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# TCE Field-Scale Simulation Using Immobile-Mobile Waste Phase Model

by

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Groundwater contamination resulting from releases of chlorinated volatile organic compounds into the environment is commonplace. Industrial solvents, such as trichloroethylene (TCE), were historically released into top soils as a means of disposal. At numerous sites nationwide, cleanup efforts are underway. To evaluate the benefits associated with proposed remediation alternatives, flow and transport modeling is playing an ever increasing role. In many situations site characterization of contaminant source terms is very sketchy, resulting in a lack of necessary data to develop a reliable source term model directly from a database. As such, investigators are forced into an approach of estimating the source term in an inverse modeling fashion.

Field-scale attempts are made here to predict the fate and transport of TCE under various remediation alternatives. Under a no action scenario, inverse modeling to establish the source term is performed where comparison to field measurements are made.

## **BACKGROUND**

The groundwater beneath the TNX Area located on the Savannah River (SR) Site is contaminated with TCE that is migrating towards the SR floodplain. The presence of dichloroethylene provides evidence that in-situ aerobic biodegradation of TCE is occurring. The initial quantity, location, and timing of TCE releases to the environment were not documented. Figure 1a shows an areal footprint of the model domain and key monitoring well locations, while Figure 1b provides a 3D perspective of the subject area.

The location of an immobile TCE source is inferred indirectly from measured dissolved TCE at wells TBG-5 and TBG-6. Surface released TCE flows by gravity downwards through the vadose zone exhausting its supply by leaving behind residual deposits. Subsequently, leaching and migration occurs into the mobile water-phase. Due to strong laterial flows within the watertable, dissolved TCE is transported down-gradient in shallow plumes of limited vertical extent. Upon reaching the SR floodplain, this plume is diverted upwards toward an engineered drainage ditch.

### **NUMERICAL MODEL**

A 3-dimensional numerical model was developed to evaluate the performance of various remediation alternatives. Each simulation involved the transport of dissolved TCE from 1988 to 2028. A modified version of the VAM3DCG code<sup>1</sup> was used. The Richard's equations<sup>2</sup> for variably saturated flow and contaminant transport were augmented using an immobile-mobile water-phase model<sup>3</sup>. A non-equilibrium mass transport formulation<sup>4</sup> was chosen for the source term. This model has been successfully demonstrated at the laboratory scale.<sup>5,6</sup>

## **CALIBRATION AND RESULTS**

A steady-state flow model was calibrated to match existing annual averaged hydraulic head data, known seepage faces, and observed flowpaths based on plume data. Hydraulic conductivities were adjusted until head differences were <3 feet. 3-dimensional particle tracking within the upper aquifer unit are presented in Figure 2a. Also shown in Figure 2a are TCE contours within the watertable for mid-year 1996.

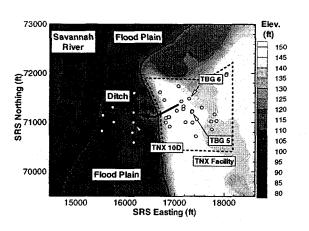
For transport modeling under a no action scenario, the source term parameters (mass transfer coefficient, initial immobile phase concentration, and location) were adjusted to match TBG-5 and TBG-6 TCE well concentrations over time. Figure 2b presents the results for these two wells along with well TNX-10D located just south of the ditch.

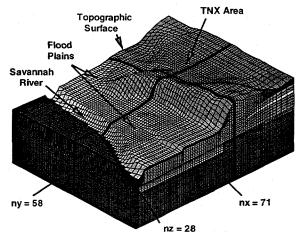
Overall, predicted TCE plumes are consistent with available monitoring data. Predicted well concentrations provide reasonable estimates for the two wells located in TNX, while predictions in the floodplain are consistently high. We believe that biodegradation is occurring at a higher rate than assumed, resulting in over estimating floodplain concentrations. An ongoing USGS project is investigating biodegradation within the SR floodplain.

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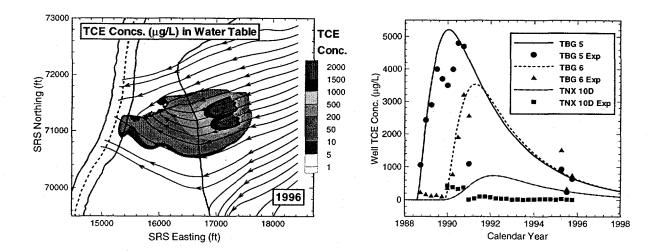




(a) Topographic surface

(b) 3D perspective

Fig. 1. TNX 3D grid showing surface features, well locations, and material zones.



(a) 1996 plume with particle tracking

(b) Well conc. comparisons

Fig. 2. flow and TCE transport results for a no action scenario case.