
Guidelines for Use of Groundwater Spreadsheet Models in Risk-Based Corrective Action Design

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ABSTRACT

For use in risk-based corrective action design, simple analytical spreadsheet models can provide a cost-effective means of predicting groundwater plume migration and developing site-specific remediation standards. Such models are therefore commonly recommended as a conservative first step in the corrective action planning process, prior to use of more complex numerical modeling methods. However, the reliability of an analytical model as a conservative predictor of potential health and environmental impacts depends upon proper characterization of key contaminant transport and attenuation parameters. This paper provides practical guidelines for the application of spreadsheet-based analytical models to exposure assessments, including a newly developed procedure for characterization of contaminant biodegradation rates.

Analytical equations can be used for analysis of contaminant transport under homogeneous, isotropic conditions, based on site-specific groundwater flow parameters and contaminant characteristics. These analytical models can be programmed in spreadsheet format, facilitating rapid estimation of potential impacts at off-site receptor points as well as back-calculation of applicable soil and groundwater clean-up standards. In this paper, guidelines for proper application of such spreadsheet models are demonstrated by comparing results of the analytical contaminant transport expression developed by Domenico and Robbins (1985) to those generated by the BIOPLUME II numerical modeling program (Rifai et al, 1987). However, the procedures outlined below can be generally applied to extend the utility of any properly validated analytical model:

- **Model Selection:** The model should be matched to the complexity of natural site conditions and to the degree of resolution provided by the existing site database. Steady-state analytical expressions provide significant advantages in terms of ease of use, speed of operation, and interactive sensitivity analysis. However, given adequate site data, numerical models may be required to properly account for flow field heterogeneities and complex biodegradation processes.

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- **Source Term Characterization:** The source term must be calculated to match current plume concentrations and to account for the presence of non-aqueous phase liquids (NAPLs). Guidelines are provided for source term characterization in the Domenico model based on a "layer-cake" approximation of the transverse plume cross-section.
 - **Aerobic Biodegradation:** Many analytical contaminant transport models incorporate a first-order decay equation to account for aerobic microbial biodegradation of organic plume constituents. However, by neglecting oxygen limitations, such first-order expressions commonly overestimate the rate and degree of natural biodegradation in groundwater systems (Borden et al, 1986a; Lee et al, 1987). Guidelines are provided for use of an oxygen superposition method with the Domenico analytical model that generates results consistent with those of BIOPLUME II.
 - **Management of Parameter Uncertainty:** For spreadsheet-based analytical models, the effect of parameter uncertainty on modeling results can be readily evaluated using companion statistical packages such as Crystal Ball. For a given site, the degree of variability observed in key modeling parameters will determine whether the deterministic or probabilistic modeling method produces the more conservative result.

RISK-BASED CORRECTIVE ACTION MODELING

Risk-based corrective action planning involves i) characterization of contaminant sources, migration pathways, and receptors, and ii) selective application of corrective measures as needed to control potential risks to human health or the environment. In this planning process, contaminant transport models are commonly employed to predict potential contaminant concentrations at possible points of exposure and to determine the media cleanup standards required to prevent exceedence of applicable human health and ecological protection criteria.

Typically, such risk assessment analyses involve application of numerical models (e.g., finite-difference, finite-element, etc.) to estimate the degree of natural contaminant dilution-attenuation occurring within a multidimensional heterogeneous flow regime. However, in recent years, efforts have been made to develop less complex risk assessment tools, both to expedite the corrective action planning process and to facilitate timely review by regulatory authorities. For example, the "ASTM Guide for Risk-Based Corrective Action Applied at Petroleum Release Sites" recommends a three-tiered planning process designed to match site investigation and risk assessment procedures to the size and complexity of the site (American Society for Testing and Materials, 1994). Under Tiers 1 and 2 of the ASTM program, if contaminant concentrations are found to exceed generic health-based limits, site-specific media cleanup standards are calculated using screening-level analytical models for soil, groundwater, and air exposure pathways. Tier 3 of the ASTM program, involving detailed numerical modeling analyses, is conducted only if the site complexity or potential remediation cost warrants the additional time and expense required for further data collection and analyses.

Analytical models, such as those identified on the ASTM Guide, are readily converted to spreadsheet format and, as such, can provide significant advantages over more complex numerical modeling methods in terms of ease of operation and interpretation. Consequently, spreadsheet-based analytical models are increasingly recommended as a conservative and cost-effective first step in the corrective action planning process. However, as can be readily demonstrated, the reliability of an analytical model as a conservative predictor of potential health and environmental impacts depends upon proper characterization of key contaminant transport and attenuation parameters. In addition, concerns remain regarding the relative accuracy of the analytical model compared to the more sophisticated numerical solutions, particularly with regard to source characterization, contaminant biodegradation, and management of parameter uncertainty.

To address these issues, this paper presents practical guidelines for 1) selecting the appropriate modeling method, based on available site information, and 2) extending the utility of spreadsheet-based analytical methods to achieve accurate and conservative results that are consistent with more complex numerical solutions.

MODEL SELECTION GUIDELINES

For use in risk-based corrective action planning, the "best" model for a given site will be the simplest model providing a reliable and reasonably conservative prediction of potential exposure. The choice between analytical and numerical modeling methods should be dictated by the adequacy of the site database and the relative degree of error likely to be introduced by the model itself. General guidelines for application of spreadsheet-based analytical models for contaminant transport analyses are provided below.

Steady-State vs. Transient Analyses

Under current EPA risk assessment guidelines (U.S. EPA 1989a, 1989b, and 1991), the potential human health or ecological resource effects associated with a contaminated site are based upon the assumption that the receptor will be chronically exposed to the contaminated environmental media. Media cleanup standards (or control methods) applied at the contaminant source zone must be designed to prevent exceedance of applicable human health and ecological protection criteria at likely points of exposure *at any future time*. To address maximum chronic future effects, the contaminant transport model(s) used to predict baseline exposure concentrations must therefore be run to determine steady-state rather than transient plume concentrations. Under steady-state conditions, numerical models, which were developed principally to simulate transient flow processes, provide results consistent with analytical solutions to the advection-dispersion equation. Consequently, exclusive of the additional considerations addressed below, for risk assessment applications, the numerical model provides no significant advantage in terms of accuracy relative to the simpler analytical model. In addition, some numerical models will require very prolonged run times in order to define steady-state conditions.

- *Summary Point:* Steady-state contaminant transport models must be used to conform with current EPA risk assessment guidelines. In steady-state applications, analytical and numerical modeling methods are in reasonably good agreement.

Inherent Modeling Error

To achieve reliable modeling results, it is important to recognize the degree of error introduced by both *external* and *internal* modeling parameters. External parameters, those variables which are matched to actual site conditions (e.g., hydraulic conductivity, soil porosity, source concentrations, etc.), must be estimated on the basis of available site data. Each estimate introduces an additional and often unquantified error into the modeling calculation, particularly when very limited or no direct site measurements are available for that parameter. Experienced modelers will also recognize the variability introduced by internal modeling parameters, i.e., those variables adjusted to define or discretize the model flow field (e.g., source input type, cell size, grid size, boundary conditions, etc.). For example, for a given site condition, (i.e., given set of external parameters), significantly different results can be obtained by variation of model cell size and grid dimensions.

Due to the greater number of both external and internal variables associated with numerical models, such tools entail a greater propensity for error than the simpler analytical model. Therefore, proper application of numerical models requires detailed characterization of site variables, as well as

sensitivity analyses for all internal parameters to ensure model stability. In this regard, analytical models, involving far fewer variables, not only prove easier and faster to use, but are more accessible to third party review. In assessing the relative accuracy of these alternative methods for a given site, the user must weigh the simplifying assumptions of the analytical model (e.g., homogeneous, isotropic conditions) against the degree of parameter "guesstimation" required for use of a numerical method.

- *Summary Point:* In terms of accuracy, the bigger model is not necessarily better. To provide reliable results, the model complexity should be matched to the degree of resolution provided by the site database.

Special Site Conditions

If the site database evidences significant nonhomogeneous conditions within the contaminant flow regime, analytical models cannot be relied upon to provide a conservative estimate of long-term exposure concentrations. For groundwater flow, such cases would include natural or man-made flow field heterogeneities, such as significant spatial variability in hydraulic conductivity and hydraulic gradient or the presence of pumping or injection wells. Numerical models will also be required to characterize complex contaminant decay or geochemical processes. For example, the BIOPLUME II model (Rifai et al, 1987) is presently being updated by H. Rifai to address anaerobic biodegradation processes that are rate-limited by alternative electron receptors, such as nitrate, sulfate, or iron.

- *Summary Point:* Numerical models should be used if long-term contaminant transport will be strongly affected by flow field heterogeneities or complex biochemical processes.

ANALYTICAL MODELING GUIDELINES

Several analytical models are presently available for 2-D or 3-D analysis of contaminant transport under homogeneous, isotropic conditions, based on site-specific groundwater flow parameters and contaminant characteristics (ASTM, 1994; Wilson and Miller, 1978; Domenico and Robbins, 1985). Although relatively simple to operate, these models can be configured to provide results that are consistent with more complex numerical modeling tools, when used for steady-state exposure assessments. The analytical modeling guidelines presented below have been demonstrated by comparing the results of the Domenico analytical transport model (Domenico and Robbins, 1985; Domenico, 1987) in spreadsheet format to those generated by BIOPLUME II (Rifai et al, 1987). However, these procedures can be generally applied to extend the utility of any properly-validated analytical model.

Source Term Characterization

To provide an accurate prediction of contaminant migration patterns within the groundwater flow system, the model source term should be calibrated to match the current plume concentrations measured in the aquifer. In most analytical flow models, the contaminant source input term is characterized as a constant-flux or constant-concentration point, line, or area source — providing limited ability to match the actual variation of contaminant concentrations within the plume. To improve the model calibration, the source zone should therefore be characterized as a set of multiple source terms (i.e., multiple points, lines, or areas) configured to match the transverse cross-sectional concentration distribution of the actual plume.

An example of this source zone characterization for the Domenico analytical contaminant transport model is illustrated on Figures 1 and 2. As shown on Figure 1, the transverse plume cross-section at the source zone location can be approximated by a stacked set of area source terms, resembling a

"layer-cake" configuration. Steady-state plume concentrations predicted by the Domenico model for cases of a single source term and multiple source term are compared to the output of BIOPLUME II (without biodegradation) for equivalent aquifer conditions on Figure 2. As shown, the "layer cake" source configuration significantly improves the agreement of the Domenico analytical model with BIOPLUME II for this steady-state, no-biodegradation case.

In establishing the model source term, the presence or absence of non-aqueous phase liquids (NAPLs) must also be addressed. Prior field studies have shown NAPL dissolution to occur at a relatively slow rate, comprising a long-term source of contaminant release to the groundwater flow system (Newell, Connor, Wilson, 1990). Consequently, if NAPLs are known or suspected to be present in the subsurface, the source term should be calibrated to existing plume concentrations and assumed to remain constant over time. Guidelines for evaluation of the impact of NAPLs on groundwater remediation efforts are provided by Newell, Bowers, Rifai (1994).

- *Summary Point:* The source term in an analytical model can best be matched to the transverse plume cross-section using a multi-source configuration (e.g., "layer-cake" for the Domenico model). If NAPLs are present within the subsurface, the source term should be assumed to remain constant, with no significant attenuation over time, to obtain a conservative value for risk assessment or design.

Simulation of Contaminant Biodegradation

Research has demonstrated that, under appropriate conditions, many organic compounds are subject to aerobic biodegradation by microbial organisms during transport within the subsurface groundwater flow regime (Wilson et al, 1983; Bedient, Rifai, Newell, 1994). For risk assessment applications, proper characterization of the rate and degree of such contaminant biodegradation is required for accurate estimation of potential long-term exposure levels. As demonstrated in prior studies, biodegradation of amenable organics is principally limited by the concentration of dissolved oxygen within the saturated zone (Borden and Bedient, 1986a; Lee et al, 1987). Because microbial biodegradation kinetics are fast in comparison to the rate of oxygen transport in the groundwater flow system, Borden has demonstrated that the biodegradation process can be simulated as an instantaneous reaction between the organic contaminant and oxygen. This simplifying assumption was incorporated into the BIOPLUME I numerical model which calculated organic loss by superposition of background oxygen concentrations onto the organic contaminant plume. In BIOPLUME II, a dual-particle mover procedure was incorporated to more accurately simulate the separate transport of oxygen and organic contaminants within the subsurface (Rifai et al, 1987; Rifai, et al, 1988).

In most analytical modeling applications, contaminant biodegradation is estimated using a first-order decay equation, with the biodecay half-life values determined from research literature or site data. However, by ignoring oxygen limitation effects, such first-order expressions can significantly overestimate the rate and degree of biodegradation, particularly within low-flow regimes where the rate of groundwater plume reaeration is very slow (Rifai, 1994). As a more accurate method of analysis, C. Newell has recommended incorporation of the concept of oxygen superposition into an analytical model, in a manner similar to that employed in BIOPLUME I. By this method, contaminant mass concentrations at any location and time within the flow field are corrected by subtracting 1 mg/L organic mass for each 3 mg/L of background oxygen, in accordance with the instantaneous reaction assumption. Borden et al (1986b) concluded that this simple superposition technique was an exact replacement for more sophisticated oxygen-limited expressions, as long as the oxygen and hydrocarbon had the same transport rates (e.g., retardation factor, $R = 1$).

For an equivalent flow system and plume concentration, Figures 3A and 3B alternately compare the results obtained from the Domenico analytical model using i) the traditional first-order decay

equation and ii) the new oxygen-superposition method to the output of BIOPLUME II. As shown on Figure 3A, the steady-state benzene concentration predicted along the plume centerline by the Domenico model using first-order decay differs dramatically from BIOPLUME II results. In this case, even though the benzene decay half-life was matched to the upper-range (i.e., slowest) value reported in the literature (Howard et al, 1991), use of the first-order decay relationship significantly overestimated biodegradation effects in comparison to BIOPLUME II. In contrast, for this same case, incorporation of the simple oxygen-superposition function into the Domenico model provides a steady-state plume prediction in close agreement with the BIOPLUME II model (see Figure 3B).

In their original work, Borden et al (1986b) noted that, for highly sorptive contaminants, the oxygen-superposition method might erroneously characterize biodegradation due to the differing transport rates of dissolved oxygen and the organic contaminant within the aquifer matrix. However, as illustrated on Figure 4, BIOPLUME I (oxygen superposition method) and BIOPLUME II (dual particle transport) are in reasonable agreement for contaminant retardation factors as high as 6. Therefore, the oxygen-superposition method can be employed as a reasonable approximation of BIOPLUME II regardless of contaminant sorption characteristics.

- *Summary Point:* Due to oxygen limitations, aerobic biodegradation of organic contaminants in groundwater cannot be accurately characterized using a first-order decay equation. Rather, a much more accurate prediction of biodegradation effects can be achieved by modifying a steady-state analytical flow model to incorporate the simple oxygen-superposition method. This superposition method works well even for sites with retardation factors greater than 1.

Management of Parameter Uncertainty

For spreadsheet-based analytical models, the effect of parameter uncertainty or variability on model results can be readily evaluated by coupling the spreadsheet model with a companion statistical package such as Crystal Ball (Decisioneering, 1993). Based on the variability of each input parameter, Crystal Ball calculates a cumulative probability distribution for each specified output value (e.g., contaminant concentration, carcinogenic risk, etc.). When applied to exposure assessments, this application constitutes *probabilistic* risk assessment, as opposed to the more traditional *deterministic* assessment in which a unique result is obtained for each output value.

This probabilistic approach provides the user with very sophisticated information regarding the possible level of risk posed to a receptor. An example of Crystal Ball output for the Domenico model, for the same case addressed above, is presented on Figures 5A and 5B. For the purpose of this example, three critical modeling parameters (i.e., hydraulic conductivity, plume source concentration, and background oxygen concentration) have been assumed to vary in accordance with the range and type of distribution commonly observed for these parameters at actual sites. Figure 5a presents a probability distribution for the carcinogenic risk associated with human ingestion of groundwater from a well located 100 ft downgradient of the contaminant (benzene) source zone, calculated for a residential exposure scenario per EPA guidelines (U.S. EPA, 1989b). As shown, for a well at this location, model results indicate the probability of exceeding an excess lifetime carcinogenic risk of $1.0E-4$ to be 84%, based on standard exposure factors specified in EPA guidelines. By comparison, the deterministic risk value calculated for this well location (based upon mean parameter input values) is $3.0E-4$, corresponding to a 49% value on the probability distribution (i.e., 51% chance of exceedance), which is in reasonable agreement with the probabilistic result.

The predicted carcinogenic risk level versus distance from the contaminant source is plotted for various probability percentiles (i.e., 50%, 85%, 95%) on Figure 5B. As shown for this case, deterministic risk values calculated on the basis of upper 95% distribution values for the critical modeling parameters correspond to probabilistic values in the 85% to 95% probability range. No

guidelines have yet been issued by the EPA regarding the "acceptable" probability level for this type of risk analysis. However, in development of the Toxicity Characteristic threshold values for RCRA hazardous wastes, the EPA used the 85% probability level to define anticipated health risks.

- *Summary Point:* For evaluation of parameter uncertainty, spreadsheet-based analytical models can be easily converted for probabilistic risk assessment, using a companion statistical package such as Crystal Ball. For a given site, the degree of variability observed in key modeling parameters will determine whether the deterministic or probabilistic modeling method produces the more conservative result.

CONCLUSION

For use in risk-based corrective action planning, spreadsheet-based analytical contaminant transport models offer significant advantages over more complex numerical modeling methods in terms of ease of operation and interpretation. For appropriate site conditions, these analytical models can be operated in accordance with the general guidelines provided above to provide results that are in good agreement with more complex and time-consuming numerical modeling methods.

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Figure 1

Schematic of Multiple-Term Source Configuration for Domenico Model

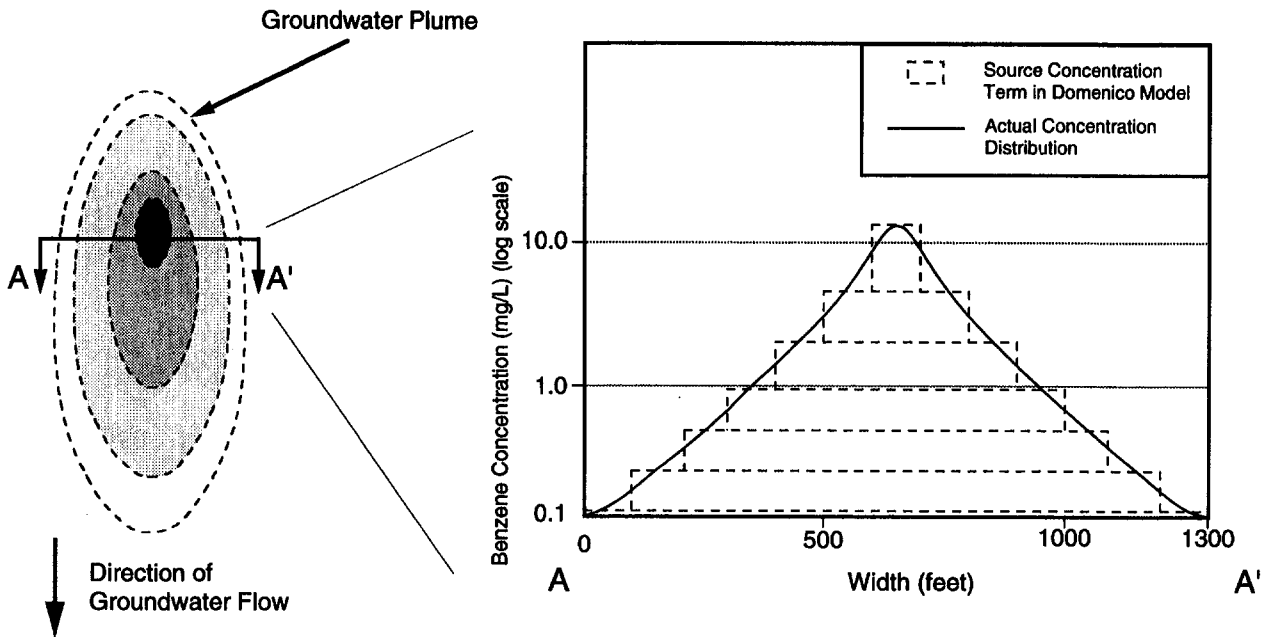
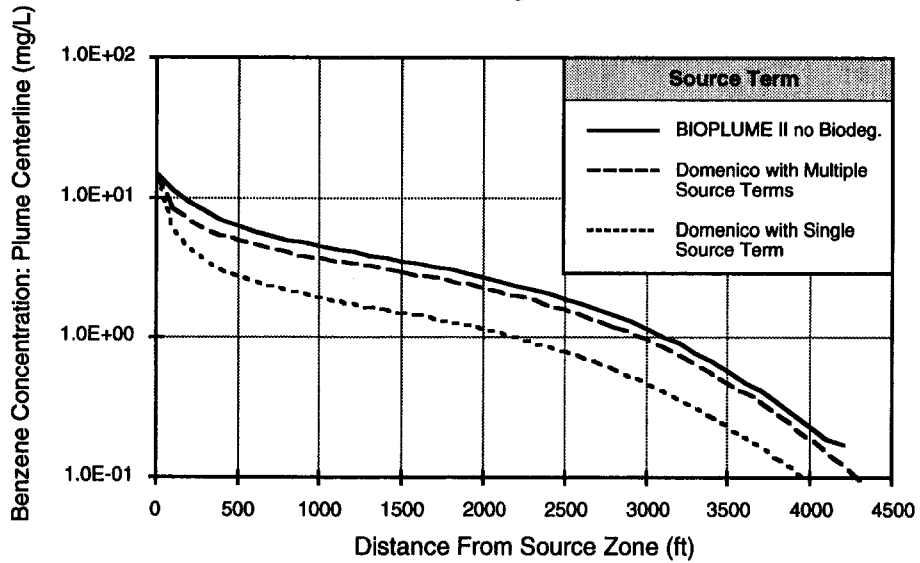


Figure 2

Comparison of Domenico Model with Single-Term and Multi-Term Source Configurations to BIOPLUME II



Parameters Used in Domenico Model

Hydraulic Conductivity = 1.0E-3 cm/sec
 Hydraulic Gradient = 0.013 ft/ft
 Porosity = 0.25
 Longitudinal Dispersivity = 150 ft
 Transverse Dispersivity = 45 ft
 Time = 50 yr
 Constituent Half-Life = 730 day
 Background Oxygen Concentration = 4.0 mg/L
 Source Depth = 5.0 ft

Source Parameters Used in Domenico Model

Source Width (Single Source) = 100 ft
 Source Concentration (Single Source) = 15.1 mg/L
 Multiple-Term Source:

Source Width (ft)	Source Concentration (mg/L)
100	15.1
300	4.8
500	2.0
700	0.9
900	0.4
1100	0.2
1300	0.1

Figure 3A

Comparison of Domenico Model w/ First-Order Decay Method to BIOPLUME II

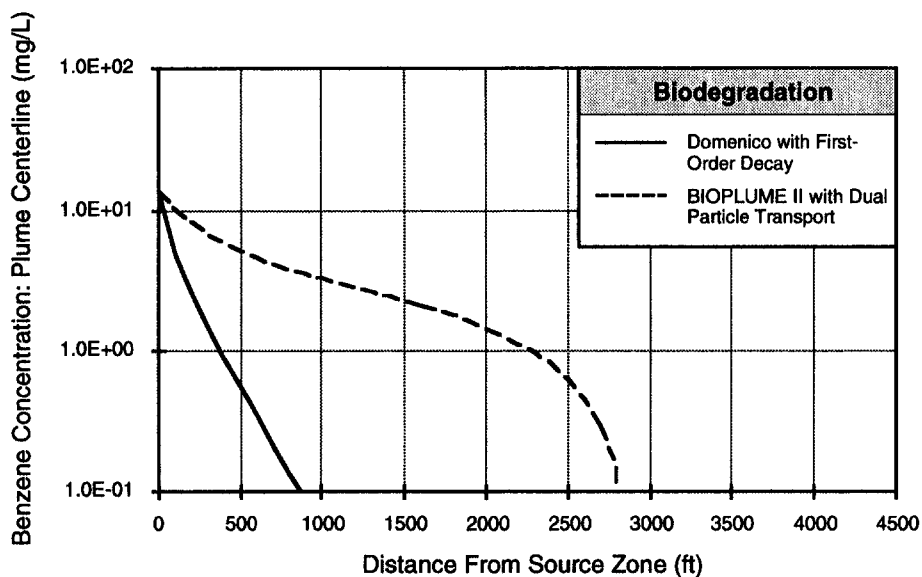
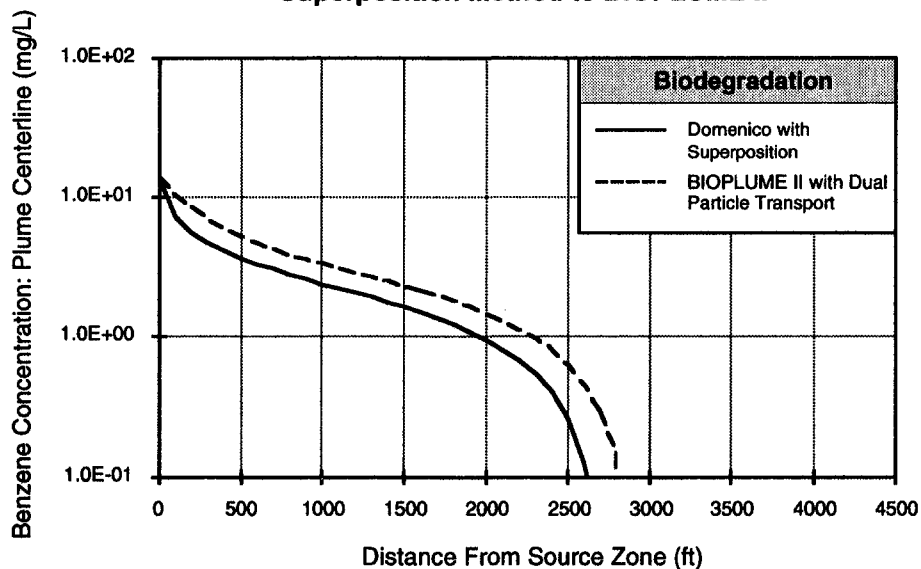


Figure 3B

Comparison of Domenico Model w/ Oxygen Superposition Method to BIOPLUME II

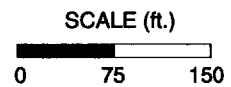
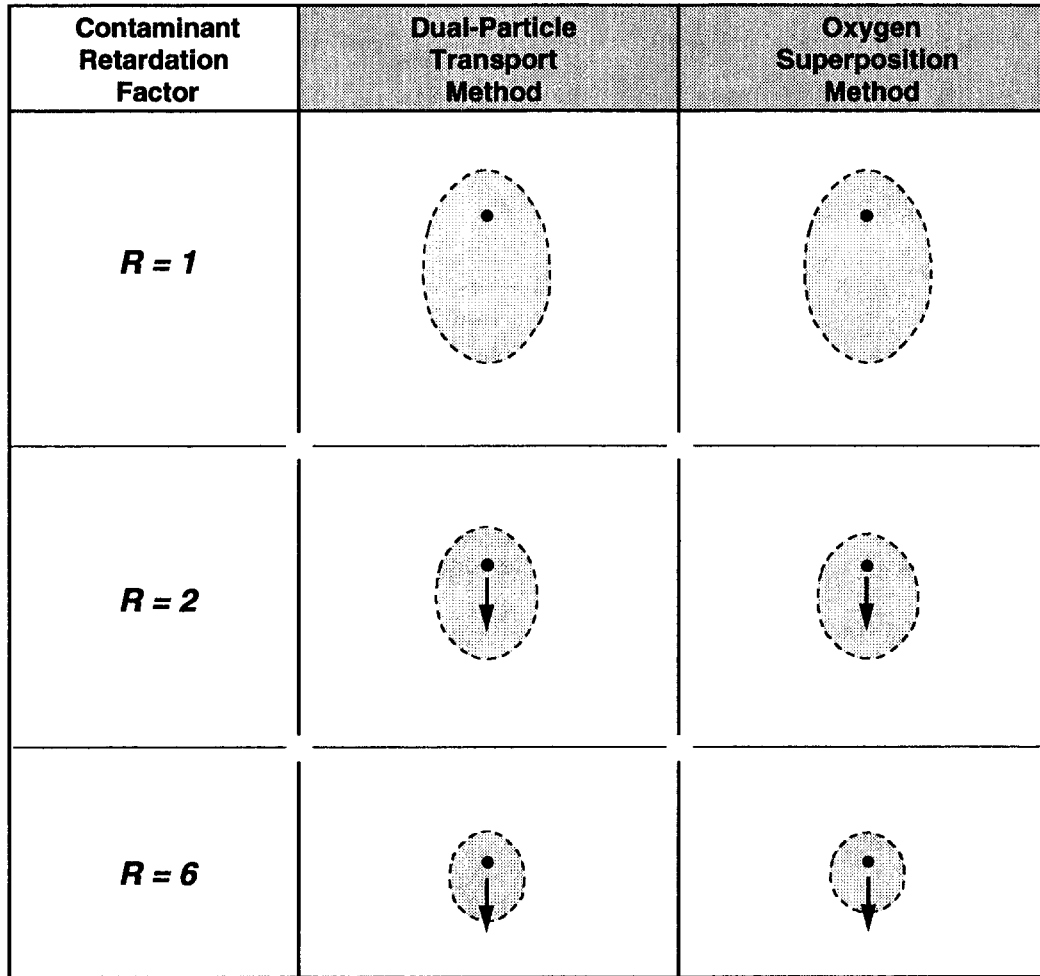


Parameters Used in Domenico and BIOPLUME II Models

Hydraulic Conductivity = 1.0E-3 cm/sec	Time = 50 yr
Hydraulic Gradient = 0.013 ft/ft	Constituent Half-Life = 730 day
Porosity = 0.25	Background Oxygen Concentration = 4.0 mg/L
Longitudinal Dispersivity = 150 ft	Domenico Source Term: See Figure 1.
Transverse Dispersivity = 45 ft	

Figure 4

Steady-State Plume Concentration Contours Predicted by Optional Biodegradation Methods Using BIOPLUME II Model



Input Parameters for Hypothetical Case Simulated on BIOPLUME II:

Plume Contour: 0.005 mg/L
 Grid Size: 25 x 50 Cells
 Cell Size: 10 ft x 10 ft
 Thickness: 5 ft
 Transmissivity: $1.5E-4 \text{ ft}^2/\text{sec}$
 Hydraulic Gradient: 0.017 ft/ft
 Source Injection Rate = $0.0001 \text{ ft}^3/\text{sec}$
 Injection Concentration = 30 mg/L

Dual Particle Transport Method

Background Oxygen Concentration: 4 mg/L

Oxygen Superposition Method

Oxygen Utilization Factor: 3

Reference for BIOPLUME II: Rifai et al, 1987

Figure 5A
Probabilistic Distribution of Risk 100 feet
Downgradient of Source Zone

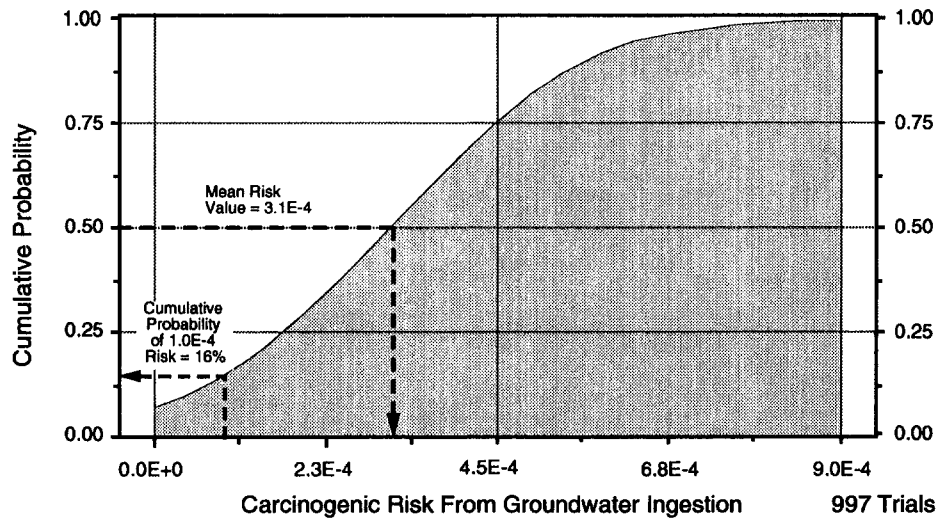
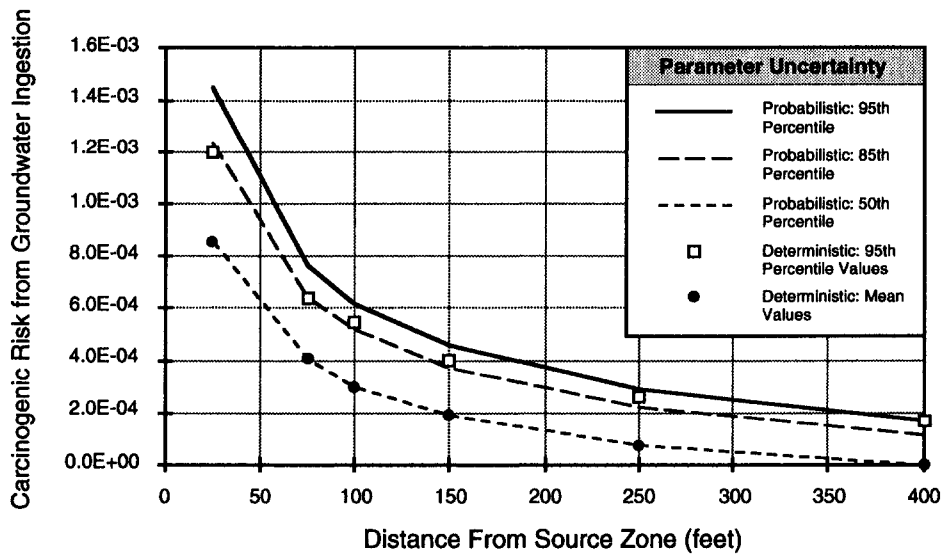


Figure 5B
Comparison of Risk Calculations: Deterministic
vs. Probabilistic Runs of Domenico Model



Parameter Distributions Used in Probabilistic Model

Parameter	Distribution	Mean	Standard Deviation
Hydraulic Conductivity	Lognormal	1.0E-3 cm/sec	5.0E-5 cm/sec
Benzene Concentration	Normal	6.0 mg/L	1.8 mg/L
Oxygen Concentration	Normal	3.0 mg/L	0.5 mg/L

Exposure Parameters Used in Probabilistic Model

Averaging Time = 70 yr
 Exposure Frequency = 350 d/yr
 Exposure Duration = 30 yr
 Body Weight = 70 kg
 Ingestion Rate = 2.0 L/d
 Slope Factor = 0.029 kg•d/mg (Benzene)