into the system. The NAPL was assumed to be residing in the fine grain materials, held by capillary pressure. NAPL in the form of a residual saturation of approximately 0.001 was deposited in a horizontal grid row of clay residing between two layers of "clean" clay. The closed system was then allowed to come to equilibration (through diffusion for a period of five years). Relatively steady states were achieved within 30 days. The system's water, gas, and NAPL distribution at a time of one year was used as the initial condition for the modeling of barometrically produced flows in and out of a well in the otherwise closed system. The well was placed at the center of the radial system. The injection parameters were defined by dividing the total mass flow (as measured by the mass flow meter) between water and air assuming a constant temperature equivalent to the relatively constant temperature of the SRS subsurface at this depth (19 degrees C) and a relative humidity of 50%. This prevented rapid drying of the system during flow. The mass flow data were converted from slpm to kg/sec and input at the same intervals as the data were obtained, i.e., every 10 minutes.. The program was forced to solve the system matrices at least as often as the flow rate data were read (every 600 seconds). As a result, gas phase concentrations of contaminant at the well grid blocks were available for each 10 minute interval. The simulations were run on a Pentium II computer with microprocessor clock speed of 300 MHz. The average time for each simulation was approximately 6 hours. Table 1 contains the relevant grid data input to the model.

	CPT RAM 16 as built.		Model	
			Idealized	CPT RAM 16
	Elevation MSL (m)	Depth (m)	Depth (m)	Depth (m)
Ground surface.	109.0	0.0	---	---
Top of upper clay.	79.4	-29.6	0.0	0.0
Bottom of upper clay.	78.8	-30.2	-0.15	-0.6
Top of well screen.	76.6	-32.4	-0.3	-2.65
Bottom of well screen.	75.1	-33.9	-0.45	-3.0
Top of lower clay.	76.4	-32.6	-1.95	-3.0
Bottom of lower clay.	75.8	-33.2	-2.05	-3.6
Water table.	69.4	-39.6	-7.45	-10.1

Table 1. Input parameters for model.

The model concentration time plots were compared with experimental concentration time plots in an inverse modeling approach. Fitting parameters were the properties of the two different types of sediment material and the spatial distribution and amount of NAPL. Some trends in behavior became apparent after running multiple simulations, i.e., the smaller the lateral extent of the NAPL distribution, the more rapidly the decline in concentration. Similarly, the slower the diffusion through a material, the more rapid the decline in concentration given a scenario in which the well is allowed to inspire and expire. In addition, the lower the intrinsic permeability of the material, the more sensitive it was to flow variations.

RESULTS AND DISCUSSION

Model results and field data for the idealized model are compared in figure 2. From the figure, it is clear that this conceptual model accurately matches the subsurface contaminant behavior. Although this scenario depicts a sand layer with a well screen sandwiched between two clays, it is a bit different than the more realistic scenario depicted in the second simulation. In this first scenario, the well is assumed to be nearer to the upper clay and was given an effective screen length of 0.1 meters. The table of flow rates was reduced by a factor of 0.1 to compensate. DNAPL was assumed to be in the upper clay zone.

In this idealized simulation, a better match to the actual initial concentration was not attempted. The initial concentration could be increased in the model by changing the location of the DNAPL and/or the residual water saturation of the clay, (i.e., the type of clay). The model concentration and field concentration data are plotted on two different scales simply to compare the relative concentration behavior through time.

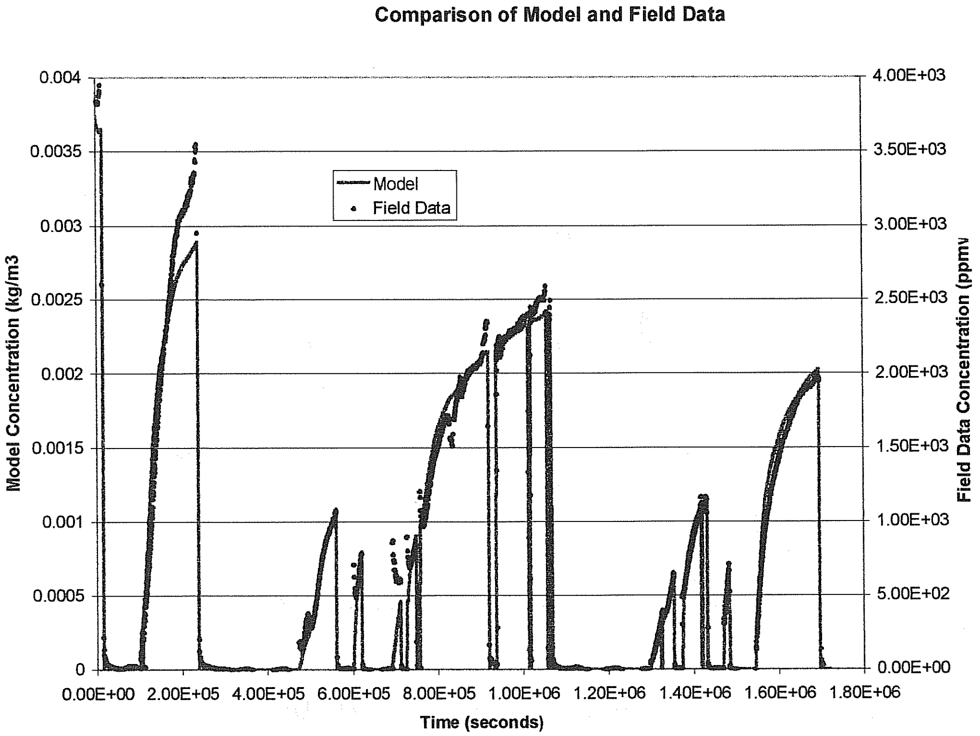

Figure 2. Idealized model comparison with field data.

The second simulation, although still somewhat idealized, more closely matched the actual subsurface conditions as measured. The clay-sand-clay interval between depths of 29.6 m and 33.2 m were matched to the well log to more accurately create the grid. The 0.35 meter long well was placed just above the clay to mimic the as-built placement of the well with approximately 1.2 meters of screen set in the clay and 0.35 meters just above in the sand. Flow rates used for this model matched the flow rates measured but were divided proportionally based on the grid block size of the well element. The DNAPL was postulated to be in the lower clay and several different combinations of materials were tested for the sand and clay zones. All of the materials were modeled after actual data of sediment samples collected at the site and analyzed in the laboratory. All of the sediment samples are from an interbedded sand and clay unit of approximately the same age.

From the close match of the model to the experimental data (Figure 3), we can conclude that the generalized conceptual model for the system is accurate. Shorter outflow events are not precisely matched but the longer intervals are well fit. The higher concentrations of the shorter intervals may be caused by small heterogeneities in the DNAPL distribution not accounted for in this simulation. The ability of the model to track the concentration profile through several in- and outflow events signifies an accurate description of the effective diffusion rate through the system and the response of the system to advective flow. Using the parameters derived from this simulation, projections of removal under various conditions can be used to determine optimum remediation strategies.

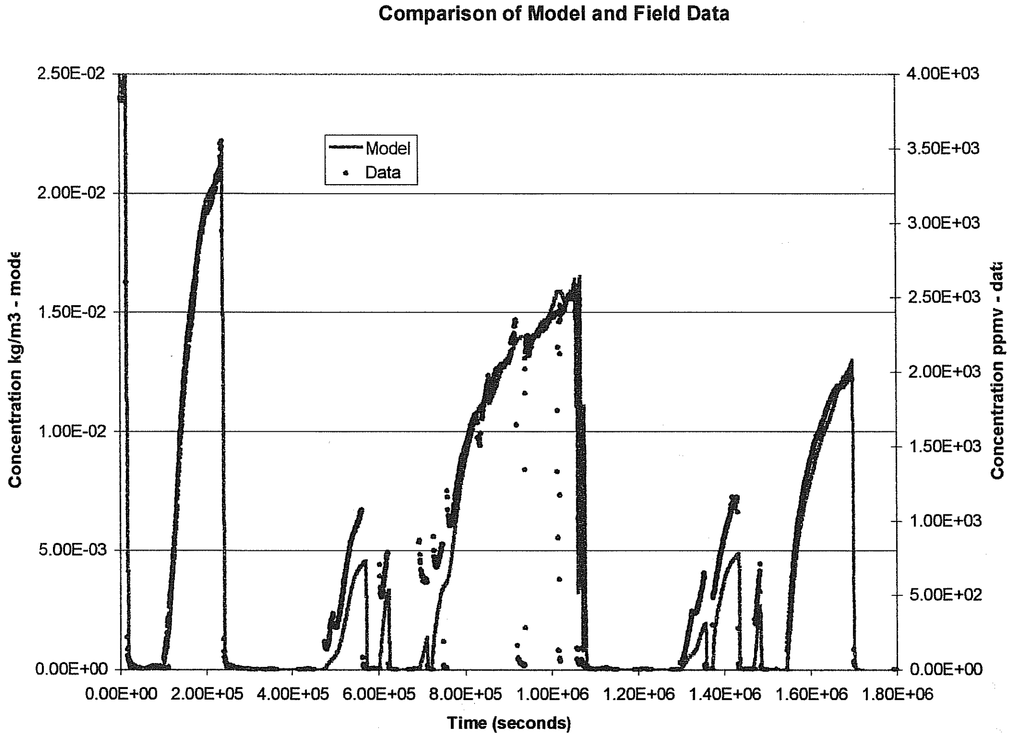

Figure 3. CPT RAM 16 model comparison with field data.

The match of the model to the data during the period when the Baroball was used to constrain flow from the subsurface to the surface and not vice versa can be used to refine the estimate of the extent of the source and relative proximity to the barometric pumping well. For example, if concentrations remain relatively constant during several cycles of outflow, we can conclude that the gaseous plume has diffused over a large volume in the more permeable zone or that diffusion through the less permeable source zone to steady state is occurring at a rate comparable to the frequency and magnitude of the volume depleted by barometric flow, or some combination of the above. Figure 4 shows the comparison between model and field data for the period when the Baroball prevented inflow. Overall, the model matches the data fairly well. The first outflow period seems to follow the behavior of the field data very closely. During the second brief outflow period (4.75E5 seconds), the model and field data do not match well. This deviation is most likely caused by the monitoring configuration. During the third outflow period, the model and field data begin to diverge. This period seems to indicate that the source may be a small distance away from the well or that there are heterogeneities of DNAPL disposition that are not accounted for in the model.

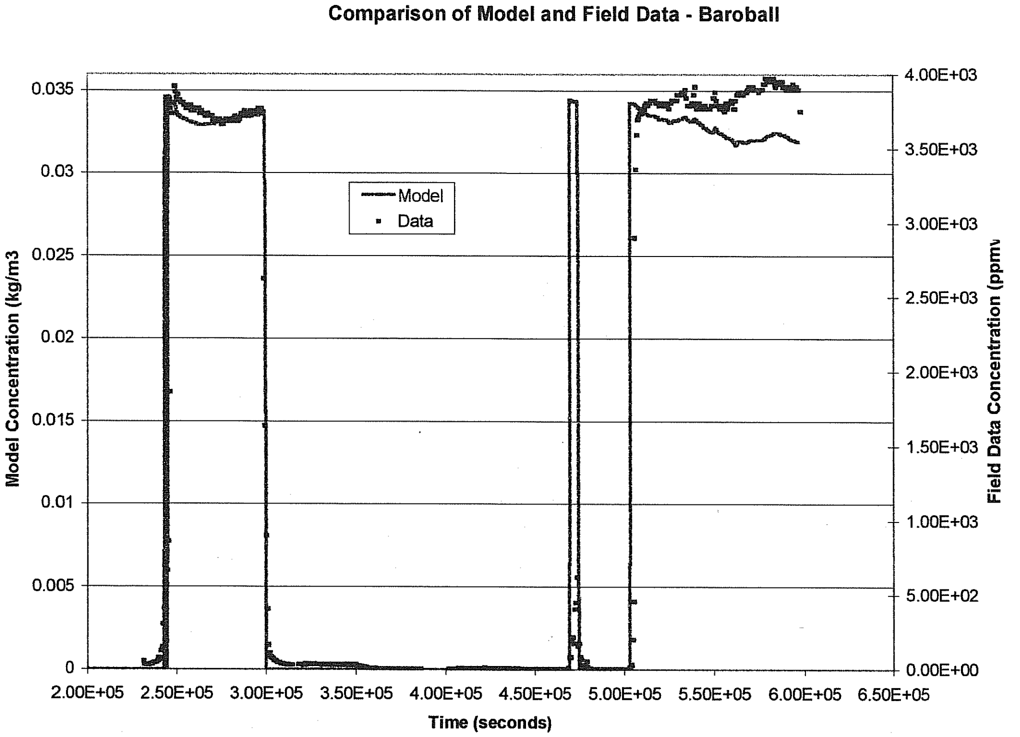

Figure 4. CPT RAM 16 model comparison with field data for Baroball operation.