

SIMULATING THE SIMULTANEOUS MOVEMENT OF WATER, JET FUEL AND BTEX COMPONENTS IN SOIL

J. Zhang, Ph.D.
E. W. Harmsen, Ph.D.
IT Corporation

ABSTRACT

Soil beneath the liquid fuel storage area at a federal facility in Arizona has become contaminated with Jet propulsion fuel (JP-4). The contamination has resulted from numerous spills and leaks occurring over a period of many years. The contamination extends from the surface to the water table at a depth of 215 feet. The distribution of JP-4 and BTEX (benzene, toluene, ethylbenzene and xylene) with depth were determined during an extensive soil boring and sampling program. Geotechnical information including grain size, porosity, bulk density and vertical hydraulic conductivity were also measured as part of the field program. As part of the risk assessment to determine if soil remediation is required, a model was developed to determine if the JP-4 is still moving downward or is in an immobile residual state, and whether the BTEX components entering the aqueous phase are a potential threat to the underlying groundwater. The finite-element model for multiphase organic chemical flow and multispecies transport (MOTRANS) was employed to model water and JP-4 flow, and BTEX transport. Simulation results from 30 year simulations are presented. Estimates of the resulting groundwater BTEX concentrations are also provided. This modeling project presented numerous challenges owing to the complex nature of the problem being solved. A detailed discussion is presented on the specific difficulties encountered and recommendations are provided for solving similar problems.

INTRODUCTION

The contaminated site studied is located in Arizona. The liquid fuel storage facility has been used to store liquid fuels since 1942. Starting in 1960's, the facility was used to store jet propulsion fuel (JP-4). In 1966, when updating the fuel delivery system, approximately 3,600 linear feet of 4- and 6-inch-diameter delivery pipe that remained buried was abandoned. If full, an estimate 4,400 gallons of fuel could have been abandoned with the lines. These lines were removed along with fuel tanks in 1991. Four major spills and leaks have been documented in the

liquid fuel storage area between 1977 and 1983. In addition, three other leaks of unknown volume were reported in 1987 through 1989. Based on the size of the petroleum hydrocarbon plume and free floating JP-4 in six monitoring wells, it has been estimated that between 650,000 and 1,400,000 gallons of JP-4 may be present on the water table (approximately 215 feet deep). Fuel recovery has been ongoing since 1990. After one year's efforts, approximately 8000 gallons of fuel were recovered.

The objective of this project was to model the migration of JP-4, water and BTEX in the vadose or unsaturated zone beneath the liquid fuel storage area. Questions which needed to be addressed by the model included: Will JP-4 in the unsaturated soil continue to migrate to the water table? If so, to what extent, and what groundwater BTEX concentrations can be expected in the next 100 years. To achieve the objective of this study, a JP-4 and water flow and BTEX transport model was developed for the site employing a two-dimensional finite element computer model MOTRANS[1]. MOTRANS simulates multiphase flow (i.e., water, oil and air) in soil. In this study, only water and oil flow were simulated since air pressure gradients in the system are negligible. MOTRANS also simulates the interphase transfer and transport of up to five oil constituents within each of the three phases. In this study, the transport of the four BTEX constituents were simulated. A field program was developed prior to the modeling effort to provide field data for determination of modeling parameters. A total of 15 soil borings were completed in vicinity of the liquid fuel storage area (5.4 acres) and the samples were collected from ground surface to the water table at 5 foot intervals. The distribution of JP-4 and BTEX (benzene, toluene, ethylbenzene and xylene) as well as soil characteristics were obtained from the field data. Contamination was found to extend from the surface to the water table.

EVALUATION OF DATA AND SITE CONCEPTUALIZATION

The site conceptual model was developed based on existing data presented in the Final Remedial Investigation Report, county soil report, and field data collected as a part of the present effort. Where model parameters pertaining to the fuel flow and BTEX transport were required but unavailable from the site study, literature values were utilized.

Climate

The study area receives an average of 8.9 inches of rainfall per year. This small amount of rainfall is distributed fairly uniformly throughout the year. Water deficiency for the site is several times the average annual rainfall. Because of the small annual rainfall and large water deficiency, the potential for downward seepage of precipitation through the unsaturated zone is very small. Storms in summer tend to be intense, usually less than 30 minutes in duration, but produce little total precipitation. Some infrequent storms produce the equivalent of the entire summers average rainfall within a 24-hour period.

Maximum and minimum daily temperatures range from around 65° and 40° Fahrenheit(°F), respectively, in December and January to around 105° and 70° F, respectively, in July and August. During mid-summer, the air is extremely dry and solar heating is at a maximum. Average lake evaporation in the area is 70 inches per year. The area is considered one of the most wind-free areas in Arizona. Wind speeds remain less than 10 miles per hour (mph) throughout most of the year. Eighty-six percent of the possible sunshine is received in the area. The infiltration rate in the area was estimated to be between 0 to 1 inch per year.

Surface Soils and Subsurface Conditions

Surface soils consist of the Mohall-Contine association. This association is well-drained, nearly level loams, clay loams, and sandy clay loams on old alluvial fans. The specific mapped soil type in the liquid fuel storage area is Mohall loam. The permeability is considered moderately low, ranging from 0.20 to 0.63 inches per hour (1.4×10^{-4} to 4.4×10^{-4} centimeters per second [cm/s]). The soil moisture holding capacity of this soil is high, averaging 2.2 inches per foot of soil. Mohall loam has a moderate shrink/swell potential.

The subsurface material is characterized by alternating beds of fine and coarse grained sediment. Geotechnical information, including grain size distribution, porosity, bulk density, and vertical hydraulic conductivity, were determined as part of the field program. Undisturbed samples were collected at six depths in selected boreholes for laboratory analysis. The soil physical properties measured for the six depths are shown in Table 1. The vertical hydraulic conductivities listed were measured from undisturbed cores using a laboratory permeameter method.

The measured vertical hydraulics were much lower than typically associated with these materials. Many thin calcium carbonate cemented layers were encountered during boring which may account for the low values of vertical conductivity. A cobble zone exists between about 145 and 170 feet below land surface which appears to be highly transmissive and sufficiently well sorted so that the material is probably isotropic. An undisturbed sample could not be obtained from this interval for laboratory analysis. Based on an evaluation of boring logs and laboratory results, the soil profile was divided into five zones of different soil types or zones. Table 2 lists the soil type profile and physical properties associated with each of the soil zones. The vertical hydraulic conductivity and porosity values shown in Table 2 are average values based on laboratory data. Horizontal hydraulic conductivity was generally assumed to be one orders of magnitude greater than the vertical conductivity. However, the cobble layer was assumed to be isotropic. Other parameters given in Table 2 will be discussed below.

Hydrogeology

The upper unconfined aquifer is located approximately 215 to 240 feet below ground surface. The aquifer is underlain by a very low permeability, laterally extensive, fine grained layer, which is approximately 20 feet thick. Immediately below the confining layer at a depth of approximately 265 feet below ground surface, is a coarse-grained sand and gravel which is saturated. The underlying confined aquifer and the upper shallow unconfined aquifer do not appear to be in hydraulic connection. The shallow aquifer has excellent water-bearing capacity, however, its ability to supply water in the area has been reduced, owing to groundwater development that began in the 1940s. The hydraulic conductivity for the shallow aquifer ranges from 0.1 to 10 ft/day (4×10^{-5} to 4×10^{-3} cm/s). Groundwater flow in the shallow aquifer is from west to east. The estimated average linear velocity is 0.01 to 0.15 ft/day. The source of recharge to the shallow unconfined aquifer is probably due to infiltration of irrigation water.

JP-4 and BTEX Distribution

The movement of JP-4 and BTEX in soil is a complex process. Most chemical components of JP-4 show a low solubility in water. Consequently, JP-4 acts as a separate phase, water and air being the other phases in the soil. Movement of the oil (JP-4) is controlled by soil characteristics and the relative saturation of water and oil within the pore spaces. Simultaneous with the movement of the oil as a separate phase, chemical components of the oil which are soluble in water or volatile to a greater or lesser degree, partition into the water and air phases. In this way, components of the oil, such as BTEX may be transported to the water table with infiltrating water.

Soil Sample No.	Depth (ft)	Soil Class (USDA)	Soil Class (USCS)	Dry Density (g/cm ³)	Saturation (%)	Vertical Hydraulic Conductivity (cm/s)	Porosity (%)
1	23-24	sil. cl. loam	ML	1.86	75.7	4 x 10 ⁻⁸	30
3	23-24	loam	SM	2.05	77.3	2 x 10 ⁻⁸	22
2	83-84	silt loam	ML	1.80	79.3	6 x 10 ⁻⁷	32
4	83-84	loam	ML	1.77	62.2	7 x 10 ⁻⁸	33
5	83-84	loam	ML	1.91	70.9	--	28
6	83-84	silt loam	ML	1.61	--	5 x 10 ⁻⁷	39
8	83-84	silt loam	ML	1.57	78.5	6 x 10 ⁻⁷	40
12	83-84	loam	ML	1.67	66.3	2 x 10 ⁻⁵	37
14	83-84	loam	ML	1.57	88.4	1.8 x 10 ⁻⁵	41
18	83-84	loam	--	1.72	88.1	1.2 x 10 ⁻⁷	33
7	143-144	sand	SW-SM	2.04	48.2	1 x 10 ⁻⁷	22
9	143-144	loam	ML	1.99	91.5	1 x 10 ⁻⁷	25
13	143-144	loam	ML	2.04	44.3	1.4 x 10 ⁻⁶	23
16	143-144	loam	ML	1.78	78.8	1.2 x 10 ⁻⁶	33
20	143-144	loam	--	1.78	79.5	1.4 x 10 ⁻⁷	30
24	143-144	loam	--	1.86	69.6	1.1 x 10 ⁻⁵	31
19	173-174	loam	--	1.80	100	8 x 10 ⁻⁸	25
10	180-181	silt loam	ML	1.77	100	1 x 10 ⁻⁶	34
15	180-181	loam	ML	1.75	90.6	3 x 10 ⁻⁷	34
22	180-181	silt loam	--	1.85	50.6	--	30
11	200-201	silt loam	ML	1.67	94.5	1.7 x 10 ⁻⁷	38
17	200-201	silt loam	ML	1.57	100	2.2 x 10 ⁻⁶	40
21	200-201	silt loam	--	1.70	48.6	7.9 x 10 ⁻⁸	36
23	200-201	loam	--	1.73	66.7	4.3 x 10 ⁻⁶	34

Table 1. Physical Properties of Fuel Storage Area Soils. The samples were collected at the different locations.

The JP-4 (or total petroleum hydrocarbons [TPH]) field analytical data were provided as a concentration in micrograms of JP-4 per kilogram of bulk soil. The JP-4 concentration was measured at 5 feet intervals in all 15 soil borings. JP-4 concentration was converted to percent saturation by multiplying TPH by soil dry bulk density and dividing by soil porosity and JP-4 density. The vertical distribution of JP-4 contamination has been plotted in Figure 1 at the boring located at the center of the JP-4 plume. The JP-4 distribution is characterized by two major peaks at approximately 40 and 180 feet below the surface. The deeper peak appears to occur just below the cobble zone. The finer material between the cobble zone and the water table appears to be impeding downward to JP-4 migration.

Concentrations of BTEX components were also sampled at 5 feet intervals in the field program. The data represents BTEX in the water, oil and solid phases. Water phase concentrations of BTEX components were obtained using partition coefficients between the different phases. A similar distribution of BTEX concentrations with depth to JP-4 distribution was found at the center of the plume. Toluene and xylene concentrations in soil were significantly greater than the benzene and ethylbenzene concentrations. Benzene showed the most uniform concentration distribution of the BTEX components. Concentrations near the surface for each compound were relatively low.

Soil Type Zone	Depth (feet)	Soil Type	K_{rwx} (cm/s)	K_{rwy} (cm/s)	ϕ	S_m	S_{or}^{max}	α (m ⁻¹)	η
1	98 - 118 176 - 190	loamy sand	1×10^{-2}	1×10^{-3}	0.28	0.15	0.15	4.0	2.3
2	72 - 85 118 - 145 203 - 215	loam	1×10^{-3}	1×10^{-4}	0.35	0.16	0.15	1.26	1.6
3	0 - 72 85 - 98 190 - 203	silty loam	1×10^{-4}	1×10^{-5}	0.30	0.16	0.15	0.45	1.4
4	145 - 176	sand	1×10^{-2}	1×10^{-2}	0.32	0.09	0.15	4.15	1.95
5	215 - 241	loamy sand	2×10^{-3}	2×10^{-4}	0.30	0.15	0.15	1.84	2.3

Table 2. Soil Physical Properties Used in the Computer Model. K_{rwx} is horizontal hydraulic conductivity, K_{rwy} is vertical hydraulic conductivity, ϕ is porosity, S_m is residual moisture saturation, S_{or} is maximum residual oil saturation for water imbibition, α and η are van Genuchten air-water capillary retention parameters.

probably due to increased biological activity and volatilization. Around 190 feet below the surface, all BTEX components increased. Xylene showed the largest increase in concentration reaching a maximum value of over 600,000 $\mu\text{g}/\text{kg}$.

MODEL DEVELOPMENT

Preliminary Modeling Approach

The preliminary model was developed to simulate the JP-4 plume with the highest concentration. The plume was assumed to be radially symmetric and the multiphase and multicomponent transport were simulated in a radially symmetric vertical section. The initial JP-4 saturation and concentrations of BTEX components were interpolated from data obtained from 5 soil borings. The origin of the coordinate system was located at the center of the plume. A uniform grid spacing of 2 meters was assigned to both vertical and radial directions. The simulation region is a cylinder with a radius of 48 meters and a height of 68 meters. A total number of 875 nodes were used in the finite element mesh. Due to the size of the grid system, and also because seven coupled differential equations were required to be solved simultaneously, tremendous computation effort was required. A 486DX-66 personal computer system was employed for the simulation. After seven days of continuous run time, a five-year simulation was completed.

The calculated JP-4 and BTEX distributions showed that there was no significant movement of the plume in the horizontal direction. Whereas the plume exhibited downward migration towards the water table. In order to

increase the efficiency of the modeling effort, the preliminary model was converted to a one-dimension model to simulate vertical movement of JP-4 and BTEX only.

Model Parameters

The required input for flow analyses consist of initial conditions, soil hydraulic properties, fluid properties, boundary condition data and mesh geometry. Three-phase permeability-saturation-capillary pressure relations are defined by an extension of the van Genuchten model. The model requires specification of parameters defining the air-water capillary retention function, nonaqueous phase liquid (NAPL) surface tension and interfacial tension with water, NAPL viscosity, NAPL density, maximum residual NAPL saturation and soil hydraulic conductivity. The model allows for anisotropic conditions and spatial variation of soil properties. For transport analysis, additional input data were porous media dispersivity, initial water-phase BTEX concentrations, component densities, diffusion coefficients, first order decay coefficients, mass transfer coefficients (non-equilibrium analyses) or partition coefficients (equilibrium analyses) and boundary conditions.

Soil hydraulic properties used in the model are listed in Table 2. Soil vertical saturated hydraulic conductivity (K_{rwy}), porosity (ϕ) and texture (i.e., soil type) were determined by laboratory analyses of soil samples and boring log data collected at the site. The parameter S_m (irreducible water content) and η (van Genuchten air-water capillary retention parameter) for similar type soils were obtained from the literature[1]. The values of α (van Genuchten air-water capillary retention parameter) used in

Bulk Fluid Properties:				
β_{ao}	= 2.5	β_{ow}	= 1.66	
η_{ro}	= 0.84	ρ_{ro}	= 0.75	
Dispersion Parameters:				
A_L	= 1 m	A_T	= 0.5 m	
Component Properties:				
	Benzene	Toluene	Ethylbenzene	Xylene
D_{oa}	0.76	0.68	0.61	0.61
D_{ow}	9.42×10^{-5}	8.21×10^{-5}	6.21×10^{-5}	6.21×10^{-5}
D_{oo}	1.12×10^{-4}	9.75×10^{-5}	7.37×10^{-5}	7.37×10^{-5}
Γ_{oa}	0.23	0.28	0.306	0.26
Γ_{oo}	493	1683	5703	5789
Γ_{os}	.015	.015	.015	.03

Table 3. Bulk Fluid Properties, Dispersion Parameters, and BTEX Component Property Data Used in Computer Model. β_{ao} and β_{ow} are the air-oil and water capillary retention scaling factors, respectively. A_L and A_T are longitudinal and transverse dispersivity, respectively; D_{oa} , D_{ow} , and D_{oo} are air, water, and oil diffusion coefficients, respectively; Γ_{oa} , Γ_{oo} , Γ_{os} are the air, water, oil-water, oil-water and solid-water partition coefficients.

the model were calculated from the following relation given by ES&T[1]:

$$\alpha = (K_{ow}/0.5)^{1/2} \quad (\text{Eq. 1})$$

The maximum residual oil saturation for water imbibition (S_{or}^{max}) defines the maximum relative percentage of oil that can become trapped in the water phase. The typical range of (S_{or}^{max}) is 0.15 to 0.35[1]. In the simulation, a value of 0.15 was used. This lower value tends to be more conservative because more oil will be available for leaching.

Longitudinal dispersivity (A_L) is a parameter which represents the degree of mechanical dispersion and has been correlated with the scale of the contaminant plume[2]. The vertical travel distance at the site is approximately 200 feet. Gelhar et al. [2] present a plot of longitudinal dispersivity for unsaturated soils versus plume scale. For a travel distance of 200 feet (66 m), longitudinal dispersivity is about 1 m or 3.3 feet. A value of 1 m was used in the model.

The bulk fluid properties, dispersion parameters and BTEX component properties used in the computer model are shown in Table 3. JP-4 properties were obtained from the Installation Restoration Program Toxicology Guide published by A. D. Little, Inc.[3]. The report lists the physical-chemical properties for a typical JP-4 jet fuel. Values of the capillary curve scaling factors, β_{ao} and β_{ow} ,

were calculated as functions of the oil and water surface tensions and the oil-water interfacial tension. Average values of the BTEX diffusion coefficients in air and water (D_{oa} , D_{ow} , respectively; the symbol α refers to the BTEX component) were obtained from ES&T [1]. The diffusion coefficient of BTEX in oil (D_{oo}), were calculated by dividing the BTEX diffusion coefficients in water by the relative oil viscosity [1].

In this study the partitioning of BTEX between the water, oil, air and soil were assumed to be equilibrium processes. The air-water, oil-water and solid-water partition coefficients are listed in Table 3 as Γ_{oa} , Γ_{os} , Γ_{os} , respectively. These parameters are commonly known as Raoult's constant, Henry's law constant, and the distribution coefficient (k_d). Alternatively, the model allows specification of kinetic rate coefficients. However, these data are not available to allow this type of simulation. Data presented by ES&T [1] suggest that for the typical rate of movement of oil and BTEX in the soil, the equilibrium assumption is quite satisfactory. Furthermore, the assumption of equilibrium conditions will provide a

more conservative result in terms of a risk evaluation. The values of Γ_{oo} and Γ_{os} in Table 4 were obtained from ES&T[1]. The values of Γ_{os} was calculated from total soil organic carbon data collected as part of the field program

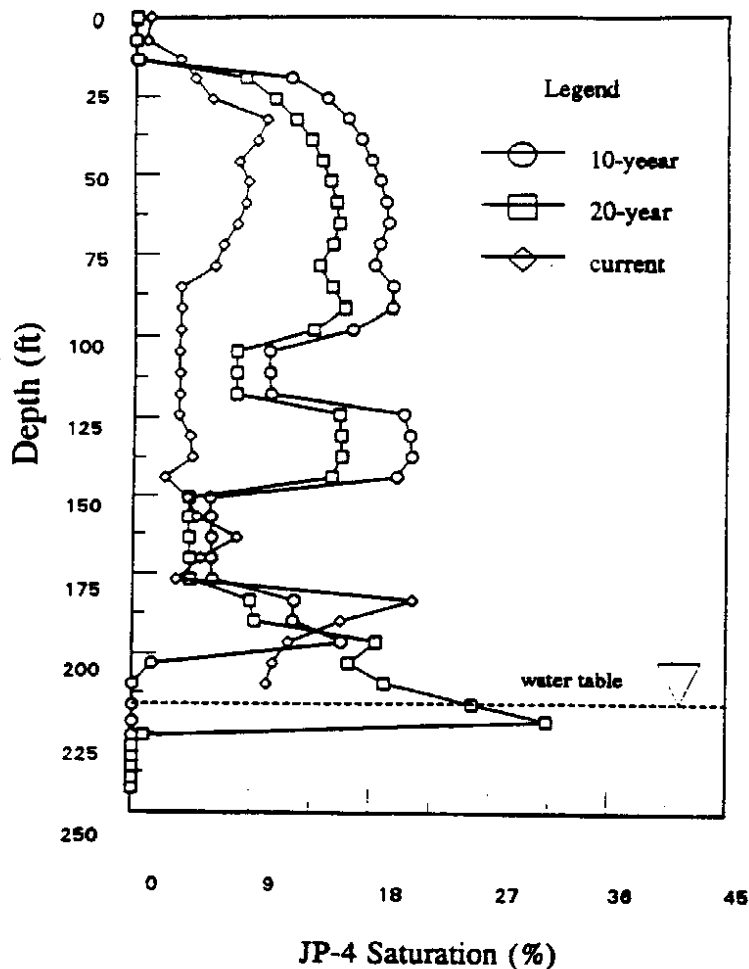


Figure 1. Simulated JP-4 saturation with depth at times 10- and 20-years after leaking began. Current JP-4 saturation obtained from the field program was plotted for comparison.

and organic carbon partition coefficients (k_{oc}) obtained from the literature[3]. The average total organic carbon content of the soil was extremely low (0.014 percent). Consequently, the dimensionless distribution coefficient values (T_{oc}) were very low. Using the estimated k_d values and applicable values of soil bulk density and porosity to calculate retardation factors, resulted in a maximum value of 1.14. This low value of retardation coefficient suggests little or no solute partitioning to the soil material.

The first order decay constants for BTEX in air, oil and water μ_{air} , μ_{oil} , μ_{water} respectively, were set to zero during the simulations. Under certain conditions, degradation of BTEX in soil is known to occur, however, chemical and biological processes controlling the degradation process are very complex. Therefore, decay of BTEX was not simulated in this study. As with the assumption of equilibrium partitioning, assuming zero decay will provide a more conservative result in terms of risk evaluation. Because BTEX can not leave the system via decay, the estimated groundwater BTEX concentrations will tend to be higher.

Model Calibration

The vertical hydraulic conductivity values obtained from laboratory analysis (Table 1) are much lower than typical associated with these materials. The question arises, if these values were used, can the model simulate JP-4 to the water table in 30 years, as is known to have actually occurred at the site? Another parameter, the infiltration rate from precipitation, needs also to be determined in the model calibration. The migration of JP-4 and BTEX is very sensitive to this parameter as shown in the preliminary modeling effort.

Since the actual JP-4 spill and leaking pattern versus time was complex and unknown, the simulation was simplified to two stages. In stage 1, JP-4 leaking to oil-free soil from a pipe 15 feet under the ground surface was simulated. The leaking JP-4 was represented by a constant oil head node under a water-equivalent oil head of -0.1 m. In stage 2, the leaking was terminated and JP-4 migrated under natural gradient. BTEX transport was not considered in stage 1. The soil water content in the region, was only determined at six depths in the field program (Table 1), and was characterized by significant variability.

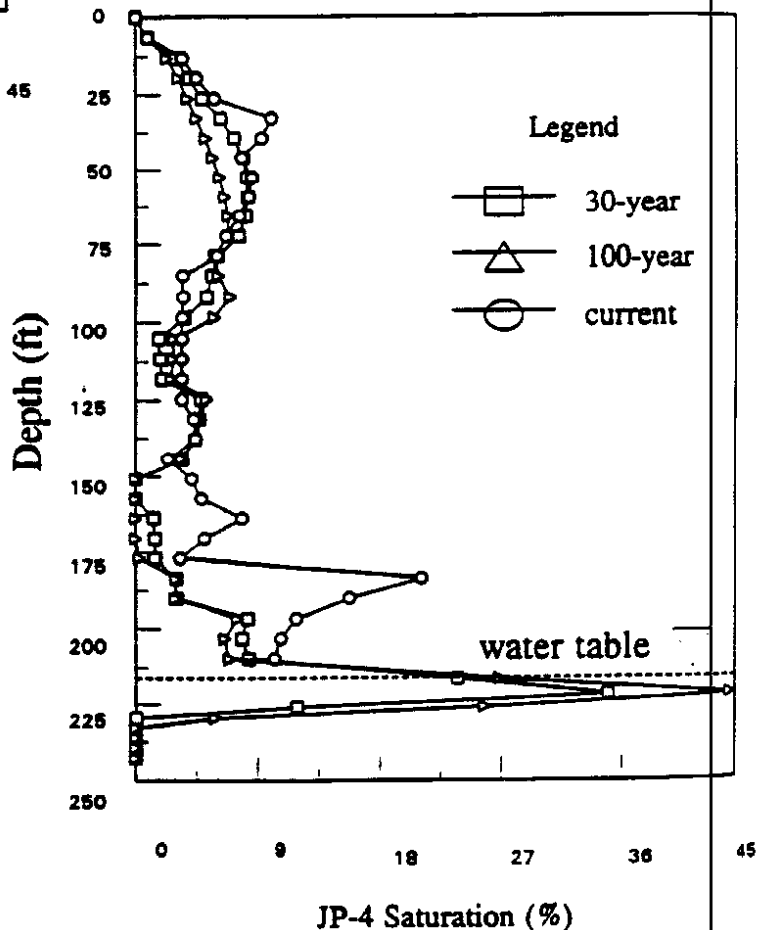


Figure 2. Simulated 30-year, 100-year and initial JP-4 saturation with depth.

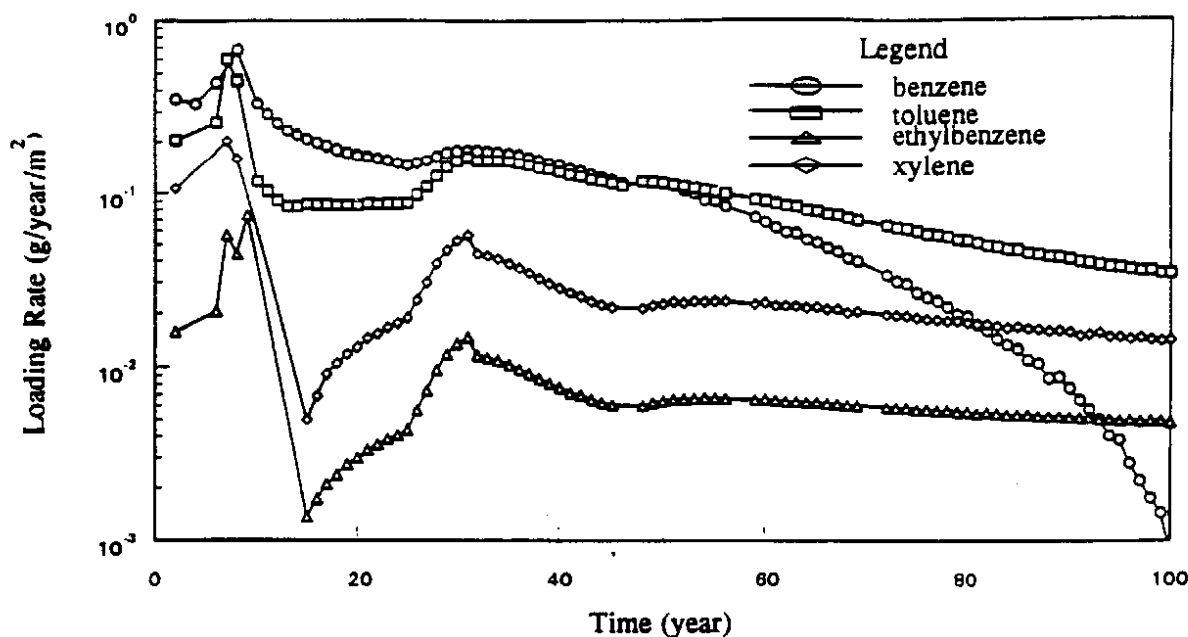


Figure 3. Estimated water phase BTEX loading rate to the groundwater system as a function of time for the next 100 years.

Therefore, to produce the initial water saturation distribution for the model, long term simulations with water flow only, were performed in order to obtain the steady-state water saturation distribution. This simulated vertical distribution was then used as the initial water saturation condition for the multiphase flow simulation. A constant head of 25 feet was assigned to the two lowest element nodes 241 feet below the surface. This resulted in the water table being located at approximately 216 feet below the ground surface. Using a constant head boundary at the bottom of the model allowed water to leave the system if seepage from the unsaturated zone resulted in a build-up of hydraulic head in the aquifer greater than 25 feet.

The earliest spill or leak of JP-4 may have happened around the later 1960s or early 1970s. The shallow groundwater system is seriously contaminated by JP-4 currently. Therefore, a reasonable time scale for JP-4 reaching the water table should be less than 20 years. In the first calibration attempt, laboratory hydraulic conductivity values were used and the duration of stage 1 was extended to 20 years. During this period, JP-4 infiltrated less than 8 meters, which implied that the laboratory values were too low. Finally, when hydraulic conductivity values in the vadose zone were increased to a factor of 100, JP-4 migrated to the water table after 15

years, and the duration of stage 1 was 2.2 years. An infiltration rate of 0.5 inch per year was used and the distribution of steady state water content reasonably matched the field data. Figure 1 shows the distribution of JP-4 with depth at 10 years and 20 years after the leak began. The pattern of the 20-year JP-4 distribution, approximately matched the current JP-4 distribution at the site.

JP-4 and BTEX migration

Long-term flow and transport simulations were performed to evaluate the likelihood of JP-4 and BTEX migration to the water table. Performing long-term simulations provided temporal information from which potential trends (e.g., increasing or decreasing groundwater BTEX concentrations) could be considered.

Figure 2 shows the calculated percent JP-4 saturation with depth after 30 years and 100 years using the calibrated model. The initial JP-4 saturation is also plotted for comparison purposes. Since there was no JP-4 saturation data available in the saturated zone, only initial data in the vadose zone were plotted. In the simulation, JP-4 contamination in the groundwater system was assumed to be removed, and the model only simulated the JP-4 and BTEX migration to groundwater system. The results indicate that from the surface to about 140 feet depth there

was less JP-4 movement. It would appear that the JP-4 in this zone, under the specified conditions (i.e., 0.5 in/year recharge), is close to a residual, immobile state and does not represent a serious threat to the groundwater. In the region of the cobble zone (145 to 175 feet depth) and the region underlying (loam sand, 175 to 200), there was an apparent decrease in oil saturation. The net result of the JP-4 movement was a build up of JP-4 floating on the water table. The JP-4 saturation at the water table increased to 45% by the end of simulation.

Figure 3 shows the estimated loading rate of the water phase BTEX components into the groundwater system with time. Benzene, the most soluble of the constituents, exhibited the maximum loading rate in the first 40 years, and then drastically decreased by two orders of magnitude by the end of simulation. The other BTEX components also demonstrated a steady decrease in their loading rates to the groundwater system after 50 years. The loading rate peaks correspond to the higher concentration of BTEX arriving at water table. The loading rate shown here only represents the impact of the center of JP-4 and BTEX plumes to the groundwater system. In order to assess the threat of the entire plume, the same calculation must be performed for other locations where field data are available. The loading of the plume at the different locations can be interpolated. Utilizing this loading as input to a separate model which simulates the flow and transport in the saturated region, the concentration distribution of BTEX components in the groundwater system will be calculated.

Summary and Comments

A model was developed to simulate the migration of JP-4, water and BTEX in soil at a liquid fuel storage area in Arizona. Due to the minimal potential lateral migration, a one-dimensional (vertical) model was developed. The multiphase flow and multicomponent transport model MOTRANS was used. The area modeled represented the area of highest contamination at the site. Soil information, initial JP-4 saturation and BTEX concentrations were obtained from the field program and used in the model. Assumptions were made (e.g., no BTEX decay and equilibrium chemical partitioning) in developing the model which tended to lead to more conservative results for the purposes of risk evaluation.

Based on a comparison of the simulated and field-measured soil water saturation data, the actual infiltration rate at the site is estimated to be around 0.5 inch per year. Model calibration suggested the effective hydraulic conductivity should be much higher than that laboratory analysis provided. The results of the simulation showed that minimal JP-4 migration occurred within the top 140 feet of the soil profile over the 100-year simulation. JP-4 migration did occur in the lower half of the soil profile, resulting in product ponding on the water table. The BTEX

component loading rates to the groundwater system were estimated. Based on the simulation results, a potential threat to the groundwater system from JP-4 and BTEX in the vadose zone may exist in the future.

Great computational effect is required when using MOTRANS due to the complex nature of simulating simultaneous multiphase flow and multi-component transport in soil. A simplified model should be developed first to ensure that the simulations can be completed during a reasonable period. Numerous parameters are required for this type of simulation. Some can be obtained from the site investigation. Some may only be found from a literature review. Uncertainty in the estimate of these parameters induces uncertainty in the modeling results. A series of sensitivity analyses must be performed in combination with the model calibration to narrow down the uncertainty. The model then can be gradually increased in complexity to simulate more realistic conditions.

REFERENCES

- 1 ES&T, MOTRANS A Finite Element Model for Multiphase Organic Chemical Flow and Multispecies Transport, Technical and User's Guide, 1992.
- 2 Gelhar, L.D., Mantoglou, A., Welty, C., and Rehfeldt, K.R., A Review of Field-Scale Solute Transport Processes in Saturated and Unsaturated Porous Media, EPRI EA-4190, Project 2485-5, 1985.
- 3 Montgomery, J.H. and L.M. Welkom, Groundwater Chemicals Desk Reference, Lewis Publishers, Inc., 1989.