

EVALUATION OF COMPUTER MODELS FOR PREDICTING THE FATE AND TRANSPORT OF HYDROCARBONS IN SOIL AND GROUNDWATER

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SUMMARY

This report was prepared by MDH Engineered Solutions Corporation (MDH) for Alberta Environment (AENV) to document Phase I through Phase III of a three-phase project to evaluate computer codes applied to predicting the fate and transport of hydrocarbons in soil and groundwater.

The first stage of the process consisted of a literature review to identify modelling codes applicable to the simulation of natural attenuation of various groups of hydrocarbons for typical Alberta soils, landscape and climatic conditions. A database was constructed based on readily available documentation, some discussion with model developers, and in-house expertise and experience of MDH personnel. The results of the review identified over 250 software packages.

During Phase I, an initial ranking matrix was devised to assist in determining the functionality of the codes. Over 130 codes were initially rated on a scale of 1 to 10 to determine their ability to model the fate and transport of hydrocarbons in groundwater and soil. Results from the preliminary review of the models indicated that there was no single model that would be suitable for all the possible scenarios applicable to the fate and transport of hydrocarbons.

Discussion with AENV personnel resulted in a modification of the scope of the project to more precisely define their specific requirements. Processes identified as important included volatilization, degradation, sorption, and transport within the saturated zone. The code was required to be capable of simulating 3D movement of hydrocarbons by advection, dispersion and diffusion. A model that can incorporate heterogeneity and irregular geometries was also required, given the variability of the surficial geology in Alberta. The modelling of free product (LNAPL or DNAPL) was not considered to be critical, as it was not expected to be a typical contaminant phase at the sites where the codes will be applied. Because monitored natural attenuation (MNA) remedies require source management, LNAPL (a potential source of dissolved phase contamination) should ideally be removed. Finally, for the volatilization component of the modelling, the scope was limited to an evaluation of what component of the hydrocarbon might partition into the vapour phase, rather than a full analysis of vapour transport.

Phase II of the project involved rating modelling codes based on 17 objective criteria. The rationale of the ranking scheme and the weighting of the 17 components are detailed in this report.

All the highly ranked codes were suitable for modelling the fate and transport of hydrocarbons if vapour phase transport was excluded as a requirement. During the ranking procedure, limited emphasis was placed on the ability to account for vapour/solid/liquid partitioning. Typically, codes that are designed to predict vapour phase partitioning are not designed to simulate the movement of dissolved hydrocarbons in both the unsaturated and the saturated zones. MDH initially recommended that a separate code be used to determine the amount of hydrocarbon that partitions into the aqueous and vapour phases.

TOUGH2v2 (T2VOC) was the only code that would simulate vapour phase transport and still allow the user to simulate unsaturated/saturated 3D conditions. TOUGH2v2 (T2VOC) was

purchased by MDH for further evaluation during Phase III. The principal objective of Phase III was to document the strength and weaknesses of TOUGH2v2 (T2VOC). A generic scenario was derived from examples provided in the TOUGH2v2 (T2VOC) users manual.

The results from TOUGH2v2 (T2VOC) were verified against the widely used and established FEMWATER code. Both codes performed well but gave somewhat different results. Differences in the results were expected given the differences in the application of boundary conditions, description of sources, the ability to model vapour phase transport (not accounted for in FEMWATER), and element geometry. The trials performed using T2VOC (an adaptation of TOUGH2v2 for modelling volatile organic compounds) were restricted to establishing the ease-of-use of the code and verification of the code against a “standard” model for saturated-unsaturated flow. MDH recommend that T2VOC be further evaluated by application to “real world” problems but initial results suggest that the code (and its successor TMVOC) have the potential capabilities to predict the fate and transport of many fractions of oil F1 (C₆-C₁₁), F2 (C₁₁-C₁₆), F3 (C₁₆-C₃₄), and possibly F4 (>C₃₄) petroleum hydrocarbons (PHC) together with many refined products.

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This project was funded by the Water Research Users Group, Alberta Environment.

1.0 INTRODUCTION

This report was prepared to document Phase I through Phase III of a project to research computer codes for predicting the fate and transport of hydrocarbons in soil and groundwater for Alberta Environment (AENV). The project evaluates a wide range of existing computer codes for their ability to predict the shallow movement of hydrocarbons in soil and groundwater.

During Phase I and Phase II of the project, a two level ranking procedure was used to compare over 250 codes. The first stage of the process was based on review of readily available documentation and in-house expertise and experience of MDH personnel. A pre-screening stage eliminated over half of the codes. The remaining codes were ranked based on 17 objective criteria. The most highly ranked codes were further evaluated to determine which code would be most applicable to the AENV hydrocarbon release scenarios. TOUGH2v2 (T2VOC) was the code recommended for detailed analysis in Phase III.

Phase III evaluates the TOUGH2v2 (T2VOC) code for its ability to predict movement of hydrocarbons in the subsurface. The code was evaluated against another independent, saturated-unsaturated flow and transport code. This report compares the performance of TOUGH2v2 (T2VOC) and FEMWATER for one generic scenario.

The principal objective of Phase III of the project was to document the strengths and weaknesses of each code for a specific task of simulating the transport of hydrocarbons in soil and groundwater in climatic regimes characteristic of the Alberta Foothills and Prairies.

2.0 SCOPE

The scope of the project was to compile a list of numerical computer codes that are suitable for site-specific risk assessment or for the development of generic risk-based scenarios that can be used to guide remediation of soil and groundwater. The project is divided into three phases:

- Literature review and code identification;
- Initial screening and comparative ranking of codes; and,
- Generic code testing.

This report contains the literature review and code identification portion (Phase I), the ranking matrix portion (Phase II), and the testing and evaluation portion (Phase III) of the project.

3.0 RISK-BASED CORRECTIVE ACTION (RBCA) PROCEDURES

Risk-Based Corrective Action (RBCA) integrates United States Environmental Protection Agency (EPA) risk assessment practices with traditional site investigation and remedy selection activities in order to determine cost-effective measures for protection of human health and environmental resources. The ultimate endpoint of the RBCA planning process is the cleanup/closure of sites in an expedient, protective, and cost-effective manner. The purpose of this section is to place the model evaluation process in the RBCA context.

3.1 RBCA Applied to Hydrocarbon Components

Under this integrated approach, hydrocarbon release sites are characterized in terms of sources, transport mechanisms, and receptors. Remedial measures are then applied as needed to prevent environmental exposure to harmful levels of contaminant. Such risk-based corrective action can be achieved by addressing any step in the exposure process:

- Removing or treating the source;
- Interrupting contaminant transport mechanisms; and,
- Controlling levels at the point of exposure.

Under RBCA, risk management strategies are developed and implemented as a standardized procedure. Based upon available site information, a site classification step is first completed to characterize the relative magnitude and immediacy of site risks and prescribe immediate response actions. After any short-term hazards have been properly addressed, risk-based cleanup standards are developed to protect against potential environmental impacts associated with long-term exposure to low levels of contaminants.

To provide for economical use at both small and large facilities, the RBCA process is designed to match the planning effort to the relative risk or complexity of each site. For this purpose, a tiered approach is employed for calculation of risk-based cleanup levels, involving increasingly sophisticated levels of data collection and analysis. Upon completion of each tier, the user reviews the results and recommendations and decides if further analysis is required. To achieve the final risk management goals, the remedial action program may involve:

- Source removal/treatment;
- Containment measures;
- Institutional controls; or,
- Some combination of all three.

RBCA represents a risk management system that must be customized to fit the specific environmental concerns and legal/regulatory constraints of each provincial or federal regulatory program.

3.2 Model Evaluation for RBCA

Modelling is an integral part of the RBCA procedure. To facilitate efficient processing of site remediation/closure applications, clear guidance is required regarding pre-approved modelling and risk characterization protocols. A tiered approach is recommended. An overview of the recommended tiered approach is provided in Section 3.2.1 through Section 3.2.3.

3.2.1 Tier 1 Assessment

At this very preliminary level, only an estimate of maximum concentrations and total mass at the point of exposure (POE) and identification of receptors are required. A simple look-up table might be sufficient to decide whether the maximum concentration and/or total mass, or the site and/or the specific receptors, justify Tier 2 analysis.

3.2.2 Tier 2 Assessment

At this level, the affected porous media needs to be delineated together with determination of the site-specific transport processes and pathways from POE to receptor. Simple analytical models can be applied to screen site-specific cases. Simple analytical models form a basis for the decision whether or not to proceed to Tier 3 analysis.

3.2.3 Tier 3 Assessment

For a Tier 3 assessment, the affected porous media needs to be delineated further together with more thorough determination of site-specific transport processes and transport pathways from POE to receptor. Numerical models can be applied at this level to investigate the extent of the problem and evaluate remediation alternatives.

4.0 COMPILATION OF SOFTWARE LIST

A two stage screening process was adopted. For the first stage, a comprehensive list of codes was assembled together with readily available documentation. The codes were reviewed for their applicability to the specified AENV scenarios and their costs. At this stage, a large number of codes were eliminated based on generic pre-screening criteria as determined by MDH. The Stage I pre-screening is discussed in Section 4.1

For the second stage, a preliminary ranking matrix was created, with particular emphasis on their ability to meet AENV criteria for modelling hydrocarbon movement. The Stage II matrix is discussed in Section 4.2.

4.1 Literature Review and Pre-screening

The investigation involved a literature review to locate available codes that appeared to be applicable to hydrocarbon fate and transport modelling. Software included in the list was located from the review of readily available model documentation, some search on the internet, and the in-house expertise of the assembled MDH team who have utilised and previously compared many of the available software packages.

At this stage a large group of codes were not included in the list because they were considered inappropriate for the intended application:

- Models with no solute transport capabilities (flow only) were not included;
- Models primarily designed for surface water flow were not included;
- Geochemical speciation models with limited or no flow simulation capabilities were not included;
- Codes that were primarily databases or pre-and post-processing interfaces were not included; and,
- Heat flow codes and codes concerned primarily with evapotranspiration only were not included.

The software packages excluded during this phase of the project are listed in Appendix A. A comprehensive list of the modelling codes that remained after this preliminary screening process will be discussed further in section 4.3 and are listed in Appendix B.

MDH would like to emphasise that elimination of codes should not be interpreted as an indication that those codes are in any way defective or inadequate. Codes were ranked against specific criteria, judged to be important for application to a specific set of practical problems.

4.2 Phase II Ranking Matrix

Once hydrocarbons enter the groundwater system, they have the potential to be transported long distances to possible receptors such as lakes, streams, and water supply wells. The rate at which hydrocarbons will reach the receptor will be dependent upon the geology, hydrology, and degradation kinetics of the PHC.

The ranking matrix took into consideration factors such as biodegradation of the compounds in a contaminant plume, dispersion, diffusion, geometric dilution of contaminant concentrations, and limitation by sorption processes. BTEX mass loss from groundwater to the unsaturated zone due to volatilization and anaerobic degradation in the capillary zone is another factor contributing to natural attenuation. Most 3D models that simulate both the unsaturated and saturated zones, adsorption, decay and biodegradation do not simulate volatilization. These codes still ranked highly because a pre-processing step could be developed using a simple code to estimate volatilization losses.

The scope of Phase II did not account for aqueous phase density dependent flow. In order to have any density effect, there must be a density contrast between contaminated water and fresh water. If there is not significant contrast between the contaminated water and fresh water, then the problem is essentially a normal transport problem involving advection, hydrodynamic dispersion, and diffusion. After discussion with AENV, it was concluded that the density gradients would be small for the scenarios being considered, and therefore, density dependent aqueous phase flow could be neglected. This does not imply that multiphase segregation would be neglected, but such processes are clearly excluded in single-aqueous-phase codes.

An initial ranking matrix with the following summary criteria was proposed to complete the initial screening of the software list created during Phase I:

- Mass balance (Chemical/Water);
- Flow model (Unsaturated/Saturated);
- Transport mechanisms;
- Biodegradation models;
- Sorption/volatilization;
- Dimensionality;
- Domain variability;
- Mesh flexibility;
- Data requirements;
- Computational requirements;
- Program availability;
- Source code availability;
- Program installation;
- Code validation;
- Code Support;
- Documentation quality; and,
- Ease of use.

Each code was rated on a scale of 1 to 10 for each of the above criteria. An objective weighting factor can be applied to each of the criteria to customize the matrix to the requirements of specific scenarios that are expected to be modelled. A default ranking value of 5 was applied if information on a particular category was unavailable without purchasing the program. The proposed ranking scale for each criterion is provided in Tables B1 to B16 in Appendix B.

TOUGH2v2 and FEMWATER were chosen for further analysis in Phase III. TOUGH2v2 was the only code that would simulate vapour phase transport and still allow the user to simulate unsaturated/saturated 3D conditions. FEMWATER was selected as a typical single-aqueous-phase transport code that would simulate unsaturated/saturated 3D conditions, but only tracks dissolved mass in the aqueous phase.

TOUGH2v2 (Pruess et al. 1999) is 3D finite difference program including numerous equations of state modules for gas pressure-volume-temperature (PVT) relationships. The T2VOC module (Pruess et al. 1995) was used for this analysis. T2VOC is a three-dimensional numerical simulation program that models the transport of organic chemical contaminants in non-isothermal multiphase systems (Pruess et al. 1995). The code was designed to simulate processes such as the migration of hazardous non-aqueous phase liquids in variably saturated media, evaporation and diffusion of chemical vapours in the unsaturated zone, and direct pumping of contaminated water and free product. T2VOC is specialized module for TOUGH2v2, and is used in conjunction with and as part of the TOUGH2v2 program. A more advanced module TMVOC is also available to simultaneously track multiple components. TMVOC was not evaluated in this study. TOUGH2v2 was developed and is maintained by the Lawrence Berkley National Laboratory (LBNL) and distributed by the U.S. Department of Energy.

FEMWATER (Yeh et al. 1992) is a 3D finite element program. FEMWATER simulates the transport of organic and inorganic contaminants in a single aqueous phase system. The code was designed to simulate processes such as the migration of contaminants in variably saturated media, with Fickian diffusion and dispersion of contaminant in the saturated zone. FEMWATER is a public domain code that can be used with GMS, the U.S. Department of Defence graphical interface. FEMWATER is currently maintained by the U.S. Army Corp. of Engineers, Waterways Experiment Station (WES).

Both FEMWATER and TOUGH2v2 are high-quality computer codes developed and maintained through research programs funded by the U.S. government. They have been extensively validated and verified by a wide range of government agencies, consultants and universities.

5.0 CODE EVALUATION

For the third phase of the project, the computer codes TOUGH2v2 (T2VOC) and FEMWATER were evaluated for their applicability for modelling hydrocarbon movement mainly in the saturated zone. TOUGH2v2 was verified against the FEMWATER code because it is a widely established code typical of many saturated / unsaturated flow codes commonly used in modelling groundwater contamination. The results from Phase III are discussed in Section 5.1.

5.1 Phase III – Code Evaluation

The scope of Phase III of the project was to:

- 1) Evaluate two numerical codes that were highly ranked in the pre-screening process.
- 2) Develop generic risk based scenarios to illustrate movement of hydrocarbons in the subsurface accounting for:
 - Biodegradation;
 - Sorption; and,
 - Advection / dispersion.
- 3) Provide a report documenting:
 - Information requirements for each generic scenario;
 - Ability of the codes to simulate the scenario;
 - Ease of use of each code; and,
 - Major strengths and weaknesses of each code.

5.1.1 *Generic Scenario*

The preliminary generic scenario comprised a simple 3D mesh with a water-soluble contaminant. The initial comparison was completed using this generic scenario based on an example from the T2VOC User's Guide. The 3D model domain was a simple rectangular block. The source was placed at the surface in the geometric centre of the block.

For T2VOC, the source was applied as mass flux (MT^{-1}) of NAPL. The source applied to the T2VOC program represented 20,000 kg of o-xylene over a 55.5 day period. The source was distributed evenly over 6 cells (1 m x 1 m) at the surface of the model. O-xylene was chosen because it is one of the BTEX groups of compounds commonly transported in the aqueous phase in groundwater systems.

For FEMWATER, the source was applied as an initial concentration (M/L^3) in a specified aqueous fluid flux (LT^{-1}). The initial concentration applied to the surface of the FEMWATER model represents o-xylene entering the system as a dissolved aqueous phase. FEMWATER does not simulate the gas or NAPL phases; therefore, the amount of dissolved o-xylene and the source concentration was estimated from the results of the T2VOC mass balance giving o-xylene masses present in each phase. The total mass of o-xylene in the aqueous phase after 55.5 days

was 10 kg (from a total injected mass of 20,000 kg). After 55.5 days, the o-xylene source was removed from the surface and the contaminant was allowed to disperse for 10 years.

5.1.2 Mesh Properties

The mesh for the generic scenario was 6 m deep, 15 m wide and 20 m long. The water table was assumed to be at a constant depth of 2.7 m below ground surface. The simulations were initially run as “flow only” problems to obtain an approximate steady-state initial condition for the transport simulation. After the steady-state initial hydraulic condition was obtained, a source with a concentration representing a hydrocarbon spill was applied to the surface of the model for 55.5 days. After 55.5 days, the source was removed and the model was run for an additional 10 years to simulate movement and attenuation of the source.

The material properties for the generic silty sand soil are shown in Table 5.1.

Table 5.1 Material properties for homogeneous isotropic silty sand

Input Parameter	Value	Units	Dimension
Hydraulic Conductivity	1.00×10^{-6}	m/s	L/T
Saturated Water Content (Porosity)	0.40	fraction	dimensionless
Residual Water Content	0.10	fraction	dimensionless
Residual NAPL Content	0.05	fraction	dimensionless
Soil Density	2650	kg/m ³	M/L ³

The material properties in Table 5.1 were chosen to be characteristic of a clean fine sand or silt. The soil density of 2650 kg/m³ was used to be consistent with the T2VOC example, but a more representative value would be $(1 - 0.4) \times 2650 = 1590$ kg/m³ for the dry density of a fine sand or silt with a porosity of 0.40.

The material property curves are shown in Figure 5.1. Relative permeability is the ratio of the permeability at a particular saturation to that of the saturated soil. At saturation, it has a value of unity and at residual moisture content the value approaches zero.

T2VOC requires the soil water characteristic data to be entered as relative permeability and capillary pressure curves.

The solute transport parameters used in the generic FEMWATER model are listed in Appendix C. Table 5.2 lists a range of transport parameters. Diffusion coefficients for porous media were estimated by multiplying the self-diffusion coefficient by porosity. A single (low) value was applied for longitudinal dispersivity. Dispersivity is generally regarded as a scale-dependent property and the value used is appropriate on the tens-of-meters scale. For solute transport on a scale of hundreds of meters, a second value is included in the table.

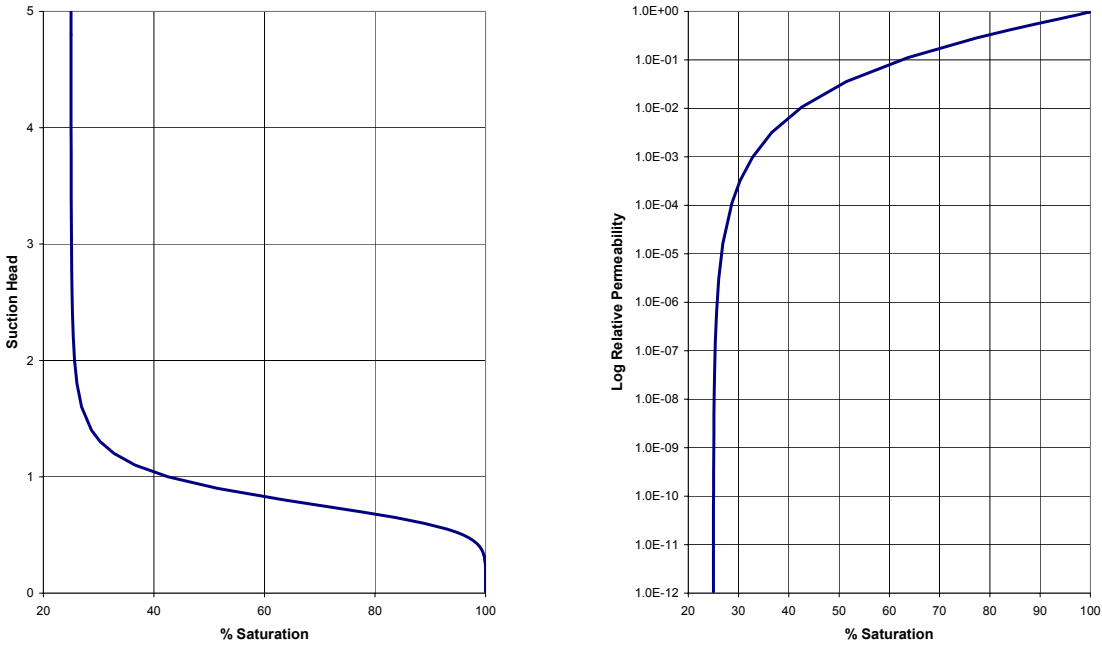


Figure 5.1 Soil water characteristic curves for a silty-sand.

Table 5.2 Solute transport parameters

Input Parameter	Value	Units	Dimension
Self Diffusion Coefficient Chloride Ion	1.44×10^{-4}	m ² /d	L ² /T
Self Diffusion Coefficient O-xylene	1.00×10^{-6}	m ² /d	L ² /T
Longitudinal Dispersivity (10 m scale)	0.5	m	L
Longitudinal Dispersivity (100 m scale)	5.0	m	L

Dispersivity is the property of a porous medium that characterizes mechanical mixing in a flow field. Longitudinal dispersivity (α_L) quantifies mixing in the direction of flow and transverse dispersivity (α_T) characterizes mixing normal to the mean flow direction. In common with hydraulic conductivity, dispersivity varies with the scale of measurement. A reasonable rule of thumb is that macroscopic dispersion (field scale) is approximately 2 orders of magnitude greater

than microscopic dispersion (lab scale). At the lab column scale, longitudinal dispersivity is typically between 0.01 and 1.0 cm. In field studies, values from 0.1 to 2.0 m are observed over short distances in well-controlled experiments. Longitudinal dispersivity values >10m are reported over longer distances, but data is very sparse and based on the back-analysis of documented plumes.

The famous Borden experiment (Sudickey, 1986; Mackay *et al.*, 1986) carried out field scale dispersivity measurements. The study found that medium-grained, fine-grained, and silty fine-grained sand, gave a field dispersivity value of 0.45 m over a travel distance 58 m. Transverse dispersivity is generally at least an order of magnitude smaller than longitudinal dispersivity. Table 5.3 summarizes the information used to estimate dispersivities.

Table 5.3 Solute transport parameters.

Dispersivity Scale	Value Range (m)
Laboratory homogeneous sand column experiments	10^{-4} to 10^{-2}
Natural-gradient tracer field experiments	10^{-2} to 10^0
Empirical fitting or matching of field plumes	10^0 to 10^2

It is well established that the apparent dispersivity, used to compute the dispersion coefficient in the advection-dispersion equation, exhibits scale effects. The apparent dispersivity grows with the plume size until the size of the plume reaches 10-15 times the size of the largest scale of heterogeneity (Howington *et al.*, 1997). For typical sand aquifers, interpreting the largest heterogeneity as lenticular bodies with a length scale of 1-5 m, an appropriate choice for dispersivity would seem to be about 10 to 50 m.

Although TOUGH2v2 can model Fickian diffusion and dispersion in the same way as FEMWATER, this capability is not available in the T2VOC module (or TMVOC) at this time. T2VOC (and TMVOC) can model macroscopic dispersion generated by inhomogeneities in the velocity field. The procedure is described by Pruess *et al.*, 1985.

The information common to all the codes is provided in Tables 5.1 to 5.3. However, each code requires the input data in a different form. A detailed description of the information specific to each modelling code is provided in Appendix C.

The 3D mesh block for the model domain is shown in Figure 5.2. The rectangular mesh block was 6 m deep x 15 m wide x 20 m long for both FEMWATER and T2VOC. In FEMWATER the block was broken down into a system of triangular prism-elements. In T2VOC, the domain was represented by a system of rectangular cell blocks. The difference in discretization arises from the requirements of the finite-element and finite difference formulations used by FEMWATER and T2VOC, respectively.

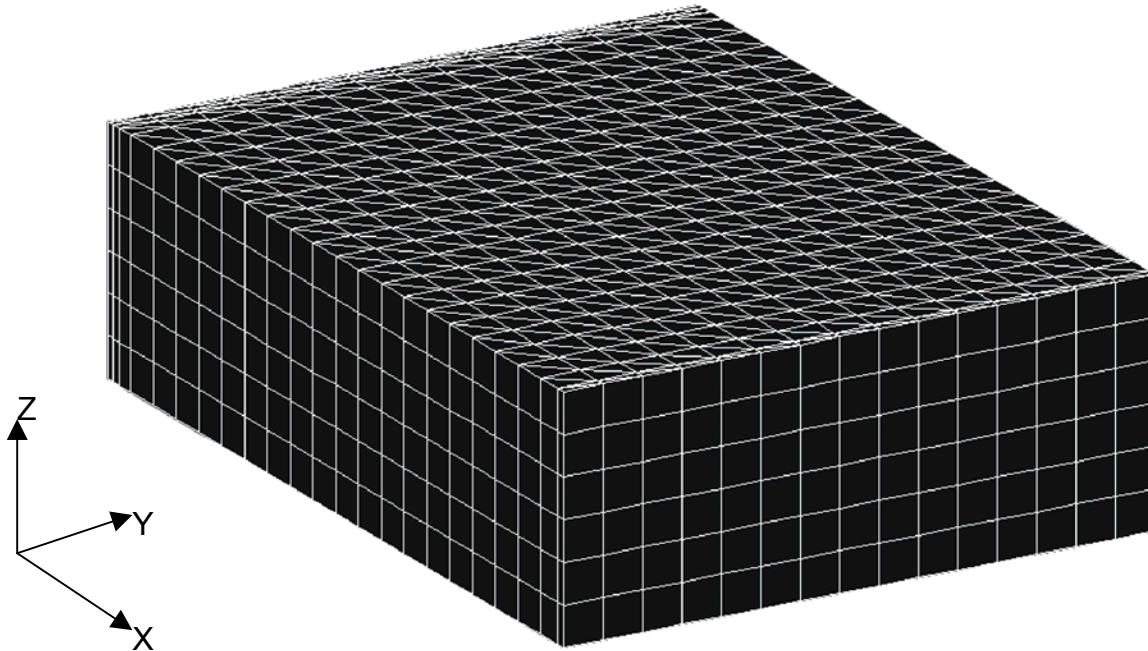


Figure 5.2 3D Mesh.

5.1.3 *Simulation Results*

This section provides the results in the form of contours along a 2D vertical cross-section. The cross-section isolates a row of cells through the middle of the model meshes at $Y = 7$ m.

Figures 5.3 and 5.4 show pressure contours after 55.5 days of source application for T2VOC and FEMWATER models respectively. The differences in the pressure contours are a result of the different surface source boundary conditions applied to the two models. T2VOC applies a mass flux of o-xylene and accounts for NAPL phase pressures where there is NAPL between the water table and the unsaturated (gas saturated) zone. FEMWATER applies an initial concentration that enters the system with a prescribed flux in aqueous solution. For this reason, the pressures are not expected to be identical between the two models.

Any asymmetry in the results can be attributed to contouring artefacts. For both models, the results are essentially symmetrical about the centre line at an X-value of 10 m.

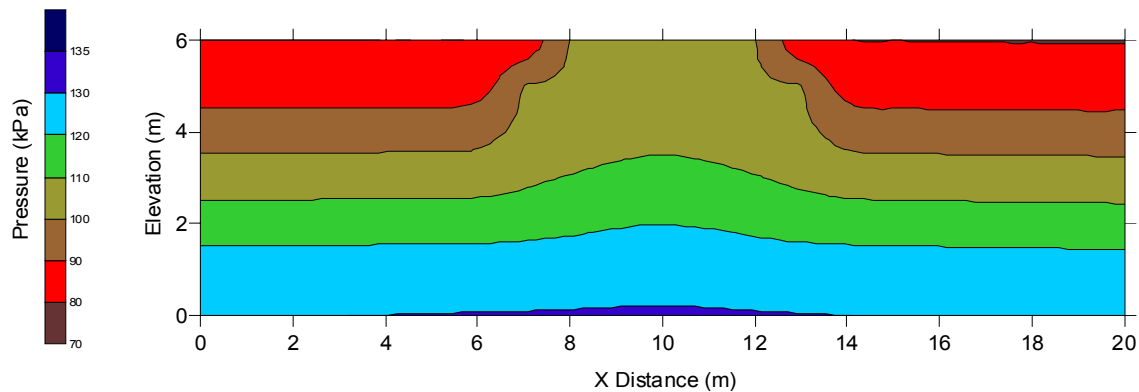


Figure 5.3 Pressure contours for T2VOC at 55.5 days.

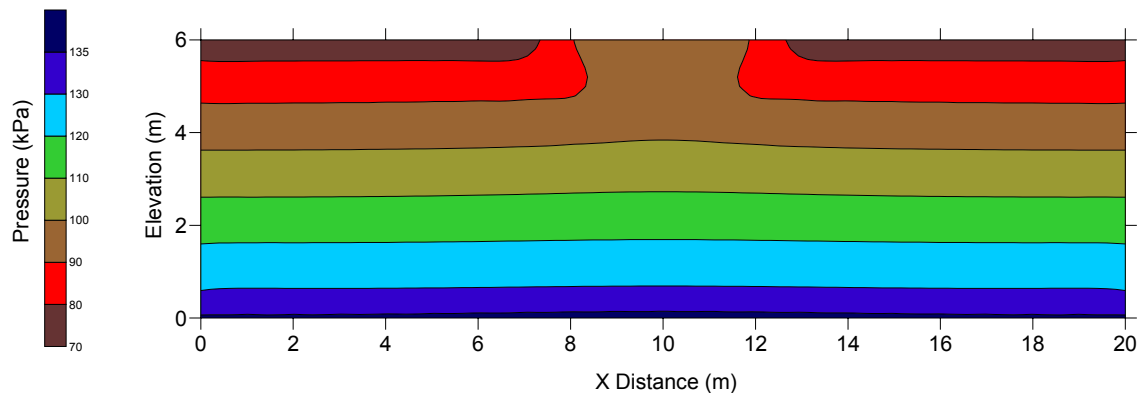


Figure 5.4 Pressure contours for FEMWATER at 55.5 days.

Both models should show a uniform pressure gradient with depth at the boundaries. The higher heads in the T2VOC prediction result from the addition of NAPL that is not accounted for in the single-aqueous-phase FEMWATER model.

Figures 5.5 and 5.6 show pressure contours after 10 years of source application for T2VOC and FEMWATER respectively. Once again there is a difference in predicted pressures as a result of the boundary conditions applied to the surface of the models. In T2VOC, 20,000 kg (or 20,000 kg / 880 kg/m³ = 22.4 m³) of free product o-xylene (density 880 kg/m³) was added to the system and 10 kg entered the aqueous phase. In FEMWATER, the source was applied as 22.4 m³ of aqueous solution containing 10 kg of o-xylene.

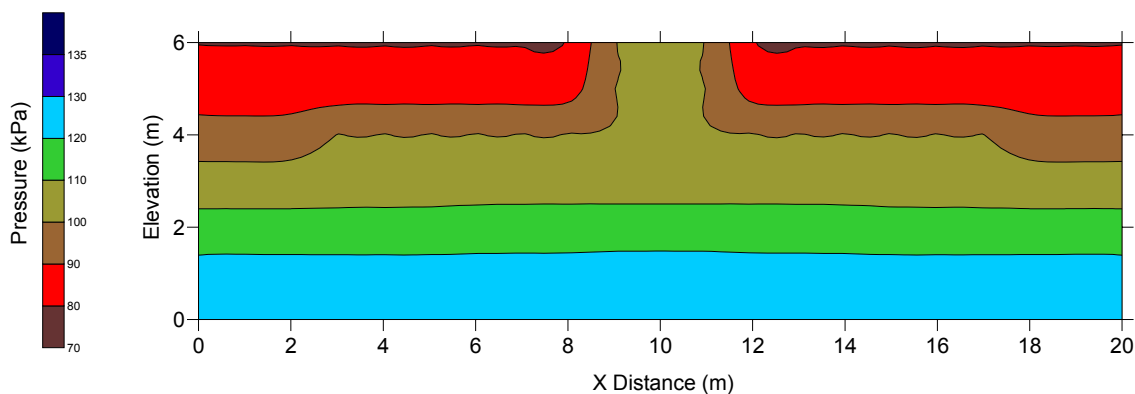


Figure 5.5 Pressure contours for T2VOC at 10 years.

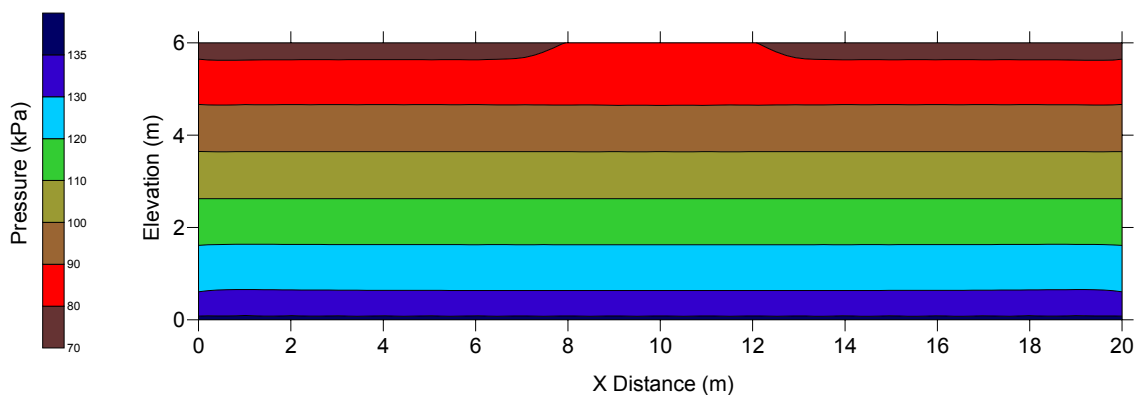


Figure 5.6 Pressure contours for FEMWATER at 10 years.

T2VOC produces a much larger aqueous-phase pressure perturbation than FEMWATER. The contribution of the NAPL column is not added into the pressure for T2VOC whereas the added aqueous solution contributes to aqueous-phase pressure in FEMWATER.

Figures 5.7 and 5.8 show mass of o-xylene after 55.5 days of source application for T2VOC and FEMWATER respectively. In terms of mass distribution, the results also show differences arising from the way the surficial source is added to the model. The source is added to T2VOC as free product o-xylene, which partially dissolves in the aqueous phase. The source is added to FEMWATER as an equivalent volume of aqueous solution containing o-xylene, with the same volume as the free product. The total mass o-xylene added to the aqueous phase is similar for FEMWATER and T2VOC after 55.5 days. The initial distribution of NAPL in aqueous solution in T2VOC is concentrated below the original water table. In FEMWATER, the dissolved NAPL in aqueous solution is mounded above the original water table. The equivalent mound in T2VOC is mostly NAPL free product. Because T2VOC accounts for gas, water and NAPL

saturations, the water saturation near the surface is lower in T2VOC than in FEMWATER. Therefore, the calculated mass in aqueous solution near the surface of the model is lower in T2VOC than in FEMWATER.

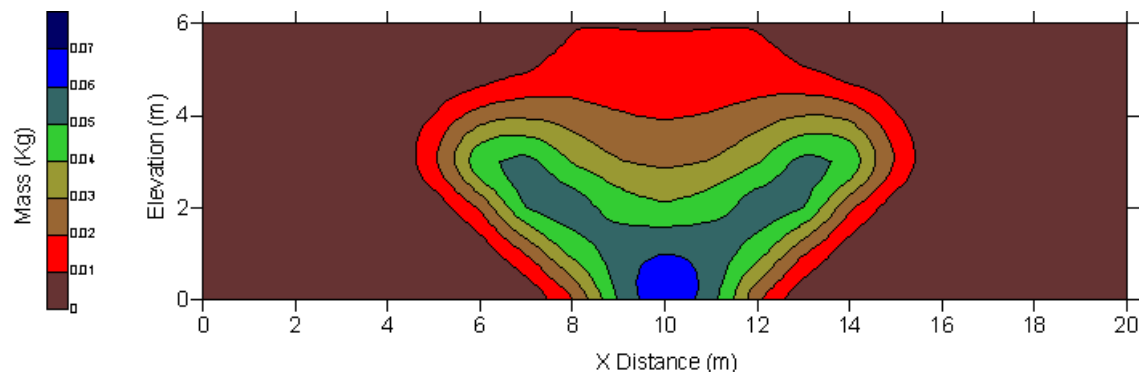


Figure 5.7 O-xylene mass in the aqueous phase. T2VOC at 55.5 days.

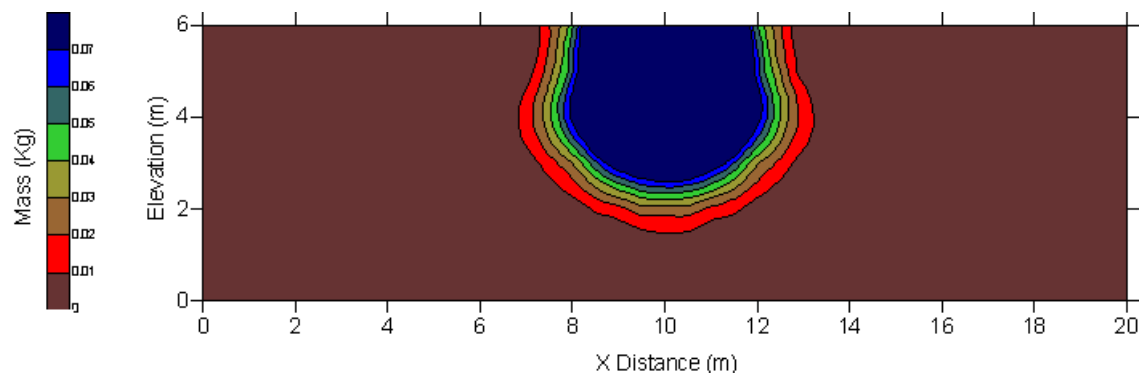


Figure 5.8 O-xylene in the aqueous phase. FEMWATER at 55.5 days.

In T2VOC, the distribution of mass is related to the spreading of the NAPL mound along the water table creating a secondary soluble plume in the saturated zone. As a result, the T2VOC plume is “widest” at the water table (at a depth of 3.32 m). No such effect is modelled with the FEMWATER code.

Figures 5.9 and 5.10 show mass of o-xylene after 10 years with no additional source applied at the surface in either T2VOC or FEMWATER. After 10 years, the original mass of o-xylene in FEMWATER disperses a small distance almost spherically from the original source location. The difference between Figure 5.8 and Figure 5.10 is relatively small. There is a slight mass balance error in the FEMWATER computation such that a small apparent loss of contaminant

mass occurs. This is a discretization problem that occurs when concentration (M/L^3) is multiplied by element volume (L^3) to obtain an estimate of mass.

In T2VOC, additional o-xylene enters aqueous solution from the NAPL mound created during the first 55.5 days and continuously dissolves into the aqueous phase. A large increase in the mass of o-xylene in the aqueous phase is predicted. The final mass of o-xylene in the aqueous phase in T2VOC after 10 years is approximately 3 times that added during the first 55.5 days and approximately 3 times the mass present in the FEMWATER model.

To simulate further dissolution of o-xylene in FEMWATER it would be necessary to apply an appropriate variable source term for the entire 10-year period. This was not attempted for the current simulations. As a result the o-xylene plume predicted by FEMWATER has a constant mass that is redistributed by diffusion over the ten years.

In T2VOC the plume grows as more o-xylene is dissolved. Notice that most of the mass in the aqueous phase is concentrated in the saturated zone beneath the footprint of the original surface source.

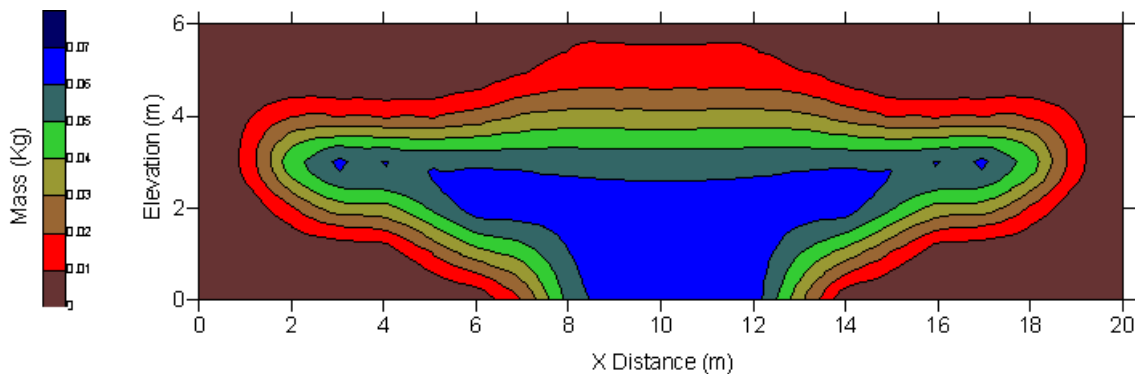


Figure 5.9 O-xylene mass in the aqueous phase. T2VOC at 10 years.

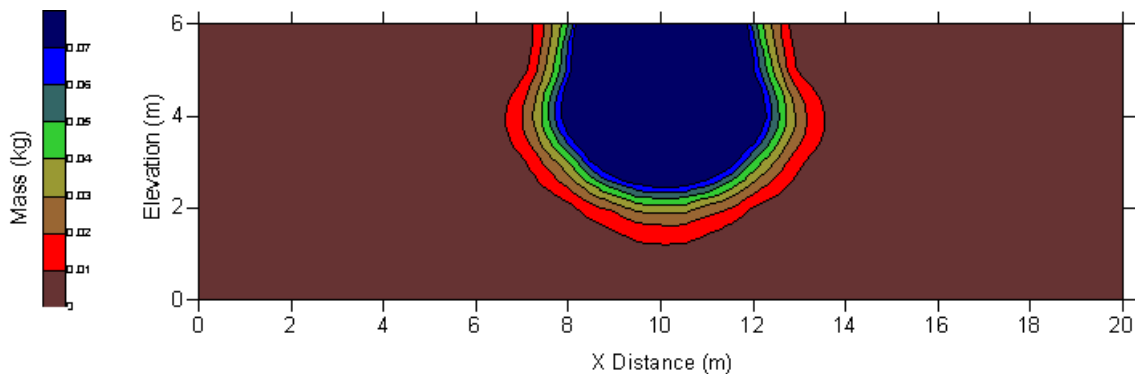


Figure 5.10 O-xylene mass in the aqueous phase. FEMWATER at 10 years

Additional generic solutions to show the influence of sorption and biodegradation parameters are shown in the figures below. These simple simulations establish the potential application of T2VOC to a wide range of petroleum hydrocarbon (PHC) problems. A more complex application of the T2VOC code is described by Fagerlund and Niemi (2003). They examine gasoline spills by independently modelling the behaviour of eight molecular weight fractions.

5.1.4 Additional Generic Simulations

Additional generic simulations were prepared by MDH Engineered Solutions Corp. (MDH) to illustrate the effects of natural attenuation, decay and adsorption and free-product removal on plume migration.

For each code, two additional simulations were run. The first simulation applies a decay constant of 0.002 (1/day). The second simulation applies a decay constant of 0.002 (1/day) and an organic carbon/water partition coefficient (K_{oc}) of 240 (ml/g) for total xylenes, and a fraction of organic carbon (F_{oc}) of 0.001 for the silty sand soil.

5.1.4.1 First Order Decay

Figures 5.11 to 5.14 show the results when a first order decay constant is applied, using T2VOC and FEMWATER. T2VOC shows less than 3% decrease in o-xylene in solution after 10 years (Figure 5.13). The effects of attenuation by decay are masked in the T2VOC simulation because a large mass of free product o-xylene (19,988 kg) that remained in the model after 55.5 days. The o-xylene remaining in the NAPL-phase after 55.5 days provided an internal source that dissolved over the 10 years after the surface source was removed. The FEMWATER solution, which has no free product remaining in the model after 55.5 days, indicates that after 10 years, o-xylene mass in solution would decrease by approximately 97% (Figure 5.14).

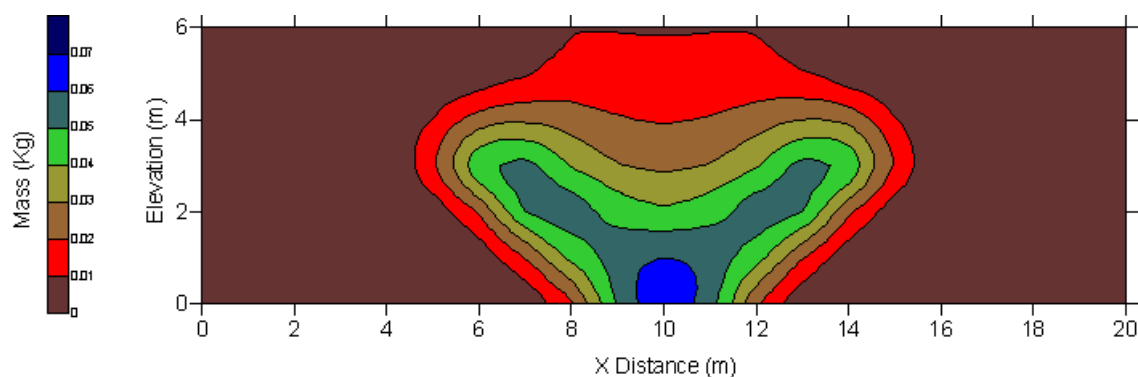


Figure 5.11 O-xylene mass in the aqueous phase accounting for decay. T2VOC at 55.5 days.

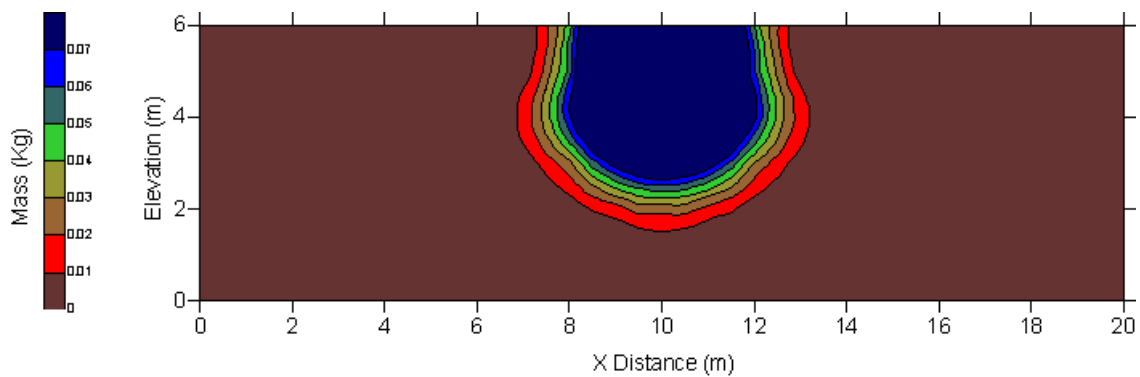


Figure 5.12 O-xylene mass in the aqueous phase accounting for decay. FEMWATER at 55.5 days.

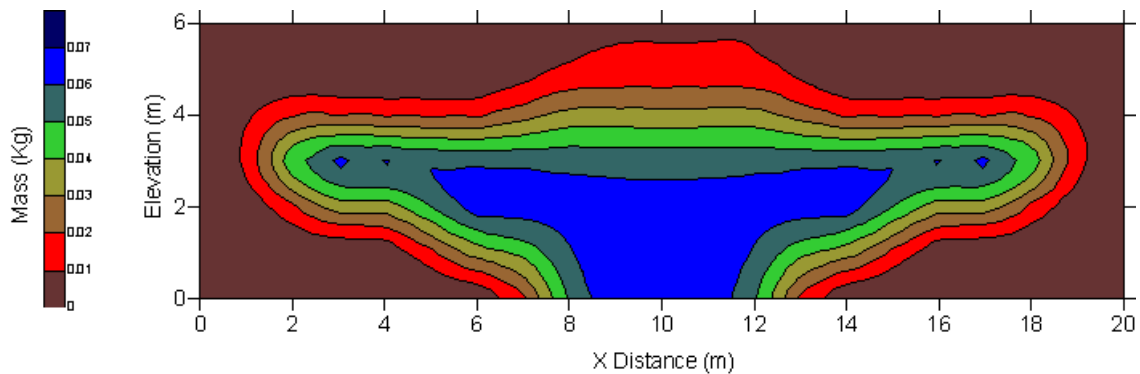


Figure 5.13 O-xylene mass in the aqueous phase accounting for decay. T2VOC at 10 years.

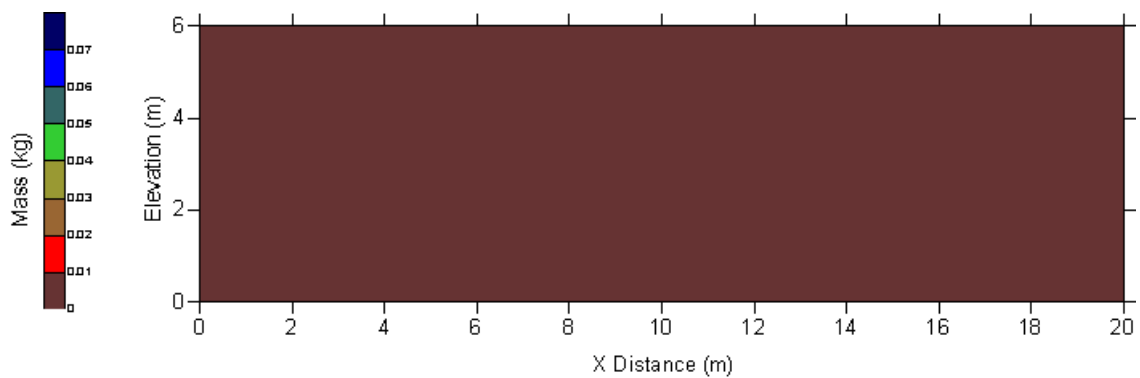


Figure 5.14 O-xylene mass in the aqueous phase accounting for decay. FEMWATER at 10 years.

5.1.4.2 First Order Decay and Adsorption

Figures 5.15 to 5.18 show the results when both a first order decay constant and adsorption constants are applied, using T2VOC and FEMWATER. When both decay and adsorption are accounted for, the o-xylene mass remaining in solution is reduced relative to the decay only case. For this analysis a K_{oc} of 240 ml/g xylene and an F_{oc} of 0.001 was used. After 10 years, T2VOC still shows less than 3% decrease in the mass of o-xylene in solution (Figure 5.17). The limited attenuation processes can once again be attributed to the mass remaining in the NAPL phase after 55.5 days (19,973 kg). FEMWATER, which only models the aqueous phase, shows a decrease of almost 99 % in the mass of o-xylene in solution after 10 years (Figure 5.18).

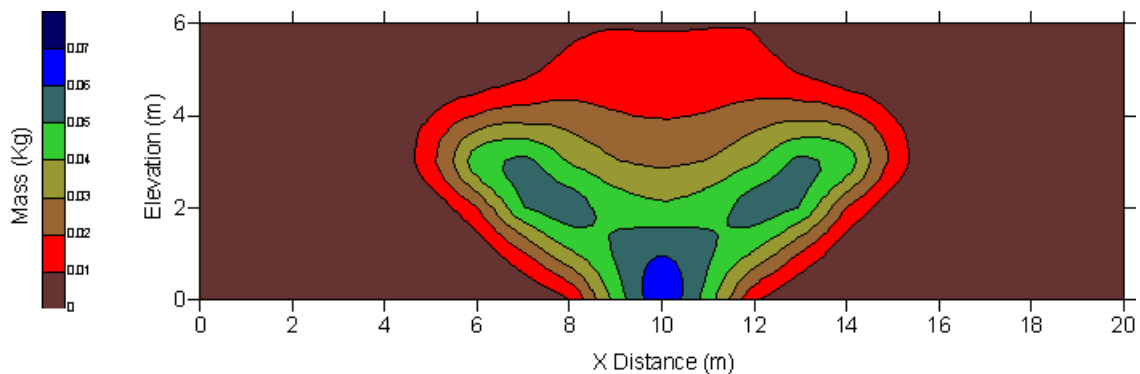


Figure 5.15 O-xylene mass in the aqueous phase accounting for decay and adsorption. T2VOC at 55.5 days.

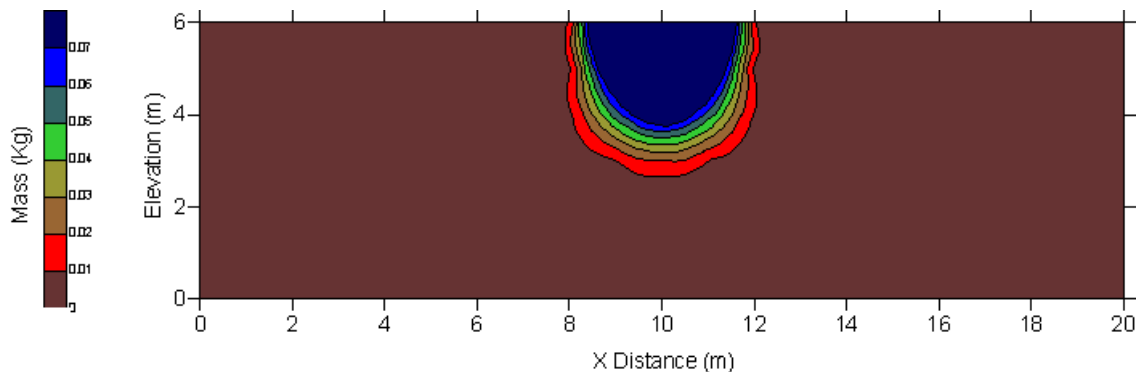


Figure 5.16 O-xylene mass in the aqueous phase accounting for decay and adsorption. FEMWATER at 55.5 days.

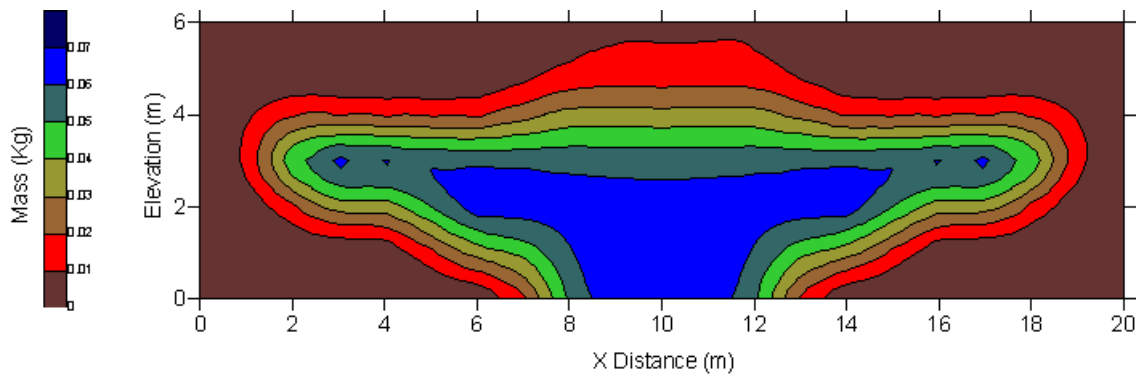


Figure 5.17 O-xylene mass in the aqueous phase accounting for decay and adsorption. T2VOC at 10 years.

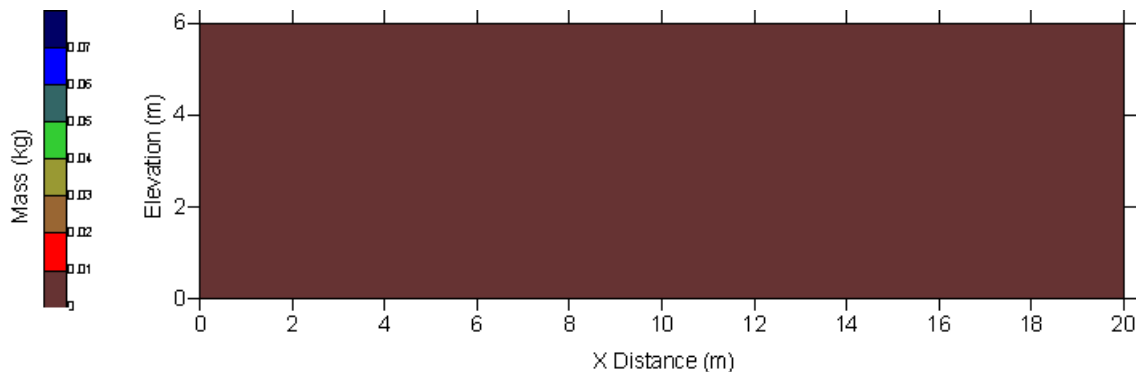


Figure 5.18 O-xylene mass in the aqueous phase accounting for decay and adsorption. FEMWATER at 10 years.

5.1.4.3 Free Product Removal

A simulation was run applying soil vapour extraction wells to T2VOC to remove some of the free product o-xylene. Approximately 50% of the o-xylene mass in the NAPL phase was easily removed using soil vapor extraction wells (Figure 5.19). Removing a larger fraction of the o-xylene mass in the NAPL phase is difficult and has not been completed at this time. Figures 5.20 and 5.21 illustrate the mass in solution 10 years after the NAPL phase for a base case and when a decay function was added to the simulation respectively. Figure 5.19 illustrates when only 50 % of the NAPL phase was removed, the mass of o-xylene in solution increased by approximately 6%.

Figure 5.20 illustrates that when a decay function is applied to the model, the mass of o-xylene in solution decreased by just under 4% after 10 years. Once again, a large mass of o-xylene remained in the NAPL phase (10,649 kg), which is significant enough to continue masking the effects of attenuation.

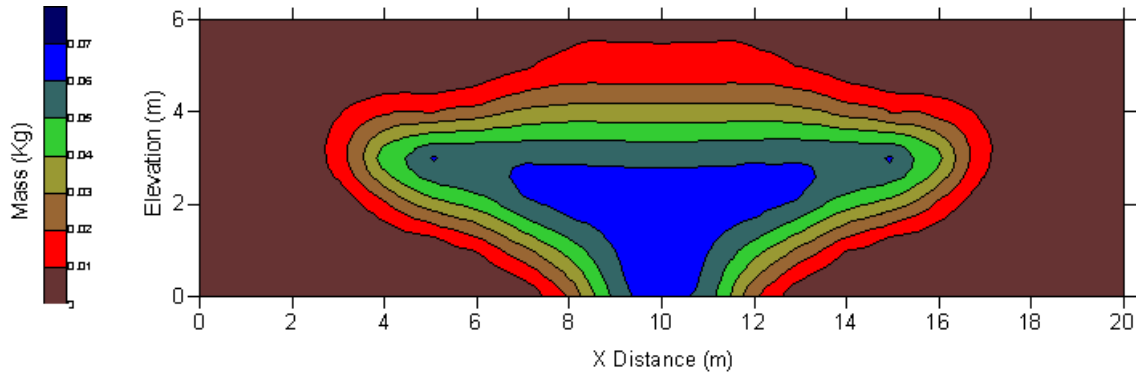


Figure 5.19 O-xylene mass in the aqueous phase after 50% of residual NAPL removed. T2VOC initial condition.

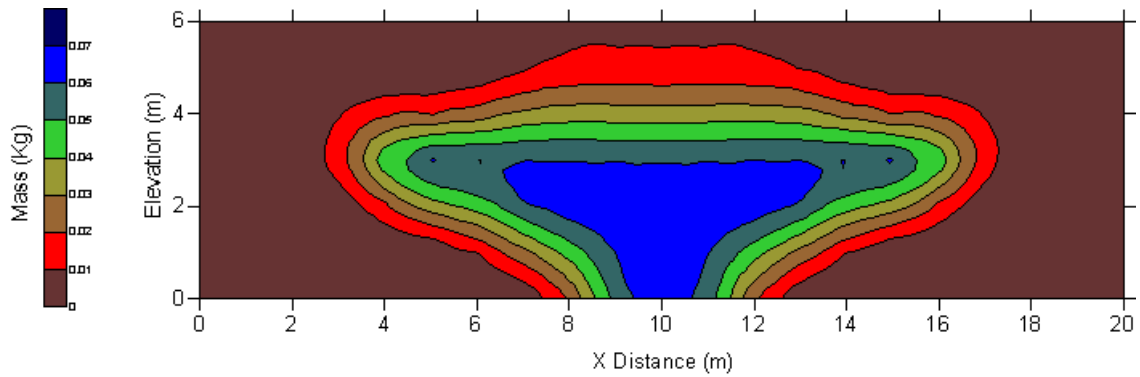


Figure 5.20 O-xylene mass in the aqueous phase after 50% of residual NAPL removed. T2VOC at 10 years.

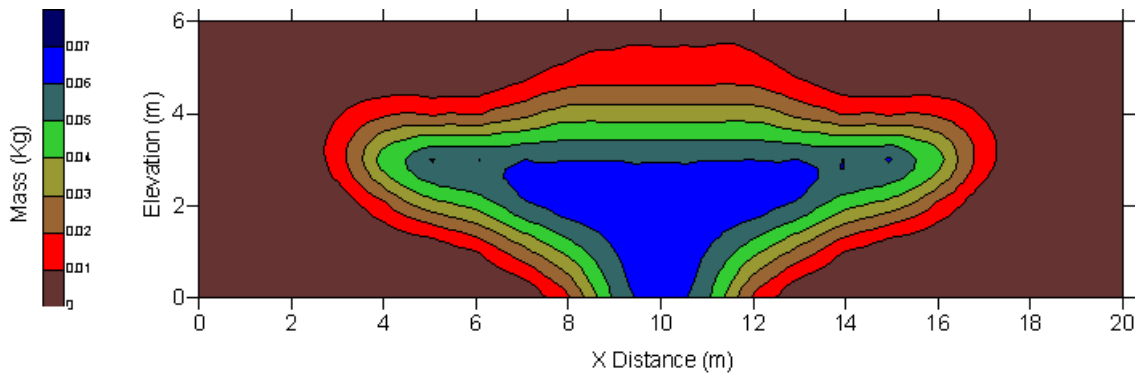


Figure 5.21 O-xylene mass in the aqueous phase after 50% of residual NAPL removed accounting for decay. T2VOC at 10 years.

5.1.4.4 *Additional Model Runs*

Additional simulations were run using T2VOC where the mass applied to the model was decreased. This generally just resulted in a smaller plume with lower masses in the aqueous phases. Because in each of these cases, NAPL remained above the water table, the effects of decay were still masked by dissolution of the NAPL phase. The results are not included in this report.

6.0 DISCUSSION OF RESULTS

Results confirm that T2VOC and FEMWATER produce consistent but different solutions to the same simple problem. Unlike FEMWATER, T2VOC tracks the distribution of the contaminant both in the aqueous and vapour phases.

The main advantage of FEMWATER is its ability model the movement and natural attenuation of o-xylene in the both the unsaturated and saturated zones by Fickian diffusion and dispersion. The main disadvantage of FEMWATER is its inability to simulate multiphase transport or to model continued solution from the NAPL phase to the aqueous phase. The source must be applied to FEMWATER as an equivalent aqueous solution. To use FEMWATER (or other saturated / unsaturated flow codes) to model aqueous phase NAPL, programs such as T2VOC, CONTAM, MOFAT, NAPL Simulator, R-UNSAT, VLEACH are required to provide a modified source term to account for the partitioning of phases between vapour and aqueous solution. If NAPL free product was removed from the system by soil vapour extraction (SVE) or other means, 3D codes like FEMWATER, SUTRA, FEFLOW and MODFLOW are capable of predicting advective and dispersive transport of an aqueous phase plume.

The main strength of TOUGH2v2 (T2VOC) is its ability to provide results for both simple 2D analysis and more complex 3D analysis. T2VOC is one of the few widely established 3D codes that can simulate vapour phase transport without sacrificing transport in the saturated zone. This is a valuable feature when modelling transport of volatile organic compounds. The capabilities present in T2VOC are required for cases where residual NAPL remains in the aquifer, at or above the water table after the surficial source has been removed.

The simple generic simulations completed in this report have shown that significant NAPL continues to dissolve after the surficial source has been removed. This NAPL source cannot be readily simulated using codes such as FEMWATER, SUTRA, FEFLOW and MODFLOW, which do not account for multiphase transport.

TOUGH2v2 is an effective tool for Tier 2 analysis and can be applied for most Tier 3 problems. General knowledge of the hydrostratigraphy, potentiometric surfaces, groundwater recharge rates, and aquifer material properties are the minimum required parameters to run TOUGH2v2 for 2D and 3D problems.

The main disadvantage of TOUGH2v2 is the lack of a high-quality, pre- and post-processing graphical interface. A graphical interface called PetraSim can be purchased, but it has limited functionality and does not have the same sophistication and maturity as GMS, ARGUS or the Visual MODFLOW interfaces.

Some further restrictions and limitations of T2VOC are as follows:

- The “basic” mesh generator supplied by the U.S. Department of Energy has limited functionality. The mesh has to be created using text editors and/or a command line interface. Specifying a mesh with variable spacing is tedious.

- Source code is not provided for TOUGH2v2 unless it is purchased from the U.S. Department of Energy.
- Even with the PetraSim interface, post-processing requires the use of external packages such as Surfer or Excel.
- To use TOUGH2v2 (T2VOC) for large problems with detailed geology, it is essential to be able to recompile the code. A FORTRAN compiler and associated expertise is needed to effectively use the code.
- T2VOC does not account for Fickian dispersion or molecular diffusion in the aqueous and NAPL phases (although gas phase diffusion is modelled). Macroscopic dispersion can be accounted for using the procedure described by Pruess et al. (1985).

Overall, TOUGH2v2 is a well-written and reliable numerical code that produces accurate results on all verification problems. Its major limitation is a relatively poor graphical user interface (GUI) compared to those available for popular 3D groundwater modelling codes such as MODFLOW, SUTRA and FEMWATER.

Results from the additional generic solutions indicate that single-phase flow models, such as FEMWATER, are adequate when 100% of the LNAPL is removed by techniques such as soil vapour extraction. If complete removal of the LNAPL does not occur, single-phase models may overestimate the rate of mass loss from aqueous solution by attenuation processes. The assumption that all LNAPL is removed would tend to result in the prediction of smaller plumes by single-phase programs. For cases where LNAPL remains above the water table, multiphase codes such as T2VOC are required to model the fate and transport of hydrocarbons. Preliminary model results indicate that it is very difficult to remove a fraction close to 100% of the LNAPL from a contaminated site. Residual NAPL will act as a source that will continue to dissolve into the aqueous phase with time. Multiphase programs such as T2VOC are required to identify potential sources (residual NAPL plumes) that exist beneath the ground surface. Multiphase programs are advantageous because they would tend to provide more conservative predictions on the fate and transport of hydrocarbons in the subsurface.

7.0 CONCLUSION

Over 250 codes were found and over 130 codes were initially rated on a scale of 1 to 10 to determine their ability to model the fate and transport of hydrocarbons in the groundwater and soil. The preliminary ranking matrix provides an indication of the functionality of each model with respect to the scenarios requested by AENV personnel. Changes in the ranking criteria or the relative weighting of components can be readily incorporated into the ranking matrix if different objectives are defined.

TOUGH2v2 and FEMWATER were recommended for further analysis in Phase III. The two recommended codes were reviewed in detail for their strengths, weaknesses, and applicability to the AENV hydrocarbon scenario during Phase III of the project.

TOUGH2v2 (T2VOC) is code that is supported by the Lawrence Berkeley National Laboratory and distributed by the U.S. Department of Energy. The T2VOC module of TOUGH2v2 was used in the analysis. TOUGH2v2 is an effective tool for Tier 2 analysis and can be applied for most Tier 3 problems. General knowledge of the hydrostratigraphy, potentiometric surfaces, groundwater recharge rates, and aquifer material properties are the minimum required parameters to run TOUGH2v2 for 2D and 3D problems.

TOUGH2v2 (T2VOC) is recommended for modelling the transport of hydrocarbons in soil and groundwater. TOUGH2v2 (T2VOC) accounts for partitioning between the vapour, water and NAPL phases. Modules of TOUGH2v2, such as T2VOC, have the ability to simulate the movement of fractions of crude oil and a variety of refined hydrocarbon products in aqueous systems. In T2VOC, each fraction has to be modelled as a separate run. In the TMVOC module, functionality is added to model multiple fractions in the same simulation. Regardless of the particular code chosen, multiphase programs have significant advantages over single-aqueous-phase codes such as FEMWATER because they simulate movement of both the NAPL and aqueous liquid phases and the gas phase together with the interactions between the liquid and gas phases.

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Appendix A List of Models Excluded from Evaluation

List of models designed primarily for NAPL simulations

HSSM	BIOPLUME III	RT3D
SPILLCAD	UTCHEM	NAPL SIMULATOR
MOFAT	BioSVE	RITZ
VENT2D	ARMOS	BIOF&T-2D
AIRFLOW/SVE	BIOF&T- 3D	ROAM
SEAM3D	MARS	SWANFLOW
MAGNAS	BIOTRANS	TOUGH2
BIOVENTING	HYPERVENTILATE	TMVOC
VENT3D		

List of models with no solute transport capabilities (flow only)

ABCFEM	MODFLOW	SOIL COVER
CAPZONE	MOD-HMS	SVFLUX2D
FEMWATER 2D	MODPATH	SVFLUX3D
FLAC	MODRET	TETRA
FLOWTHRU	NETFLO	THWELLS
FRAC2D	PAT	TWODAN
GFLOW	PATH2D	VADOSE/W
GWDIVIDE	PLASM	WATERMOD2
GWFLOW	QUICKFLOW	WhAEM2000
HELP v.3.0	RADFLOW	WHPA
HOTWTR	SEEP/W	WINFLOW
INFIL	SEEP2D	whPROFILE
JOB2D-3D	SEEP3D	

List of surface water models

AGNPS	BREACH	DISPERS
FLDWAV	HYDRA	

List of geochemical speciation models with limited or no flow simulation

HYDROCHEM	MINTEQA2	NETPATH
PHREEQC	PHREEQE	PHRQPITZ

List of codes that were primarily databases

BORDEN DATA SET	PEST2000	STF
ENVES&T	ROSETTA	VISUAL PEST
LIMS	SOIL VISION	

List of codes that were primarily pre-and post-processing interfaces

ARGUS ONE	MFI	SUTRA-GUI
EIS-GWM	MODIME	VISUAL MODFLOW
GMS	SEQUENCE	VS2DI
GROUNDWATER VISTAS	SHOWFLOW 2	

List of heat flow codes and codes concerned with evaporation only

HT	UNSAT2	VS2DH
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List of codes that no longer appear to be sold

EXPRES	KYSPILL	UNSAT2
FEMSEEP	MULAT	
FTRAN	TDPLUME	

List of flow only models that could not be located by diligent searching

2PAR_DEGRADE	FRACNET	SEEPS2D
ADE 3D	GEOFLOW	SPLIT
ANALYT	MOTIF	SWIFT II
AQUIFEM-N	NEFTRAN II	TBC
CADIL_AGTEHM	PERCPLAN	VaMP
FRACFLO	POLUTE2D	VSAFT2
FRACFLOW	SANGRE	

List of flow only models that do not have a North American distributor*

2D_V_HYDRO_S	GGU-SS FLOW3D	SEFTRANS
BEAVER	MACRO	SIMULAT
FEHM	MARTHE	
FLOW2D	MSEEP	

**or where documentation and/or support in the English language is a concern*

List of codes that have become obsolete or succeeded by later versions

ASM	FEMW-FEMA	SATURN
BALANCE	MOTRANS	SOILCO2
BIOPLUMEII	PRZM	
FEMWASTE	PRZM2	

Appendix B Preliminary Ranking List

Table B1 Water balance.

Ranking	Explanation
10	Computes flow and chemical mass balance.
8	Computes chemical mass balance but flow balance can be added.
6	Computes flow balance but chemical balance can be added.
5	No information found.
4	Computes chemical mass balance only.
3	Computes flow balance only.
1	Does not compute flow or chemical mass balance.

Table B2 Flow model.

Ranking	Explanation
10	Unsaturated and saturated flow, vertical and lateral flow, transient state simulations.
9	Saturated flow, vertical and lateral flow, transient state simulations..
8	Unsaturated and saturated flow, vertical and lateral flow, steady state simulations.
7	Saturated flow, vertical and lateral flow, steady state simulations.
6	Unsaturated and saturated flow, vertical flow, transient state simulations.
5	No information found.
4	Saturated flow, vertical flow, transient state simulations.
2	Saturated flow, vertical flow, steady state simulations.
1	Unsaturated flow simulations.

Table B3 Transport mechanisms.

Ranking	Explanation
10	Advection, dispersion, diffusion.
8	Advection, dispersion.
6	Dispersion, diffusion.
5	No information found.
1	Advection, particle tracking only.

Table B4 Biodegradation model.

Ranking	Explanation
10	Monod biodegradation, first order decay, instantaneous reactions.
9	Monod biodegradation, first order decay.
8	Monod biodegradation.
6	First order decay.
5	No information found.
4	Instantaneous reactions.
3	Type of decay function not specified.
1	No decay option.

Table B5 Sorption / volatilization.

Ranking	Explanation
10	Sorption, volatilization.
8	Sorption.
6	Volatilization.
5	No information found.
2	Other reactions.
1	No reactions.

Table B6 Dimensionality.

Ranking	Explanation
10	3D flow.
7	2D, axisymmetric flow.
5	No information found.
3	2D, planar flow.
1	1D flow

Table B7 Domain variability.

Ranking	Explanation
10	Heterogeneous, anisotropic.
7	Heterogeneous, isotropic.
5	No information found.
3	Homogeneous, anisotropic.
1	Homogeneous isotropic.

Table B8 Mesh flexibility.

Ranking	Explanation
10	Irregular mesh boundaries, variable element block size and shape.
8	Irregular mesh boundaries, fixed element block size and shape.
7	Irregular mesh boundaries, unknown element block size and shape.
5	No information found.
3	Simple (rectangular) mesh boundaries.
1	Pre-made mesh for specific problem.

Table B9 Data requirements.

Ranking	Explanation
10	Provides default data/recommended values and units.
8	Provides units for parameters, but no default data.
5	No information found.
4	Provides default data but no guidance on units.
1	Provides no default data or units for parameters.

Table B10 Computational requirements.

Ranking	Explanation
10	Standard desktop CPU, Windows GUI (Graphical User Interface).
9	Standard desktop CPU, Windows GUI, EXCEL.
7	Dedicated fast CPU, Windows GUI.
6	Dedicated fast CPU, Windows GUI, added memory.
5	No information found.
3	CPU, Windows GUI, C/Fortran compilers.
1	Standard desktop CPU, non-windows OS.

Table B11 Code availability.

Ranking	Explanation
10	Readily available from free website, automatic installation.
9	Readily available from free website, requires manual installation.
8	Readily available from commercial website, automatic installation.
7	Readily available from commercial website, manual installation.
6	Available after email request.
5	No information found.
4	Commercially available via email and/or order form processing.
3	Available but difficult to install (needs compilation and editing).
2	Available but obsolete or too old to readily install.
1	MDH could not locate installable version.

Table B12 Source code availability.

Ranking	Explanation
10	Free.
5	No information found.
1	Not available.

Table B13 Program installation.

Ranking	Explanation
10	Code downloaded and installed successfully.
9	Code downloaded and compiled successfully.
8	Program downloaded, not compiled, no problems expected.
7	Demo version downloaded and installed successfully.
6	Program downloaded, not installed, may be difficult to install.
5	No Information available.
4	Code downloaded and compiled with many changes.
3	Code/demo version downloaded, will not install or compile.
2	Code or demo requested by email, not received.
1	Code or demo not available, or no download available.

Table B14 Code validation.

Ranking	Explanation
10	Established widely used code.
9	New version of established code.
8	Extensively tested code.
6	New program validated against more established codes.
5	No information found concerning validation.
4	Regulatory program intended for screening purposes.
3	Older, obsolete or little used code.
1	Educational and/or development code.

Table B15 Support availability.

Ranking	Explanation
10	Unlimited professional support.
8	Commercial support at cost.
7	Government agency support.
5	No information found.
4	Email author support.
3	Government agency maintenance.
2	Author maintenance, limited support.
1	No support

Table B16 Documentation quality.

Ranking	Explanation
10	Good up-to-date manual, many sample data sets, available online.
9	Good manual, some sample data sets, available online.
8	Adequate manual, many sample data sets, available online.
7	Manual not available online, but well documented.
6	Adequate manual, some sample data sets.
5	No information found.
4	Manual not available online, documentation quality unknown.
3	Poor manual, some sample data sets, available online.
2	Poor documentation and availability.
1	Documentation unavailable or in language other than English.

Table B17 Ease of use.

Ranking	Explanation
10	Windows GUI (Graphical User Interface).
8	Non Windows GUI.
5	No information found.
4	Windows/Dos CLI (Command Line Interface).
1	Non Windows CLI.

Table B18 Preliminary ranking of codes

PROGRAM NAME	Ranking Sum	Water Balance	Subsurface Flow Capabilities	Transport Mechanisms	Biodegradation Reactions	Sorption/Volatilization	Dimensionality	Domain Variability	Mesh Flexibility	Data Requirements	Computational Requirements	Code Availability	Source Code Availability	Program Installation	Code Validation	Support Availability	Documentation Quality	Ease of Use	Cost \$ U.S
WEIGHTING FACTOR		1	3	1	3	1	3	2	2	1	1	1	1	1	1	1	1	2	
FEMWATER with GMS	9.4	10	10	10	8	8	10	10	10	10	7	8	10	10	10	8	10	10	*
VS2DTI	9.3	10	10	10	8	8	10	10	10	8	7	10	10	10	10	4	10	10	FREE
TOUGH2v2	9.1	10	10	10	8	10	10	10	10	8	7	8	10	1	10	8	10	10	\$2300
UTCHEM with GMS	9.0	10	10	10	10	8	10	10	10	5	10	8	10	1	8	8	7	10	*
MT3D and MODFLOW with ARGUS	8.9	10	9	10	8	8	10	10	10	8	7	8	10	1	10	8	10	10	**
3DFATMIC with GUI	8.8	10	10	10	10	8	10	10	10	8	3	8	10	1	8	8	6	10	\$2000
HYDRUS-2D	8.8	10	10	10	8	8	7	10	10	10	7	8	10	10	6	8	8	10	\$600
RT3D and MODFLOW with GMS	8.8	10	9	10	10	8	10	10	10	8	7	8	1	1	10	8	10	10	*
3DFEMFAT	8.7	10	10	10	8	8	10	10	10	8	3	8	10	9	9	2	6	10	\$1000
SUTRA with ARGUS	8.7	10	10	10	8	8	7	10	10	8	7	8	10	7	10	8	6	10	**
CTRAN and SEEP/W	8.6	10	10	10	8	8	7	10	10	10	7	8	1	7	10	8	10	10	\$6000
SEVIEW	8.5	10	10	10	8	8	10	10	3	8	10	8	10	7	10	8	3	10	\$1000
FEFLOW	8.5	10	10	10	8	8	10	10	10	8	7	8	1	1	10	7	7	10	\$7000
FEMWATER no GUI	8.5	10	10	10	8	8	10	10	10	8	3	10	10	9	10	3	8	4	FREE
MT3D and MODFLOW no GUI	8.5	10	9	10	8	8	10	10	10	8	3	9	10	10	10	3	10	4	FREE
CHEMFLUX3D with SVFLUX3D	8.4	10	10	10	8	8	10	10	10	8	7	8	1	1	6	8	7	10	\$6000
SUTRA no GUI	8.4	10	10	10	8	8	7	10	10	8	10	10	10	10	10	3	6	4	FREE

PROGRAM NAME	Ranking Sum	Water Balance	Subsurface Flow Capabilities	Transport Mechanisms	Biodegradation Reactions	Sorption/Volatilization	Dimensionality	Domain Variability	Mesh Flexibility	Data Requirements	Computational Requirements	Code Availability	Source Code Availability	Program Installation	Code Validation	Support Availability	Documentation Quality	Ease of Use	Cost \$ U.S
BIOF&T 3D	8.3	10	10	10	9	8	10	10	10	8	7	8	1	1	5	8	4	10	\$2000
MOC3D and MODFLOW	8.3	10	9	10	8	8	10	10	10	8	3	10	10	8	10	3	6	4	FREE
BIOMOC3D	8.2	10	9	8	9	8	10	10	10	8	3	9	10	8	10	3	5	4	FREE
PORFLOW	8.2	10	10	10	8	8	10	10	10	8	7	8	1	1	8	5	4	10	\$5000
SWMS_3D	8.2	10	10	10	8	10	10	10	10	8	3	3	10	9	9	4	6	4	FREE
TARGET	8.2	10	10	10	8	8	10	10	10	5	10	8	1	1	5	8	4	10	\$3000
MODPATH with ARGUS	8.1	10	9	8	1	1	10	10	10	8	7	8	10	10	10	8	10	10	**
SEAM3D with GMS	8.1	10	9	8	6	8	10	10	10	5	10	8	1	1	10	8	6	10	*
CHEMFLUX2D with SVFLUX2D	8.0	10	10	10	8	8	7	10	10	8	7	8	1	1	6	8	7	10	\$4000
BIOF&T 2D	8.0	10	10	10	9	8	7	10	10	8	7	8	1	1	5	8	4	10	\$1000
WHI UNSAT SUITE	8.0	10	1	10	8	8	7	10	10	8	10	8	10	7	10	8	10	10	\$700
HST3D with ARGUS	7.9	5	9	10	8	8	10	10	3	8	7	8	10	1	10	8	4	10	**
MARS	7.9	5	10	10	9	8	10	10	7	5	10	8	1	1	5	8	4	10	\$3000
FRAC3DVS	7.9	10	10	10	5	8	10	10	10	5	10	8	1	1	5	8	4	10	\$3000
VAM2D	7.9	10	10	10	8	8	9	10	7	5	10	8	1	1	5	8	4	10	\$2000
CHAIN2D	7.8	10	10	10	8	10	9	10	8	8	3	9	10	8	3	1	6	4	FREE
3DFATMIC no GUI	7.8	10	10	10	10	8	10	10	3	8	3	9	10	8	6	1	6	4	FREE
MAGNAS	7.8	5	10	10	8	10	10	7	10	5	10	8	1	1	5	5	5	10	\$20,000
HST3D no GUI	7.8	5	9	10	8	8	10	10	3	8	10	10	10	10	10	3	3	4	FREE
UTCHEM and MODFLOW no GUI	7.7	10	10	10	10	8	10	10	3	5	3	9	10	6	8	3	3	4	FREE

PROGRAM NAME	Ranking Sum	Water Balance	Subsurface Flow Capabilities	Transport Mechanisms	Biodegradation Reactions	Sorption/Volatilization	Dimensionality	Domain Variability	Mesh Flexibility	Data Requirements	Computational Requirements	Code Availability	Source Code Availability	Program Installation	Code Validation	Support Availability	Documentation Quality	Ease of Use	Cost \$ U.S
MODPATH no GUI	7.5	10	9	8	1	1	10	10	10	8	7	10	10	10	10	3	10	4	FREE
ASMWIN	7.5	10	9	10	8	8	3	10	3	8	10	10	10	10	5	1	6	10	FREE
SWAP	7.5	10	10	10	8	8	1	7	3	5	10	10	10	10	10	8	6	10	FREE
SWMS_2D	7.4	10	10	10	8	10	3	10	10	8	3	3	10	9	9	4	6	4	FREE
FLONET/TRANS	7.3	10	9	10	8	8	3	10	10	5	10	8	1	1	5	8	4	10	\$500
MOFAT with a GUI	7.3	10	10	10	8	10	3	10	3	5	10	8	10	1	5	8	4	10	\$1000
BIOPLUME III	7.3	10	9	10	9	8	3	3	3	8	10	10	10	10	10	3	5	10	FREE
FLOWPATH II	7.3	10	9	10	8	1	3	10	10	5	10	8	1	7	5	8	4	10	\$600
FTWORK	7.3	5	9	8	8	8	10	10	7	5	10	8	1	1	5	8	5	5	\$300
BIOSLURP	7.2	10	10	10	8	8	3	10	7	5	10	8	1	1	5	8	4	10	\$2500
MOFAT no GUI	7.2	10	10	10	8	10	3	10	3	5	10	10	10	10	5	3	6	4	FREE
AQUA3D	7.1	5	9	10	5	5	10	10	5	5	10	8	1	1	5	8	4	10	\$900
HSSM	7.1	10	10	10	8	8	3	3	3	8	10	10	10	10	4	3	6	10	FREE
AT123D	7.0	10	4	10	8	8	7	10	3	8	10	6	10	10	10	2	6	4	FREE
UNSATCHEM2D	7.0	10	10	10	1	4	9	10	10	8	3	3	10	9	6	4	6	4	FREE
PATH3D	6.9	5	9	8	5	5	10	10	10	5	10	8	1	1	5	8	4	4	\$400
SWIFT-98	6.9	0	9	5	5	8	10	10	7	5	10	8	10	1	5	8	4	5	\$400
FATMIC2D	6.9	10	10	10	10	8	3	10	3	8	3	9	10	8	3	1	6	4	FREE
HYDRUS-1D	6.8	10	6	10	8	8	1	7	3	8	10	8	10	7	6	8	8	10	\$600
FRACTRAN	6.7	10	10	5	5	5	3	10	10	5	7	8	1	1	5	8	5	10	\$1500

PROGRAM NAME	Ranking Sum	Water Balance	Subsurface Flow Capabilities	Transport Mechanisms	Biodegradation Reactions	Sorption/Volatilization	Dimensionality	Domain Variability	Mesh Flexibility	Data Requirements	Computational Requirements	Code Availability	Source Code Availability	Program Installation	Code Validation	Support Availability	Documentation Quality	Ease of Use	Cost \$ U.S
HYDROGEOCHEM2	6.7	5	10	10	5	8	3	10	7	5	10	8	1	1	5	8	5	10	\$5000
STAFF3D	6.7	5	10	10	3	8	10	10	3	5	10	4	1	1	5	5	5	10	\$15,000
BIOSCREEN	6.6	10	4	8	9	8	3	3	3	8	10	10	10	10	10	3	5	10	FREE
MIGRATEv9	6.6	10	10	10	8	8	3	7	1	8	10	4	1	7	5	5	5	10	\$2000
FRACMAN SUITE	6.6	5	10	10	3	8	7	10	10	5	7	4	1	1	5	0	5	10	\$10,000 annual
RAND3D	6.6	5	9	5	8	10	10	1	3	5	10	8	1	1	5	8	4	10	\$300
POLLUTEv6	6.5	5	10	10	3	8	10	7	1	8	3	8	1	8	5	5	4	10	\$1500
BIOCHLOR	6.5	10	9	8	8	8	3	1	1	8	9	10	10	10	4	3	5	10	FREE
MOC	6.5	10	9	10	8	8	3	10	3	8	10	2	10	10	3	3	1	4	FREE
ASM	6.4	10	9	10	8	8	3	10	3	8	3	9	10	7	4	1	3	4	FREE
SOLUTRANS	6.4	5	6	8	8	8	10	1	3	5	10	8	1	7	5	5	5	10	\$400
WINTRAN	6.4	10	9	10	8	8	3	1	3	8	10	8	1	7	5	8	4	10	\$800
DSTRAM	6.4	5	9	10	3	5	10	5	10	5	10	8	1	1	5	5	5	5	\$6000
ANALGWST	6.3	5	9	8	8	5	10	1	5	5	3	9	10	8	4	3	4	4	FREE
HYDRUS 6	6.3	10	6	10	8	8	1	7	3	8	8	9	10	10	8	1	8	4	FREE
SWANFLOW	6.3	5	10	10	5	5	10	1	3	5	10	8	10	1	6	8	4	4	\$200
TRAFRAP-WT	6.3	5	9	10	3	8	3	10	7	5	10	8	10	1	5	8	4	5	\$200
CHEMFLO2000	6.2	10	1	10	8	8	1	7	5	8	10	10	1	10	10	4	6	10	FREE
MOC DENSE	6.2	5	9	10	5	4	3	7	3	8	10	10	10	10	8	3	3	4	FREE
BIOMOC	6.1	10	9	8	9	8	3	1	3	8	3	9	10	8	10	3	3	4	FREE

PROGRAM NAME	Ranking Sum	Water Balance	Subsurface Flow Capabilities	Transport Mechanisms	Biodegradation Reactions	Sorption/Volatilization	Dimensionality	Domain Variability	Mesh Flexibility	Data Requirements	Computational Requirements	Code Availability	Source Code Availability	Program Installation	Code Validation	Support Availability	Documentation Quality	Ease of Use	Cost \$ U.S
UNSATCHEM	6.1	10	6	10	1	4	1	10	3	8	10	10	10	10	6	4	6	10	FREE
R-UNSAT	6.0	5	1	10	8	10	10	3	3	8	3	10	10	8	10	3	3	4	FREE
ARMOS	6.0	5	10	5	5	5	3	10	5	5	10	5	1	1	5	5	4	10	\$4000
LEACHM	6.0	10	1	10	8	10	1	7	3	8	10	10	10	10	9	4	6	4	FREE
N3DADE	5.9	10	1	10	8	8	10	1	3	8	3	9	10	8	8	1	6	4	FREE
SESOIL	5.9	10	1	10	8	10	1	7	3	8	10	4	10	10	10	8	6	4	FREE
BIO1D	5.8	10	6	8	9	8	1	7	3	5	10	8	1	1	5	8	4	8	\$300
BIOTRANS	5.8	5	10	10	8	10	3	5	5	5	5	6	1	1	5	5	5	5	\$2600
MOVER	5.8	5	6	10	5	5	3	10	3	5	10	8	1	1	5	8	4	10	\$1900
3DADE	5.7	10	1	10	8	8	10	1	3	8	3	9	10	8	3	1	6	4	FREE
SOLUTE	5.6	5	5	5	8	8	10	1	3	5	10	8	1	1	5	8	4	4	\$200
AGU-10	5.5	5	9	10	5	8	5	1	5	5	3	8	10	1	5	8	4	4	\$200
VENT3D	5.5	10	1	10	1	8	10	10	10	5	10	4	1	1	1	4	4	4	Unknown
PRINCE	5.4	5	5	10	8	8	3	1	3	5	10	8	1	1	5	8	4	10	\$400
PRZM3	5.4	10	1	10	8	10	1	1	3	8	10	10	10	10	6	3	8	4	FREE
RBCA TIER2 ANALYZER	5.4	5	9	10	4	8	3	1	3	5	10	8	1	1	5	8	4	10	\$700
SPILLCAD	5.4	5	10	10	3	8	5	5	5	5	5	4	5	1	5	5	5	4	\$1000
CHEMFLO	5.3	10	1	10	8	8	1	7	5	8	10	10	1	10	2	1	5	5	FREE
VERTPAK-1	5.3	5	5	10	8	8	3	1	3	5	10	8	10	1	5	8	4	4	\$200
AIRFLOW/SVE	5.3	5	1	5	1	8	7	10	5	5	10	8	1	1	5	8	4	10	\$600

PROGRAM NAME	Ranking Sum	Water Balance	Subsurface Flow Capabilities	Transport Mechanisms	Biodegradation Reactions	Sorption/Volatilization	Dimensionality	Domain Variability	Mesh Flexibility	Data Requirements	Computational Requirements	Code Availability	Source Code Availability	Program Installation	Code Validation	Support Availability	Documentation Quality	Ease of Use	Cost \$ U.S
RANDOM WALK	5.3	5	5	5	8	8	3	3	3	5	10	8	10	1	5	8	4	4	\$200
FATE5	5.2	10	6	8	8	5	1	1	5	5	10	5	1	1	5	5	4	10	\$300
NAPL Simulator	5.2	10	1	10	8	10	1	7	3	5	3	9	10	8	4	3	6	4	FREE
FOCUS PRZM	5.2	10	1	10	8	10	1	1	3	5	10	10	1	10	6	1	3	10	FREE
PESTAN	5.1	10	1	10	8	8	1	1	3	8	3	10	10	6	10	8	3	4	FREE
EMSOFT	5.0	10	1	10	8	10	1	1	3	5	10	10	10	10	4	3	3	4	FREE
BEAVERSOFIT	5.0	5	4	8	5	5	3	10	3	5	10	8	1	1	5	8	4	4	FREE
PARSSIM	5.0	5	5	10	9	1	5	5	5	5	3	3	5	3	5	1	1	5	FREE
RITZ	5.0	10	1	5	8	10	1	1	3	5	10	10	1	10	4	3	3	10	FREE
DUST-BNL	4.8	5	4	10	5	2	5	5	5	5	5	5	5	1	5	5	5	5	\$1300
OILVOL	4.8	5	1	1	5	5	5	5	5	5	5	8	5	1	5	8	4	10	\$300
ONED	4.8	5	5	10	8	8	1	1	3	5	3	8	10	1	5	8	4	4	\$100
MAGNUM 2D	4.8	5	9	10	3	8	5	1	5	5	5	1	5	1	5	1	5	5	Unknown
VENT2D	4.8	10	1	10	1	8	3	10	3	5	10	10	1	10	1	4	6	4	FREE
VAPEX	4.7	5	1	10	3	10	5	5	5	5	10	4	5	1	5	5	5	5	Unknown
CMLS94	4.7	10	1	8	8	8	1	7	3	5	3	9	1	10	5	1	3	4	FREE
BIOTRENDS	4.5	5	1	5	8	5	1		5	5	10	8	1	1	4	8	5	10	\$1000
DPCT	4.5	5	5	5	1	8	5	5	5	5	5	4	5	1	5	5	5	5	\$1300
VIRALT	4.5	5	10	10	1	8	3	1	3	5	3	8	1	1	5	8	4	4	\$100
VLEACH	4.5	10	1	10	1	10	1	1	3	8	3	10	10	6	10	8	6	4	FREE

PROGRAM NAME	Ranking Sum	Water Balance	Subsurface Flow Capabilities	Transport Mechanisms	Biodegradation Reactions	Sorption/Volatilization	Dimensionality	Domain Variability	Mesh Flexibility	Data Requirements	Computational Requirements	Code Availability	Source Code Availability	Program Installation	Code Validation	Support Availability	Documentation Quality	Ease of Use	Cost \$ U.S
CONTAM	4.4	10	1	10	1	10	1	1	3	5	9	10	10	10	2	1	1	10	FREE
MULTIMED	4.4	5	6	10	8	8	1	1	3	5	3	3	1	3	8	3	5	4	FREE
BIOVENTING	4.2	5	1	5	3	5	5	5	5	5	5	6	5	1	5	5	5	5	Unknown
GETOUT	4.2	5	1	10	5	8	1	7	3	5	5	4	10	1	5	1	5	4	\$1300
BioSVE	4.1	5	1	5	4	8	1	1	3	5	10	8	1	1	5	8	4	10	\$400
SWAGMAN	4.1	10	1	10	3	8	1	7	3	8	10	1	1	1	8	1	5	4	Unknown
2D_V_HYDRO_S	4.0	5	10	10	1	8	5	5	5	5	1	2	0	2	0	1	1	1	FREE
AIR2D	4.0	5	1	5	1	5	3	5	5	5	3	9	10	6	4	3	5	5	FREE
SAM	4.0	10	1	8	3	6	1	7	3	5	8	1	10	1	5	2	4	4	FREE
BIOTRACKER	3.9	10	1	1	3	5	1	1	3	5	10	8	1	1	4	8	5	10	\$500
SUMMERS	3.9	10	1	8	1	8	1	1	3	5	10	8	10	1	4	8	4	4	\$100
PAGAN	3.8	5	6	10	3	5	1	1	3	5	10	4	1	1	5	1	5	4	\$1300
DIFMOD	3.5	10	1	10	3	5	1	1	3	5	3	4	10	1	5	1	5	5	\$1300
2PAR_DEGRADE	0.0																		
3D FE DUAL	0.0																		
ADE	0.0																		
BALANCE	0.0																		
BIOMOD3D	0.0																		
BIOPLUME II	0.0																		
BLT FEMWATER	0.0																		

PROGRAM NAME	Ranking Sum	Water Balance	Subsurface Flow Capabilities	Transport Mechanisms	Biodegradation Reactions	Sorption/Volatilization	Dimensionality	Domain Variability	Mesh Flexibility	Data Requirements	Computational Requirements	Code Availability	Source Code Availability	Program Installation	Code Validation	Support Availability	Documentation Quality	Ease of Use	Cost \$ U.S	
BTEX	0.0																			
CADIL_AGTEHM	0.0																			
CANVAS	0.0																			
Dominico	0.0																			
EPA-VHS	0.0																			
EXPRESS	0.0																			
FEHM	0.0																			
FEMSEEP	0.0																			
FEMWASTE	0.0																			
FEMWATER/LEWASTE	0.0																			
FEMW-FEMA	0.0																			
FLOW2D	0.0																			
FLOWTHRU	0.0																			
FRACFLO	0.0																			
FTRAN	0.0																			
GASSOLVE	0.0																			
HPS	0.0																			
HYPERVENTILATE	0.0																			
ICE-1	0.0																			
KYSPILL	0.0																			

PROGRAM NAME	Ranking Sum	Water Balance	Subsurface Flow Capabilities	Transport Mechanisms	Biodegradation Reactions	Sorption/Volatilization	Dimensionality	Domain Variability	Mesh Flexibility	Data Requirements	Computational Requirements	Code Availability	Source Code Availability	Program Installation	Code Validation	Support Availability	Documentation Quality	Ease of Use	Cost \$ U.S	
MACRO	0.0																			
MAP	0.0																			
MARTHE	0.0																			
MOTIF	0.0																			
MOTRANS	0.0																			
MS-VMS	0.0																			
MULAT	0.0																			
NEFTRAN II	0.0																			
PATRIOT	0.0																			
PLUME	0.0																			
PLUME2D	0.0																			
POLUT2D	0.0																			
PRZM	0.0																			
PRZM2	0.0																			
PULSE	0.0																			
ROAM	0.0																			
RWH	0.0																			
SATURN	0.0																			
SEFTRANS	0.0																			
SIMULAT	0.0																			

PROGRAM NAME	Ranking Sum	Water Balance	Subsurface Flow Capabilities	Transport Mechanisms	Biodegradation Reactions	Sorption/Volatilization	Dimensionality	Domain Variability	Mesh Flexibility	Data Requirements	Computational Requirements	Code Availability	Source Code Availability	Program Installation	Code Validation	Support Availability	Documentation Quality	Ease of Use	Cost \$ U.S
SOILCO2	0.0																		
Split	0.0																		
SWICHA	0.0																		
SWIFT II	0.0																		
T2VOC	0.0																		
TBC	0.0																		
TDPLUME	0.0																		
TMVOC	0.0																		
TRAC3D	0.0																		
TRAFRAP	0.0																		
USGS-SOL	0.0																		
VADSAT	0.0																		
VIRTUS	0.0																		
VSAFT2	0.0																		

= Insufficient data to fully verify.

* GMS Package FEMWATER, MODFLOW, MT3D, RT3D, MODPATH, UTCHEM, SEEP2D = \$7600 U.S.

GMS FEMWATER Package = \$2000 U.S.

GMS MODFLOW, MODPATH, MT3D, RT3D = \$3350 U.S.

Visual MODFLOW package for MODFLOW, MODPATH, MT3D, RT3D, and WINPEST = \$1990 U.S

** ARGUS ONE all modules = \$2475 U.S.

Codes were given a ranking of 0 for the following reasons:

- They could not be found;
- There was no North American distributor;
- They are obsolete or have been replaced by a newer code.

Appendix C 3D Detailed Input Data

Variable	Unit	Program	
		T2VOC	FEMWATER
			R
SOIL PROPERTIES:			
Moisture Content			
Saturated Moisture Content (θ_s)	--	0.4	0.4
Residual Moisture Content (θ_r)	--	0.1	0.1
Coefficient of Permeability			
Saturated Hydraulic Conductivity (Ks)	m/d	0.21	0.21
SWCC			
Relative Permeability Function	--	Modified Stone	Van Genutchen
Capillary Pressure Function	--	Parker	Van Genutchen
Compressibility	md ² /kg	none	1.58x10 ⁻¹⁸
Tortuosity	--	0	0.5
Degree of Anisotropy	--	1	1
Bulk Density	kg/m ³	2650	2650
SOLUTE PROPERTIES:			
Dispersion Properties			
Longitudinal Dispersivity	m	No Option	0
Transverse Dispersivity	m	No Option	0
Molecular Diffusion Coefficients			
Diffusion Coefficient (o-xylene)	m ² /d	No Option	1.44x10 ⁻⁶
Diffusion Coefficient (air)	m ² /d	No Option	0
Adsorption Coefficients	--	0	0
Decay Coefficients	--	0	0
Organic Carbon Partition Coefficient	--	0	No Option
Organic Carbon Fraction	--	0	0
Wet Heat Conductivity	W/m-C	3.1	No Option
Dry Heat Conductivity	W/m-C	2.85	No Option
Specific Heat	J/kg-C	1000	No Option
Temperature Dependent Parameters			
Chemical Critical Temperature	K	630.3	No Option
Chemical Critical Pressure	--	37.3	No Option
Chemical Critical Compressibility	--	0.262	No Option
Pitzers Acentric Factor	--	0.31	No Option
Chemical Dipole Moment	--	0.5	No Option
Chemical Normal Boiling Point	K	417.6	No Option
Chemical Vapor Pressure Constant	--	-7.53357	No Option
Chemical Vapor Pressure Constant2	--	1.40968	No Option
Chemical Vapor Pressure Constant3	--	-3.10985	No Option

Variable	Unit	Program	
		T2VOC	FEMWATER
Chemical Vapor Pressure Constant4	--	-2.85922	No Option
Chemical Molecular Weight	g/mol	106.18	No Option
Chemical Ideal Gas Heat Capacity Constant	--	-15.85	No Option
Chemical Ideal Gas Heat Capacity Constant2	--	0.5962	No Option
Chemical Ideal Gas Heat Capacity Constant3	--	-3.443x10 ⁻⁴	No Option
Chemical Ideal Gas Heat Capacity Constant4	--	7.528x10 ⁻⁸	No Option
Reference Density for NAPL	kg/m ³	880	No Option
Reference Temperature for NAPL	K	293	No Option
Reference Binary Diffusivity of VOC in air	m ² /s	8x10 ⁻⁶	No Option
Reference Temperature for gas diffusivity	K	273	No Option
Chemical diffusivity exponent	--	1.93	No Option
Liquid NAPL viscosity constant	--	-3.332	No Option
Liquid NAPL viscosity constant2	--	1039	No Option
Liquid NAPL viscosity constant3	--	-1.768x10 ⁻³	No Option
Liquid NAPL viscosity constant4	--	1.706x10 ⁻⁶	No Option
Chemical Critical Volume	m ³ /mol	3.690x10 ⁻⁴	No Option
Water solubility constant A	--	2.975x10 ⁻⁶	No Option
Water solubility constant B	--	0	No Option
Water solubility constant C	--	0	No Option
Water solubility constant D	--	0	No Option
Air vapor diffusion		0	No Option
Vapor air temperature dependence		1.8	No Option