
Three- and Four-Phase Partitioning of Petroleum Hydrocarbons and Human Health Risk Calculations

Technical Background Document and Recommendations

Prepared for
**Alaska Statement of Cooperation Working
Group**

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Preface

This document was created under the Alaska Statement of Cooperation (SOC), which is an agreement between the Alaska Department of Environmental Conservation (ADEC), the U.S. Environmental Protection Agency (EPA), the Departments of the Army, Air Force, Navy, Military and Veterans Affairs (Army National Guard), Interior, and the Federal Aviation Administration (FAA) and U.S. Coast Guard. The objective of the agreement is to work cooperatively to identify and resolve issues affecting human health and the environment through promoting compliance with environmental laws, preventing pollution, creating partnerships to identify and cleanup contaminants and pollution, promoting training and coordinating with affected Tribes. A subcommittee or “working group” was formed under the SOC to evaluate the characterization and fate and transport of petroleum hydrocarbons spilled in the environment, and the risks posed by petroleum contamination. FAA contracted with Geosphere and CH2M Hill to research the issues and develop eight technical issue papers. The paper titles are listed below. Staff from ADEC, FAA, the Army and Army Corps of Engineers, and the Army National Guard reviewed and provided feedback on the draft papers. These papers provide sound scientific and technical information along with recommendations for use and/or future consideration.

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Statement of Cooperation Working Group Paper Titles

1. Three- and Four-Phase Partitioning of Petroleum Hydrocarbons and Human Health Risk Calculations, Technical Background Report Document and Recommendations
2. Hydrocarbon Characterization for Use in the Hydrocarbon Risk Calculator and Example Characterizations of Selected Alaskan Fuels, Technical Background Document and Recommendations
3. Dilution-Attenuation Factors at Fuel Hydrocarbon Spill Sites, Technical Background Document and Recommendations
4. Maximum Allowable Concentration, Residual Saturation, and Free-Product Mobility, Technical Background Document and Recommendations
5. Groundwater Sampling Techniques for Site Characterization and Hydrocarbon Risk Calculations, Technical Background Document and Recommendations
6. Migration to Indoor Air Calculations for Use in the Hydrocarbon Risk Calculator, Technical Background Document and Recommendations
7. Site Conditions Summary Report for Hydrocarbon Risk Calculations and Site Status Determination, Technical Background Document and Recommendations
8. Proposed Environmental Site Closeout Concepts, Criteria, and Definitions, Technical Background Document and Recommendations

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Acronyms and Abbreviations

ADEC	Alaska Department of Environmental Conservation
EPA	U. S. Environmental Protection Agency
BTEX	benzene, toluene, ethylbenzene and xylene
mg/L	milligrams per liter
L/kg	liter per kilogram
C_{sat}	soil saturation concentration
kg/L	kilograms per liter
mg/cm ³	milligrams per cubic centimeter
NAPL	nonaqueous phase liquid
DRO	diesel-range organics
Ecology	Washington State Department of Ecology
ODEQ	Oregon Department of Environmental Quality
MTCA	Model Toxics Control Act [State of Washington]
GRO	gasoline-range organics
UCL	upper confidence limit
RRO	residual-range organics
PAH	polycyclic aromatic hydrocarbons
DAF	dilution attenuation factor
MCL	maximum contaminant level

SECTION 1

Introduction

Understanding the human health and environmental risks associated with spilled fuel hydrocarbons requires an understanding and quantification of the phase distribution, phase changes, and transport of the hydrocarbon in the environment. This technical background report describes hydrocarbon phase partitioning.

Individual petroleum hydrocarbon compounds may exist at a contaminated site in four phases:

- As hydrocarbon molecules in air-filled soil pores (the vapor phase)
- As hydrocarbon molecules in soil moisture and groundwater (the dissolved phase)
- As hydrocarbon molecules bound to the soil matrix (the adsorbed phase)
- As hydrocarbon molecules surrounded predominately by other hydrocarbon molecules (the oil phase or nonaqueous phase liquid [NAPL])

The partitioning of a hydrocarbon constituent among these four phases is dependent on the properties and concentrations of the hydrocarbon compounds present, and on the properties of the soil. In this report, the terms “oil phase,” “oil,” “free product,” and “NAPL” are used synonymously. The terms “oil,” “free product,” and “NAPL” as used in this report do not indicate that the oil phase is mobile. Indeed, most of the free product in the soil at a contaminated site is generally held in the soil pores by capillary forces as immobile, residual saturation, and even the oil that collects on the water table surface in monitoring wells often is not mobile in the soil environment at the site scale (i.e., the oil will not migrate downgradient into previously uncontaminated soils).

Phase Partitioning

Hydrocarbon phase partitioning describes the movement and redistribution of hydrocarbon molecules between the dissolved, vapor, adsorbed and nonaqueous liquid phases. The movement of molecules between the phases occurs continuously in the soil environment because of the thermal energy of the molecules. Phase equilibrium exists when the movement into each phase equals the rate of movement out of the phase. The hydrocarbon concentrations in each phase at equilibrium are defined by the phase partitioning relationships. Key terms required to understand and communicate phase partitioning are discussed below.

2.1 Solubility

The solubility of a compound (S) describes the maximum concentration of the compound that may be dissolved in water. If a given hydrocarbon compound is mixed with water at concentrations above its solubility limit, the compound will dissolve in the water to its solubility limit and the remainder of the compound will be present as free product. The solubility of hydrocarbons in water varies as a function of temperature and total dissolved solids. Solubility values for common fuel hydrocarbons range over many orders of magnitude; for example, the solubility of benzene is about 1750 milligrams per liter (mg/L) and the solubility of hexadecane (C16 aliphatic) is about 0.00005 mg/L.

Solubility data may be obtained from numerous references, such as the Alaska Department of Environmental Conservation (ADEC) Guidance on Cleanup Standards, Equations and Input Parameters (1998); chemical engineering handbooks; and U. S. Environmental Protection Agency (EPA) documents. Table 1 lists solubilities for benzene, toluene, ethylbenzene and xylene (the BTEX compounds) and for aromatics and aliphatics with equivalent carbon numbers representative of Alaskan fuels (the aromatic and aliphatic equivalent carbon solubilities were calculated from the Total Petroleum Hydrocarbon Criteria Working Group regression equations, 1998).

2.2 Vapor Pressure and Concentration

Similar to the concepts for solubility, each hydrocarbon compound has a vapor pressure that describes the maximum quantity of the compound that may volatilize in the air. If a given hydrocarbon compound is mixed with air at concentrations above its vapor pressure limit, the compound will volatilize into the air to its vapor pressure limit and the remainder of the compound will be present as free product. The concentration in the vapor phase may be calculated from the ideal gas law as follows:

$$\text{Vapor concentration (mg/L)} = \frac{(1000 * \text{vapor pressure} * \text{molecular weight} * \text{volume})}{(n * R * T)}$$

Where: n = moles of compound

R = universal gas constant = $0.082 \text{ L} \cdot \text{atm}/^\circ\text{K} \cdot \text{mole}$

T = temperature in degrees Kelvin

When water, air, and a hydrocarbon compound are present together, the concentration of the compound in the vapor phase may be related to the dissolved or aqueous concentration by the dimensionless Henry's constant (H') of the hydrocarbon compounds.

dimensionless Henry's constant (H') = vapor concentration (mg/L) / dissolved concentration (mg/L)

vapor concentration (mg/L) = dissolved concentration (mg/L) * dimensionless Henry's constant

The dimensionless Henry's constant (H') may be calculated from the Henry's constant (H), which has units of "atmosphere * meter³ / mole" as follows:

dimensionless Henry's constant (H') = $H / R * T$

Vapor pressure data and Henry's constants may be obtained from numerous references, such as the ADEC Guidance on Cleanup Standards, Equations and Input Parameters (1998); chemical engineering handbooks; and EPA documents. Henry's constants for selected fuel hydrocarbons are listed in Table 1.

2.3 Sorbed Concentrations

The concentration of the compound that is sorbed to the organic soil solids may be related to the dissolved concentration by the soil-water partitioning coefficient (K_d). The soil-water partitioning coefficient is a function of the organic carbon partitioning coefficient (K_{oc}) of the compounds and the fraction of organic carbon (f_{oc}) in the soil as follows:

Sorbed Concentration = dissolved concentration * K_d

Where: $K_d = K_{oc} * f_{oc}$ = soil-water partitioning coefficient
(liter per kilogram [L/kg])

K_{oc} = organic carbon partitioning coefficient (L/kg)

f_{oc} = fraction of organic carbon (gram of carbon/gram of soil)

Note that the K_{oc} is a property of the hydrocarbon compound, and K_d is a property of the compound in a specific soil environment. K_{oc} values may be obtained from numerous references, such as the ADEC Guidance on Cleanup Standards, Equations and Input Parameters (1998); chemical engineering handbooks; and EPA documents. K_{oc} values for selected fuel hydrocarbons are listed in Table 1.

2.4 Soil Saturation Concentration

The ability of a soil to hold dissolved, vapor, and sorbed hydrocarbon is finite, and the maximum holding capacity of the soil for dissolved-, vapor-, and sorbed-phase

hydrocarbons is described as the soil saturation concentration, which is abbreviated as C_{sat} . The C_{sat} of a compound may be calculated as follows:

$$C_{sat} = (S * n_w / \rho_b) + (S * H' * n_a / \rho_b) + (foc * koc * S)$$

Which reduces to:

$$C_{sat} \text{ (mg/kg)} = S / \rho_b * (K_d * \rho_b + n_w + H' * n_a)$$

Where: S = compound solubility in water (mg/L)

ρ_b = soil dry bulk density (kilograms per liter [kg/L] or milligrams per cubic centimeter [mg/cm³])

K_d = soil-water partitioning coefficient (L/kg)

n_w = water-filled porosity (L water/L soil)

H' = dimensionless Henry's Constant

n_a = air-filled porosity (L air/L soil)

At hydrocarbon concentrations below the saturation concentration (C_{sat}), all hydrocarbon present in the soil is distributed between the dissolved, vapor, and sorbed phases and the distribution of hydrocarbon may be referred to as a three-phase problem (Figure 1). At hydrocarbon concentrations above the saturation concentration, nonaqueous phase hydrocarbon is present in addition to the dissolved, vapor, and sorbed phases, and the distribution of hydrocarbon may be referred to as a four-phase problem (Figure 2). On the left side of Figures 1 and 2, the soil particles are represented by the brown irregular-shaped grains, while water is present as a thin layer covering the soil particles and as thick wedges or rings where the soil particles are in contact, and soil gas is present in the larger pore bodies. Hydrocarbon is represented by the red dots and red films. The diagrams on the right side of Figures 1 and 2 provide the same information, but the soil particles, water, and soil gas are shown as a contiguous block.

The understanding three- and four-phase partitioning and having a quantifiable boundary between three- and four-phase distributions is important when assessing fate and transport and risk because:

- Below C_{sat} , the risk associated with the migration to outdoor air, migration to indoor air and migration-to-groundwater pathways increases linearly with increasing bulk soil concentration.
- At concentrations above C_{sat} , the risk associated with the vapor-inhalation and migration-to-groundwater pathways does not increase linearly, but rather remains relatively constant because the vapor and dissolved concentrations do not change as the mass of free product in the system increases (Figures 3 and 4).

In Figure 3 the bulk soil concentration includes the hydrocarbon concentrations in the dissolved, vapor, adsorbed and nonaqueous phases and the bulk soil concentration is the value provided by the EPA 8021, EPA 8260, EPA 8270, AK101, AK102, and AK103 test methods.

The C_{sat} values for several fuel hydrocarbon compounds and fractions are shown in Table 1. Note that the C_{sat} values for diesel-range aliphatics are relatively low (<10 mg/kg), indicating that NAPL is present at most diesel-range organics- (DRO) contaminated sites and that four-phase partitioning is necessary to representatively characterize the distribution of hydrocarbon constituents at these sites. Typical soils hold less than about 50 mg/kg of spilled diesel fuel in the vapor, dissolved, and adsorbed phases. Hydrocarbon present in the soil above the soil saturation concentration is present as NAPL (synonymous with free product). At large spill sites, the majority of the spilled fuel is present as free product or NAPL (but, most or all of the free product or NAPL is held in the soil by capillary forces, is typically not mobile at the site scale, and often does not appear in monitoring wells as floating product). For example, in a soil with a hydrocarbon concentration of 5,000 mg/kg and a C_{sat} of 50 mg/kg, 99 percent of the oil is present as free product.

C_{sat} is dependent on the soil properties (such as moisture content, bulk density, and porosity) and the chemical compounds' properties. Hence, C_{sat} values are different in different soils and different above and below the water table, as shown in Table 1. Table 1 also shows the percentage of the hydrocarbon mass in the dissolved, vapor, and adsorbed phases at or below C_{sat} given ADEC default soil conditions (as described above, at most spill sites the bulk soil concentration is above C_{sat} and the majority of the hydrocarbon mass is present as NAPL). The example C_{sat} data in Table 1 show the tendency of different compounds to partition into the dissolved, vapor, or adsorbed phases. In the Table 1 example, most of the benzene mass partitions into the dissolved phase, while the majority of the DRO aliphatics partition into the adsorbed phase.

SECTION 3

Raoult's Law Background

Gasoline, diesel fuel, and crude oil are complex mixtures of hundreds of individual hydrocarbon compounds. When NAPL in a soil is composed of more than one compound, the effective solubility and vapor concentrations of the compounds vary from their pure-phase solubility and vapor concentration according to Raoult's Law. Raoult's Law relates the effective solubility and vapor concentration of a hydrocarbon constituent to the mole fraction of the constituent in the NAPL:

$$S_{\text{effective}} = X_i * S$$

Where S = theoretical or maximum solubility (mg/L)

X_i = mole fraction of compound X in the multiconstituent NAPL

$$= (\text{moles of } X_i / \text{total moles of NAPL})$$

The effect of Raoult's law is illustrated in Figure 5, which shows a layer of NAPL floating on water in a beaker. In the beaker on the left the NAPL is 100 percent benzene and the dissolved benzene concentration in the water is 1750 mg/L. In the center beaker 50 percent of the moles in the NAPL are benzene and 50 percent of the moles in the NAPL are toluene and the resulting dissolved benzene concentration in the water is 875 mg/L (half of its pure phase solubility). In the beaker on the right only 0.05 percent of the moles in the NAPL are benzene and 99.95 percent of the moles in the NAPL are other diesel fuel constituents and the resulting dissolved benzene concentration in the water is only 0.875 mg/L (this benzene mole fraction and solubility is typical of weathered diesel).

Because many of the most hazardous compounds in gasoline and diesel (such as the BTEX compounds) are present as only a small fraction of the fuel mass, these compounds generally are present at only a small fraction of their theoretical solubility and volatility. Because the risk associated with the vapor-inhalation and migration-to-groundwater exposure pathways is a function of the dissolved and vapor concentrations, the failure to use Raoult's Law to assess the vapor concentration and dissolved concentration may result in overestimating the risk by several orders of magnitude. Table 2 shows dissolved phase BTEX concentrations in equilibrium with soils containing 5,000; 10,000; and 15,000 mg/kg arctic diesel as calculated by the EPA three-phase partitioning equation and with four-phase partitioning equations. At the bottom of Table 2 the over-estimation of the dissolved concentration calculated by the three-phase equation is listed. In this example the dissolved concentrations calculated using Raoult's Law are generally 1 to 2 orders of magnitude lower than those calculated using the three-phase equations. Use of Raoult's Law is critical to accurately represent the phase partitioning processes and to quantitatively assess the vapor-inhalation and migration-to-groundwater pathway risks.

The four-phase partitioning following Raoult's Law is well-documented in the technical literature and is used by the Washington State Department of Ecology (Model Toxics Control Act [MTCA] Cleanup Regulation, WAC 173-340-700) and the Oregon Department of

Environmental Quality (ODEQ) to assess soil cleanup levels. Theoretical discussions of four-phase partitioning and the applicability of Raoult's Law are addressed in numerous research papers (Cline et al., 1991; Lee et al., 1992; Feenstra et al., 1991; Mott et al., 1995; Mariner et al., 1996; Park and San Juan, 2000). Note that the four-phase partitioning equations used in this document are technically valid when NAPL is present, and that the three-phase soil screening equations are not valid or accurate when NAPL is present. (The limitations of the three-phase soil screening equations are identified in the EPA's *Soil Screening Guidance: Technical Background Document*, 1996a). NAPL is typically present at the default gasoline-range organics (GRO) and DRO soil cleanup concentrations listed in Table B2 of 18 AAC 75.

SECTION 4

Forward and Backward Risk Calculations

Human health risk calculations combine phase partitioning equations, fate and transport equations, and human exposure equations to calculate risk and/or cleanup levels. Two general types of calculations are possible: forward calculations and backward calculations. Forward calculations assess the risk that is caused at some exposure point within or downgradient of the contaminant source area. Backward calculations assess the concentration of a contaminant in the source area that causes or creates some (allowable) level of risk at an exposure point in or downgradient of the contaminant source area. Backward calculations are useful for setting screening levels. Forward calculations are most useful for assessing risk. Note that when multiple contaminants and/or multiple exposure pathways are present, the backward calculated screening levels do not represent “risk-based cleanup levels” because the backward calculation typically only accounts for one compound and one exposure route; hence, the cumulative risk likely exceeds the allowable risk level when the screening level concentration is reached. The hydrocarbon risk calculator (discussed in the following section) uses existing source area concentrations as model input and performs a forward calculation of risk for each compound and each exposure route. In addition, cumulative risks are calculated in the hydrocarbon risk calculator model.

SECTION 5

Hydrocarbon Risk Calculator

A “hydrocarbon risk calculator” spreadsheet model has been developed to assess the human health risks associated with petroleum hydrocarbon-contaminated soils. The hydrocarbon risk calculator is appropriate for fuel hydrocarbon spill sites and follows ADEC Method 3 guidelines. The methods used to assess human health risk are similar to the ADEC approach for establishing the Table B1 and B2 cleanup levels in that the human health risks associated with the soil ingestion, migration to outdoor air, migration to indoor air, migration-to- groundwater and groundwater ingestion exposure routes have been calculated with partitioning and transport equations. The primary differences between the “hydrocarbon risk calculator” described here and the existing ADEC Method 3 calculator is that the hydrocarbon risk calculator model:

- Applies either three-phase or four-phase partitioning equations (whichever is appropriate for the specific situation) that account for the presence of NAPL, and use Raoult’s Law to calculate the vapor pressure and solubility of the hydrocarbon constituents when NAPL is present
- Uses the Johnson & Ettinger model to characterize risk associated with the vapor intrusion (migration to indoor air route)
- Calculates the cumulative carcinogenic and non-carcinogenic risk assuming that the soil ingestion, outdoor and indoor inhalation, and groundwater ingestion exposure pathways are complete, and calculates risk from the pathways that are complete at the present time.

5.1 Hydrocarbon Risk Calculator General Layout

The hydrocarbon risk calculator combines or uses the following: 1) a three- or four-phase solution to the partitioning equations (whichever is appropriate) to calculate the dissolved- and vapor-phase concentrations present based on the input data set; 2) the EPA soil screening equations to back-calculate risk-based concentrations associated with each compound or hydrocarbon fraction 3) a characterization of the entire mass of the hydrocarbon in the soil; and 4) a characterization of the site soil and hydrogeologic conditions using the basic ADEC site condition assumptions, site-specific measurements of site conditions, or a combination of both. The hydrocarbon risk calculator spreadsheet has been reviewed by the University of Alaska-Fairbanks environmental engineering faculty and ADEC staff, and is an accepted ADEC method 3 and method 4 calculation tool.

The spreadsheet model is divided into twelve primary sections. The purpose and type of calculations performed in each section are as follows (the following discussion assumes that the reader has the spreadsheet and is familiar with ADEC regulations and guidance documents).

1. **Hydrocarbon Concentration and Soil and Groundwater Character Model Input Parameters.** The first section is for the input of the site-specific data such as hydrocarbon concentrations, soil parameters, and aquifer data. The cells requiring input data are highlighted in yellow; all other values are calculated by the spreadsheet. All calculations follow basic hydrologic and geotechnical parameter relationships. The concentrations for soil and water contaminant input would typically be the 95 percent upper confidence limit (UCL) on the mean concentration, or the highest soil and or water concentrations measured at the subject site. The cells containing the equivalent-carbon data are derived from the hydrocarbon characterization. The site characteristics such as the bulk density, water- and air-filled porosity, and aquifer properties match the ADEC default assumptions or are based on site-specific measurements. The site characterization and hydrocarbon characterization input data are discussed in detail in the technical background documents focusing on those topics.

2. **Migration to Indoor Air Model Input Parameters.** The second section of the hydrocarbon risk calculator is for the input of soil and building parameters used in the characterization of risk associated with the migration to indoor air exposure pathway. The Johnson & Ettinger vapor intrusion model is used to characterize the human health risk. As described above the light yellow cells are for the input of site specific data and all other required values are calculated by the spreadsheet. The EPA's default building parameter values are listed to help ensure that reasonable input values are used.

3. **Phase-Partitioning Calculations.** The third section of the spreadsheet performs the phase-partitioning calculations and assesses whether a three- or four-phase hydrocarbon distribution is present. This section of the spreadsheet is white (not color highlighted) except for a block of cells (C60 to C69) that are used for input that help characterize the distribution of GRO, DRO and RRO into aromatic and aliphatic equivalent carbon groups. The four-phase partitioning equations require that several simultaneous equations be solved. An Excel spreadsheet was used to define the partitioning equations, and "Solver," an Excel add-on feature, was used to numerically converge on the unique solution to the four-phase equations. The Excel Solver approach is used by the Washington State Department of Ecology and is documented in a paper by Hun Seak Park and Charles San Juan (2000). The Solver tool is accessed by clicking on the tools pull-down menu and then clicking on the Solver option in the pull-down menu. After the four-phase equations are solved with the use of Solver, the four-phase results are automatically compared to three-phase calculations and if-then statements are used to assess whether a three- or four-phase distribution is present. The three-phase calculations and all subsequent calculations do not require the Excel Solver tool. All cells/calculations are updated and saved when the Excel Solver solution is accepted. The appropriate three- or four-phase distributions are then used to characterize the dissolved- and vapor-phase concentrations in the contaminated-soil source area of the subject site. The core four-phase equations are as follows (Park and San Juan, 2000):

$$C_i^t = x_i S_i / \rho_b (H_i n_a + K_{oc}^i f_{oc} \rho_b + n_w + (MW_i n_{NAPL} / S_i \sum (x_i MW_i / \rho_i)))$$

$$\sum x_i = 1$$

$$n = n_a + n_w + n_{\text{NAPL}}$$

Where:

Four phases of NAPL, pore water, pore air, soil sorbed, and total are represented by the subscripts NAPL, w, a, s, and t, respectively; and

M^i = mass of component i in each of the four phases and total;

C^i = concentration of component i in each of the four phases and total;

K^i_{oc} = soil organic carbon to water partition coefficient of component i;

f_{oc} = mass fraction of natural soil organic carbon within the soil matrix;

H_i = dimensionless Henry's Law constant of component i;

S_i = pure aqueous solubility of component i;

x_i = mole fraction of component i in the NAPL mixture;

n = total soil porosity;

n_w = water filled porosity = volumetric water content in soil;

n_a = air filled porosity = volumetric air content in soil;

n_{NAPL} = NAPL filled porosity = volumetric NAPL content;

MW_i = molecular weight of component i;

MW_{NAPL} = weighted average (or equivalent) of molecular weight of NAPL mixture

ρ_b = dry soil bulk density;

ρ_i = density of component i in liquid form;

ρ_{NAPL} = density of the NAPL mixture

4. **Soil-Ingestion Risk.** The fourth section of the spreadsheet calculates the soil-ingestion risks for residential and industrial land use. The cells displaying the results are highlighted in tan. The bulk hydrocarbon concentration in each hydrocarbon fraction at the subject site is displayed in cells B82 to B104. The EPA (1996a) and ADEC (1998) soil-screening equations are used without modification to back-calculate the bulk soil concentration that produces a hazard index of 1 for the noncarcinogenic compounds and a cancer risk of 1×10^{-5} for the carcinogenic compounds for the hydrocarbon compounds of interest in the contaminated soil source area (BTEX, GRO, DRO, residual-range organics [RRO], and polycyclic aromatic hydrocarbons [PAH]). The results of the ingestion-risk calculations are displayed in cells C82 to C104 for residential sites and in cells F82 to F104 for industrial sites. Note that ingestion risk increases linearly with increasing bulk soil concentration (the phase in which the hydrocarbon is ingested is not important). Therefore, the back-calculated value is the soil-ingestion cleanup level for the compound being considered whether three or four hydrocarbon phases are present. The hydrocarbon risk calculator compares the back-

calculated risk-based soil concentration to the concentration measured at the subject site to assess the fraction of risk created by the presence of each compound of interest:

$$\text{fraction of risk} = \text{concentration at subject site} / \text{risk-based concentration}$$

The fraction of risk calculations are displayed in cells D82 to D104 and G82 to G104 for residential and industrial sites respectively, are used in subsequent cumulative risk calculations, and to screen for compliance with the regulations. A check for regulatory compliance is made by using Excel “if-then” statements as follows: If the fraction of risk for a given compound is less than 1, then the site meets the compliance criteria for that compound and the spreadsheet displays a “0.” If the fraction of risk is greater than 1, then the site does not meet regulatory criteria and the spreadsheet displays a “1” as shown in cells E82 to E104 and cells H82 to H104 for residential and industrial sites respectively.

- 5. Migration to Outdoor Air Risk.** The fifth section of the spreadsheet calculates and displays the vapor inhalation risks for residential and industrial land use. The cells displaying the results are highlighted in light green. The EPA and ADEC three-phase soil-screening equations and the four-phase Excel Solver vapor concentrations are combined to assess the vapor inhalation risks.

The EPA and ADEC linear three-phase soil-screening equations are used to back-calculate the bulk soil concentration that produces a hazard index for the vapor-inhalation pathway of 1 for the noncarcinogenic compounds and a cancer risk of 1×10^{-5} for the carcinogenic compounds. The EPA/ADEC vapor inhalation conceptual model and equations (Figure 6) assume that volatiles in the soil diffuse into the outdoor air above the ground surface where they are mixed with uncontaminated ambient air. When back-calculating these risk-based inhalation levels, the concentrations were not capped at the soil-saturation concentration limit. (Note that for many hydrocarbon constituents, the three-phase equations calculate a soil concentration that is above C_{sat} for the compound, which results in a back-calculated, three-phase vapor concentration that is above the maximum vapor concentration of the compound. Risk-based vapor concentrations above the maximum vapor concentration of a compound indicate that the compound cannot present a risk to human health through the vapor- inhalation exposure pathway.

The risk-based bulk soil concentration from the three-phase soil-screening equation was then used to calculate the three-phase vapor concentration (cells C 114 to C136 and F114to F136) associated with the risk-based bulk soil concentration as follows:

$$C_a \text{ (mg/L)} = H'(C_s / (K_d + ((n_w + H' * n_a) / \rho_b)))$$

Where: C_w = compound concentration in water (mg/L)

ρ_b = soil dry bulk density (kg/L or mg/cm³)

K_d = soil-water partitioning coefficient (L/kg) = $k_{oc} * f_{oc}$

n_w = water filled porosity (L water/L soil)

H' = dimensionless Henry’s Constant

n_a = air-filled porosity (L air/L soil)

The risk-based “three-phase” vapor concentration is then compared to the four-phase Excel Solver vapor concentration (B114 to B136) to assess the fraction of risk created by the presence of each compound of interest:

$$\text{fraction of risk} = \frac{\text{vapor concentration at subject site}}{\text{risk-based vapor concentration}}$$

The fraction of risk calculation results, displayed in cells D114 to D136 and G114 to G136 for residential and industrial sites, are used in subsequent cumulative risk calculations and are used to screen for compliance with the regulations. If the fraction of risk for a given compound is less than 1, the site meets the risk-based criteria for that compound and a “0” is displayed, while if the fraction of risk is greater than 1 then the site does not meet regulatory criteria and a “1” is displayed, as shown in cells E114 to E136 and H114 to H136.

- 6. Migration to Indoor Air Risk** The sixth section of the spreadsheet calculates and displays the migration to indoor air or vapor intrusion inhalation risks for residential and industrial land use. The cells displaying the results are highlighted in olive green. The Johnson and Ettinger model and a characterization of the soil vapor hydrocarbon concentrations are combined to assess the migration to indoor air or vapor intrusion risks. The Johnson and Ettinger model is used to calculate an attenuation factor exactly as is done in the EPA’s “advanced soil gas” version of the Johnson and Ettinger model.

The soil vapor concentration in the NAPL contaminated soil source area is shown in cells B146 to B168. These vapor concentrations are from either (1) the four-phase solver solution for vadose zone sources or (2) are based on partitioning from the groundwater data if the source is in the saturated zone or (3) are direct sub-slab soil gas concentration measurements. The source area vapor concentrations are multiplied by the Johnson and Ettinger attenuation factor to predict a building vapor concentration as displayed in cells C146 to C168. Back calculated risk based residential and industrial indoor air target concentrations are listed in cells D146 to D168 and G146 to G168 respectively (these concentrations produce a hazard index for the vapor-inhalation pathway of 1 for the noncarcinogenic compounds and a cancer risk of 1×10^{-5} for the carcinogenic compounds).

The risk-based indoor air vapor concentrations are then compared to the predicted indoor air vapor concentrations to assess the fraction of risk created by the presence of each compound of interest:

$$\text{Fraction of risk} = \frac{\text{vapor concentration predicted to be in indoor air}}{\text{indoor air risk-based vapor concentration}}$$

The fraction of risk calculation results, displayed in cells E146 to E168 and H146 to H168 for residential and industrial sites, are used in subsequent cumulative risk calculations and are used to screen for compliance with the regulations. If the fraction of risk for a given compound is less than 1, then the site meets the risk-based criteria for that compound and a “0” is displayed, while if the fraction of risk is greater than 1

then the site does not meet regulatory criteria and a “1” is displayed, as shown in cells F146 to F168 and I146 to I168.

7. **Migration-to-Groundwater Risk (Calculated).** The seventh section of the spreadsheet compares the calculated dissolved-phase equilibrium concentration in the source area soil moisture to groundwater MCLs and groundwater ingestion risk based levels to assess the predicted migration-to-groundwater (groundwater) risks for residential and industrial land use. The cells displaying the migration-to-groundwater (or groundwater) results are highlighted in light blue.

The migration-to-groundwater risks are assessed using portions of the EPA and ADEC soil-screening equations combined with the four-phase Excel Solver dissolved concentrations, as shown in Figure 7 and described below.

- The equilibrium dissolved phase concentrations, calculated by Solver from the input soil concentrations, are displayed in cells B178 to B200.
- The maximum contaminant levels (MCLs) for compounds with MCLs are displayed in cells C178 to C200.
- The EPA and ADEC equations for groundwater cleanup levels are used without modification to calculate a risk-based concentration for groundwater used as drinking water. These groundwater cleanup levels are based on a hazard index of 1 for the noncarcinogenic compounds and a cancer risk of 1×10^{-5} for the carcinogenic compounds. The results for residential and industrial exposure scenarios are displayed in cells D178 to D200 and H178 to H200.
- The EPA and ADEC equations for the mixing zone thickness and dilution factor of the groundwater and infiltrating precipitation are used without modification.
- According to ADEC guidance, a dilution attenuation factor (DAF) is calculated by adding the calculated dilution factor to a fixed attenuation factor of 10:

DAF = dilution factor + attenuation factor,
 where attenuation factor = 10

- According to ADEC guidance, a target soil moisture concentration in the contaminated soil source area is calculated by multiplying the DAF by the risk-based groundwater cleanup level or MCL which ever is lower (displayed in cells E178 to E200 for a residential site and cells I178 to I200 for an industrial site):

Target soil moisture concentration = DAF * MCL or risk-based
 groundwater cleanup level (if there is not an MCL)

- The fraction of risk created by the presence of each compound of interest is calculated as follows:

Fraction of risk = calculated equilibrium soil moisture concentration
 at subject site / risk-based soil moisture concentration

The fraction of risk calculations are displayed in cells F178 to F200 and cells J178 to J200. If the predicted fraction of risk for a given compound is less than 1, the site meets the risk-based level for that compound.

- This “target soil-moisture concentration” is compared to the four-phase Excel Solver dissolved concentration to assess if the groundwater concentrations are predicted to be within regulatory limits (assuming that the DAF characterization is accurate). The result of the check for compliance with the regulations is displayed in cells G178 to G200 and cells K178 to K200. Note that because for several compounds MCLs are below groundwater ingestion risk based concentrations it is possible to be out of compliance with regulatory concentrations but to meet the groundwater ingestion risk based criteria.
8. **Groundwater Ingestion Risk (Measured).** The eighth section of the spreadsheet assesses the groundwater ingestion risk posed by the measured dissolved-phase concentrations in the source area for residential and industrial land use scenarios. The section also assesses if the measured groundwater concentrations are in compliance with regulations (which may be valuable for compounds with MCLs below risk based levels). The cells displaying the migration-to-groundwater results are highlighted in dark blue. Note that this section of the model uses both MCLs and groundwater ingestion risk based concentrations as described below.
- The measured dissolved phase concentrations that are input to the model are displayed in cells B211 to B233.
 - The maximum contaminant levels (MCLs) for compounds with MCLs are displayed in cells C211 to C233.
 - The EPA and ADEC equations for groundwater cleanup levels are used without modification to calculate a risk-based concentration for groundwater used as drinking water. These groundwater cleanup levels are based on a hazard index of 1 for the non carcinogenic compounds and a cancer risk of 1×10^{-5} for the carcinogenic compounds. The results for residential and industrial exposure scenarios are displayed in cells D211 to D233 and H211 to H233.
 - According to ADEC regulations groundwater that is not within a potable aquifer has a cleanup level 10 times the risk based level or MCL (whichever is lower). A groundwater compliance concentration for the contaminated soil source area may be calculated by multiplying the lesser of the risk-based groundwater cleanup level or MCL by either a value of 1 or 10 depending whether the groundwater is or is not within a potable aquifer. The groundwater compliance concentrations are displayed in cells E211 to E233 for a residential site and cells I211 to I233 for an industrial site:

Groundwater compliance concentration = 1 (for a potable aquifer) or 10 (for a non-potable aquifer) * lesser of MCL or risk-based groundwater cleanup level
 - For potable aquifers the fraction of risk created by the presence of each compound or fraction is calculated as follows:

$$\text{fraction of risk} = \frac{\text{measured groundwater concentration at subject site}}{\text{risk-based groundwater concentration}}$$

The fraction of risk calculations for residential and industrial sites, are displayed in cells F211 to F233 and cells J211 to J233, respectively. If the predicted fraction of risk for a given compound is less than 1, the site meets the risk-based level for that compound. Note that the groundwater ingestion risk based concentration (which is often different than the MCL) is used in the fraction of risk calculation.

For non-potable aquifers the fraction of risk is listed as zero for all compounds and fractions because by definition the aquifer and groundwater will not and/or cannot be used as a drinking water source.

A check for regulatory compliance is made by comparing the “groundwater compliance concentration” to the measured dissolved concentration to assess if the groundwater concentrations are within regulatory limits. The result of the check for compliance with the regulations is displayed in cells G211 to G233 and cells K211 to K233. If the measured groundwater concentration meets the compliance criteria for that compound a “0” is displayed, while if the measured groundwater concentration does not meet the compliance criteria for that compound a “1” is displayed.

9. **Potential Cumulative Risk Assuming All Pathways Complete.** The ninth section of the spreadsheet assesses the cumulative risks associated with fuel hydrocarbon compounds that may be expected if the soil ingestion, migration to outdoor air, migration to indoor air and groundwater ingestion exposure routes were complete at the subject site. The term “potential” cumulative risk is used to acknowledge the risk calculations are based on numerous assumptions such as the exposure factors, toxicities and fate and transport characterizations. The cells displaying the potential cumulative risk by all pathways are highlighted in purple. Cells B244 to E266 (for residential sites) and H244 to K266 (for industrial sites) summarize the fraction of risk values calculated for the soil ingestion, migration to outdoor air, migration to indoor air and groundwater ingestion pathways. The cumulative risk for each compound is calculated as the sum of fraction of risk values associated with each pathway for that compound as shown in cells F244 to F266 and L244 to L266 for residential and industrial sites respectively. The cumulative carcinogenic risks are then calculated by summing risk associated with the carcinogenic compounds as shown in cells F267 and L267 for residential and industrial sites respectively. The cumulative non-carcinogenic risks are then calculated by summing risk associated with the non-carcinogenic compounds as shown in cells F268 and L268 for residential and industrial sites respectively. Consistent with ADEC policy, the four-phase spreadsheet model uses measured dissolved-phase concentrations, not dissolved-phase concentrations calculated by the spreadsheet model, to assess the groundwater ingestion risk. Also, consistent with ADEC guidance documents (2001), the risks associated with the GRO, DRO, and RRO groups of compounds are not included in the cumulative risk calculation. According to the contaminated site regulations, the noncarcinogenic and carcinogenic cumulative risks are acceptable if the cumulative noncarcinogenic fraction of risk is less than 1 and the cumulative carcinogenic fraction of risk is less than 1. (The carcinogenic risk has been normalized. The carcinogenic risk level may be calculated by multiplying the fraction of carcinogenic risk by the acceptable

carcinogenic risk level— 1×10^{-5} .) A check for compliance with human health risk criteria is displayed in cells G244 to G268 and cells M244 to M268. If the cumulative risk meets the compliance criteria a “0” is displayed, while if the measured groundwater concentration does not meet the compliance criteria for that compound a “1” is displayed.

10. **Potential Cumulative Risk for Pathways Complete at Present Time.** The tenth section of the hydrocarbon risk calculator assesses the cumulative risks associated with all compounds and all exposure routes that are complete at the site at the present time (the time the report is prepared). The cells displaying the cumulative risks for pathways complete at the present time are highlighted in gold. The section of the spreadsheet containing the cumulative risks for pathways complete at the present time is laid out identical to the preceding section (cumulative risk assuming all pathways are complete). The values in the cumulative risks for pathways complete at the present time are calculated as the values in the previous section multiplied by: one if the pathway is complete at the present time; or by a zero if the pathway is not complete at the present time. The pathways complete at the present time are input to the calculator in the gold block of cells in the data input section of the calculator (cells J11 to J15). The purpose of calculating the cumulative risk for pathways complete at the present time is to understand if current site conditions present an acceptable or unacceptable risk, which is valuable for prioritizing remedial and/or risk management actions and for placing the site in a site status category. Note that if all pathways are complete at the present time then the hydrocarbon risk calculator sections titled “cumulative risk assuming all pathways are complete” and “cumulative risk at the present time” show the same risk values. A check for compliance with human health risk criteria is displayed in cells G276 to G300 and cells M276 to M300. If the cumulative risk meets the compliance criteria a “0” is displayed, while if the measured groundwater concentration does not meet the compliance criteria for that compound a “1” is displayed.
11. **Partitioning into Surface Water and Groundwater.** The eleventh section of the hydrocarbon risk calculator assesses if contaminated soil from the site has the potential to partition into groundwater or surface water at concentrations exceeding ADEC Table C levels or the ambient water quality criteria. To make these assessments the dissolved phase equilibrium concentration calculated from the input soil concentrations or the measured groundwater concentration (depending on whether the source is in the vadose or saturated zones) is compared to the Table C concentrations and the ambient water quality criteria using “if...then” statements. If soil has the potential to cause a compound to exceed a regulatory level then a one is printed in the column. If the soil does not have the potential to cause a compound to exceed a regulatory level then a zero is printed in the column. The information could be used to assess if the soil can be transported to another site without causing a water quality criteria to be exceeded and to assign a site closeout status (provided human health and environmental risk criteria are met) as described in the SOCWG paper titled “Proposed Environmental Site Closeout Concepts, Criteria, and Definitions” (Geosphere and CH2MHill, 2006). The partitioning into groundwater and surface water section is highlighted in turquoise. Data displayed in the partitioning into groundwater and surface water section include the following:

- The dissolved phase equilibrium concentrations for each hydrocarbon fraction as calculated from the input soil concentrations are printed in cells B308 to B332. The measured groundwater concentrations (from the input data) are listed in cells C308 to C332. The MCLs or risk based groundwater ingestion criteria are listed in cells D308 to D330.
 - Cells E308 to E330 could be used to assess whether soil from the subject site could be used as vadose zone fill at another location by 1) comparing the equilibrium partitioning concentration to the target soil moisture concentration (i.e. the MCL or risk based groundwater concentration multiplied by the DAF) if subject site is a vadose zone spill site (NAPL is only present in the vadose zone); or 2) by comparing the measured groundwater concentration to the MCL or risk concentration if the subject spill site a saturated zone site (i.e. NAPL is present in the saturated zone). The differing criteria for vadose and saturated spill sites are used because most existing sites are interpreted to be saturated zone spill sites and measured groundwater concentrations tend to have lower detection limits and fewer censored values than soils data and consequently are interpreted to provide a better measure of the concentration when a compound is present at low concentrations. If the soil can be used as vadose zone fill a "0" is printed in the column, while if the soil cannot be used as vadose zone fill a "1" is printed the column.
 - Cells F308 to F330 could be used to assess whether soil from the subject site could be used as saturated zone fill at another location by (1) comparing the dissolved phase equilibrium partitioning concentration to the MCL or risk based concentration (without considering the DAF) if subject site is a vadose zone spill site; or (2) by comparing the measured groundwater concentration to the MCL or risk concentration if the subject spill site is a saturated zone site. If the soil can be used as saturated zone fill a "0" is printed in the column, while if the soil cannot be used as saturated zone fill a "1" is printed the column.
 - The ADEC ambient water quality criteria addressing fuel hydrocarbons are listed in cells G308 to G332. The total aromatic hydrocarbon (TAH) concentration and the total aqueous hydrocarbon (TAqH) concentration are calculated as the sum of the BTEX and sum of the BTEX and PAH concentrations respectively.
 - Cells H308 to H333 could be used to assess whether soil from the subject site could be used as fill in a surface water body by (1) comparing the equilibrium partitioning concentration to the surface water criteria (without considering the DAF) if subject site is a vadose zone spill site; or (2) by comparing the measured groundwater concentration to the surface water criteria if the subject spill site is a saturated zone site. If the soil can be used as fill in surface water body a "0" is printed in the column, while if the soil cannot be used as fill in surface water body a "1" is printed the column.
12. **Site Status Summary.** The twelfth and final section of the hydrocarbon risk calculator summarizes the site status as described in the SOCWG paper on proposed site closure categories (Geosphere & CH2MHill, 2006). The spreadsheet displays the cumulative human health carcinogenic and noncarcinogenic risks assuming that all pathways are

complete (cells B341 & B342); displays the cumulative human health carcinogenic and noncarcinogenic risks for the pathways that are complete at this time (cells B343 & B344); calculates a site ranking score, which is the product of the present risk and the number of people currently exposed (cells B345 & B346); and summarizes compliance with GRO, DRO and RRO aromatic and aliphatic risk criteria (cells C348 to F353 and C354).

The spreadsheet then uses “if...then” statements to print a statement saying that risk criteria have or have not been met (cell A355) and describing the potential to use soils from the subject site as fill at other locations (cells A356 to A358).

5.2 Presentation of Results from the Hydrocarbon Risk Calculator

5.2.1 Hydrocarbon Risk Calculator Tables

The most important results of the four-phase risk calculations are presented in a 12 page long table. Table 3 is an example of the hydrocarbon risk calculator results for a hypothetical old diesel fuel spill site. The input data for this hypothetical, but reasonable calculation include the following:

- The default ADEC soil and hydrogeologic conditions.
- Table B1 migration to groundwater soil screening levels.
 - Table B2 maximum allowable DRO and GRO soil screening levels (RRO concentration was 100 mg/kg which is an arbitrary number representative of many old diesel spill sites).
 - Aromatic and aliphatic GRO and DRO percentages from a representative diesel spill site.
 - Arbitrary groundwater concentrations that are in general representative of weathered diesel spill sites (the groundwater concentration used as input are conservative given the default dilution attenuation assumptions – that is they are greater than the dissolved phase equilibrium concentration calculated by the four-phase solver model from the input soil concentrations multiplied by the default DAF).

The printed output of the hydrocarbon risk calculator (Table 3 of this report) is organized as follows:

Page 1 shows the hydrocarbon concentration and soil and groundwater model input values.

Page 2 shows the Johnson & Ettinger soil and building parameter input values

Page 3 summarizes the concentration of each hydrocarbon fraction in the dissolved, vapor, adsorbed and NAPL phases.

Pages 4 through 8 of each results table lists the risks associated with different exposure pathways. Residential site risks are shown on the left side of the table, and industrial site risks are shown on the right side of the table.

Page 4 contains the soil ingestion pathway risks and soil compliance levels for each compound or hydrocarbon fraction.

Page 5 contains the outdoor air vapor-inhalation pathway risks for each compound or hydrocarbon fraction.

Page 6 contains the indoor air vapor-inhalation pathway risks for each compound or hydrocarbon fraction.

Page 7 contains the calculated migration-to-groundwater pathway risks for each compound or hydrocarbon fraction.

Page 8 presents the groundwater-ingestion risks for each compound or hydrocarbon fraction based on the measured concentrations in groundwater samples.

Page 9 contains the results of the potential cumulative risk calculations assuming that all pathways are complete. Residential site risks are summarized on the left side of the table, and industrial site risks are summarized on the right side of the table.

Page 10 contains the results of the potential current cumulative risk calculations (this is the risk from the exposure pathways at the site that are complete at this time). Residential site risks are summarized on the left side of the table, and industrial site risks are summarized on the right side of the table.

Page 11 assesses if contaminated soil from the site has the potential to cause surface water to exceed the ambient water quality criteria or groundwater to exceed groundwater criteria. The information could be used to assign a site closeout status, as proposed in the site closure recommendations paper, provided risk criteria are met.

Page 12 summarizes the site status as defined by the SOCWG paper onsite closure (Geosphere & CH2MHill, 2005).

The following paragraphs give more detailed information about the structure and content of the hydrocarbon risk calculator tables. (The hydrocarbon risk calculator tables shown in Table 3 should be referenced as needed while reviewing the following explanations.)

Page 1, Model Input Values. Model input parameters including soil and groundwater geologic conditions and soil and groundwater hydrocarbon concentrations are shown on page 1 of the hydrocarbon risk calculator. The cells containing input values are highlighted in light yellow. Note that the input values for the soil hydrocarbon concentrations will typically be the 95 percent UCL values for the NAPL contaminated soil source area samples from the site in question; hence the calculation results may be used to conservatively assess risks associated with the soil-ingestion, outdoor air-inhalation, indoor air-inhalation, and migration-to-groundwater routes. The groundwater concentrations used as input to the calculator are typically the highest concentration measured in a recent data set, and hence these values are thought to be conservative. The soil and groundwater geologic characteristics (bulk density, moisture content, gradient, etc.) represent average conditions

or the ADEC default conditions. In the in Table 3 example calculations the soil and groundwater site conditions input values are the ADEC default conditions used when calculating ADEC Tables B1 and B2. T BTEX and PAH concentrations are the ADEC Table B1 migration to groundwater values and the GRO and DRO values are the maximum allowable concentrations from Table B2.

Page 2, Migration to Indoor Air Data Entry. Soil and building input parameters for the Johnson & Ettinger model are shown on page 2 of the hydrocarbon risk calculator output. The soil values used in the example calculation are arbitrary. The building parameter input values are in general the EPA default values.

Page 3, Phase Partitioning Results. The hydrocarbons fractions or groups used to characterize the NAPL are shown in the first column, the representative equivalent carbon number of the compound or fraction is shown in the second column, and the fraction of the DRO aromatics, DRO aliphatics and GRO aliphatics in different equivalent carbon groups is entered and shown in column 3. The columns 4, 5, and 6 show the soil concentration of each compound or fraction, the fraction of the TPH mass represented by the compound or fraction, and the mole fraction of each compound or hydrocarbon group in the NAPL, respectively. Columns 7 and 8 display the dissolved and vapor concentrations in equilibrium with the NAPL. Columns 9 through 12 list the percent of each hydrocarbon constituent in the dissolved, vapor, sorbed and NAPL phases. The example calculation clearly shows that that about 95 percent of the benzene, 98 percent of the toluene and more than 99 percent of all the other hydrocarbon fractions is present in the NAPL and not in the dissolved, vapor or adsorbed phases (as is assumed in three-phase calculations performed by the existing online calculator).

Page 4, Soil Ingestion Risks. Column 2 displays the hydrocarbon concentration in the soils of the subject site. Columns 3 and 6 list the soil concentrations that present a hazard quotient of 1 or a carcinogenic risk of 1×10^{-5} for residential and industrial sites, respectively (the risk based concentrations are calculated using equations 3 and 4 from the ADEC guidance on cleanup level calculations). Columns 4 and 7 show the fractions of the risk-based concentration that exist for each compound or hydrocarbon group. Columns 5 and 8 indicate whether the existing soil concentrations are within the risk-based criteria for each compound or hydrocarbon group (a zero in the column indicates that the ADEC compliance criteria are met, and a 1 indicates that compliance criteria have not been met). The calculations show that for a hypothetical residential site, the BTEX cleanup levels based on soil-ingestion risk are about 151 mg/kg benzene; 20,278 mg/kg toluene; 10,139 mg/kg ethylbenzene; and 202,778 mg/kg xylene. The calculations also show that for residential sites, GRO aromatic and aliphatic and DRO aromatic and aliphatic soil cleanup levels based on soil-ingestion risk are about 20,278 mg/kg GRO aromatics; 506,944 mg/kg GRO aliphatics; 4,056 mg/kg DRO aromatics; and 10,139 mg/kg DRO aliphatics. The fraction of risk calculations show that the input DRO concentration of 12,500 mg/kg is in compliance with ADEC risk criteria (given that 20 percent are aromatics) In addition, the BTEX and PAH soil concentrations used as input present only a fraction of the acceptable cumulative risk for the soil ingestion route (about 2 percent of the allowable carcinogenic risk and less than 1percent of the allowable noncarcinogenic risk). From this information, it appears that the input soil concentrations are protective of human health via the soil ingestion route under a residential land use scenario.

Page 5, Outdoor Air Inhalation Risks. Column 2 lists the vapor concentration in the source zone soils of the subject site based on three- or four-phase partitioning (as appropriate). Columns 3 and 6 list the soil vapor concentrations that present a hazard quotient for the vapor-inhalation pathway of 1 or a carcinogenic risk of 1×10^{-5} for residential and industrial sites, respectively. Columns 4 and 7 show the fractions of the risk-based concentration that exist for each compound or hydrocarbon group. Columns 5 and 8 indicate whether the existing concentrations are within the risk-based criteria for each compound or hydrocarbon group (a zero in the column indicates that the ADEC compliance criteria are met, and a 1 indicates that compliance criteria have not been met). The example calculations show that for a residential site, the soil vapor concentrations for benzene, toluene, and ethylbenzene that present an outdoor air inhalation pathway risk are about 9.75; 1186 and 2918 mg/L, respectively. (Xylene is interpreted to not pose an inhalation risk by default, ADEC Table B1.) The calculations also show that for residential sites the soil vapor concentrations for GRO aromatics and aliphatics and DRO aromatics and aliphatics that present an inhalation-pathway risks are about 852; 91752; 47 and 364 mg/L, respectively. The vapor concentrations of hydrocarbon fractions in the example soil, as calculated by the hydrocarbon risk calculator, are several orders of magnitude lower than the risk based vapor concentrations, and because there is NAPL in the soil, the soil vapor concentrations will not increase significantly as the bulk soil concentration increases. Therefore, the fraction of risk calculations shows that the example soil (containing a DRO concentration of 12,500 mg/kg and a TPH soil concentration of 14,000 mg/kg) presents only a tiny fraction of the acceptable risk (< 0.002 percent of the allowable carcinogenic risk and about <0.0015 percent of the allowable noncarcinogenic risk). The zeros in columns 5 and 8 of Table 3 show that the existing concentrations are in compliance with ADEC criteria for the individual compounds and/or compound groups. From this information, it can be concluded that the input soil concentrations are protective of human health via the outdoor air inhalation route under a residential land use scenario. (Note in all representative calculations performed to date fuel hydrocarbons appear to present relatively little risk via the migration to outdoor air pathway).

Page 6, Indoor Air Inhalation Risks. Indoor air inhalation risks are calculated using the Johnson and Ettinger equation (Johnson & Ettinger, 1991) assuming that the soil gas concentration is the vapor concentration in equilibrium with the NAPL or groundwater depending on whether the source zone extends into the saturated zone. Column 2 lists the vapor concentration in the source zone soils of the subject site based on three- or four-phase partitioning, groundwater concentrations or input soil gas data (as appropriate). Column 3 lists the building or indoor air vapor concentrations calculated by the Johnson & Ettinger equation. Columns 4 and 7 list the indoor target concentration. The vapor-inhalation target concentration is the concentration that presents a hazard quotient of 1 or a carcinogenic risk of 1×10^{-5} for residential and industrial sites, respectively. Columns 5 and 8 show the fractions of the risk-based concentration that exist for each compound or hydrocarbon group. Columns 6 and 9 indicate whether the existing concentrations are within the risk-based criteria for each compound or hydrocarbon group (a zero in the column indicates that the ADEC compliance criteria are met, and a 1 indicates that compliance criteria have not been met). The example results show that the ADEC Table B1 BTEX soil cleanup levels and Table B2 GRO and DRO maximum allowable concentrations present risks within existing regulatory standards.

Page 7, Migration to Groundwater Risks. Column 2 shows the dissolved phase equilibrium concentration that is expected in the source zone soils of the subject site based on three- or four-phase partitioning calculations (as appropriate), and the input soil concentrations. Column 3 lists the maximum contaminant levels (MCLs) for each hydrocarbon compound. Columns 4 and 8 list the dissolved concentrations that present a hazard quotient of 1 or a carcinogenic risk of 1×10^{-5} for residential and industrial sites, respectively (note that some MCLs are lower than the risk based groundwater ingestion concentration). Columns 5 and 9 show the target soil moisture concentrations given the dilution and attenuation factor calculated for the site. Columns 6 and 10 show the fractions of the risk-based concentration that exist for each compound or hydrocarbon group. Columns 7 and 11 indicate whether the existing concentrations are within the regulatory or risk-based criteria for each compound or hydrocarbon group (a zero in the column indicates that the ADEC compliance criteria are met, and a 1 indicates that compliance criteria have not been met).

Note that the BTEX, GRO, and DRO aromatics each represent a minor fraction of the moles of NAPL present in the site soils; therefore, these aromatics have much lower effective solubilities than those calculated by using the three-phase soil-screening equations. The risks associated with BTEX, GRO, and DRO aromatics via the migration-to-groundwater pathway are commonly lower than might be expected given the concentrations listed for these compounds in the ADEC regulations. Also note that the model predicts that vadose-zone DRO aromatics and aliphatics generally will not present significant migration-to-groundwater risks because the Raoult's Law solubilities of these compounds are below the risk-based concentration multiplied by the ADEC default DAF. The results show that the ADEC Table B1 and B2 soil input concentrations are unlikely to present a migration-to-groundwater risk. Finally, because some MCLs are not risk based (for example benzene), compliance criteria may not be met (the MCL may be exceeded) even though the site poses an acceptable risk.

Page 8, Groundwater Ingestion Risks. Column 2 lists the dissolved concentrations measured in the saturated source zone or directly below the vadose source zone soils of the subject site. Column 3 lists the maximum contaminant levels (MCLs) for each hydrocarbon compound. Columns 4 and 8 list the dissolved concentrations that present a hazard quotient of 1 or a carcinogenic risk of 1×10^{-5} for residential and industrial sites, respectively (note that some MCLs are lower than the risk based groundwater ingestion concentration). Columns 5 and 9 show the groundwater compliance concentrations which is the MCL or risk based concentration for sites with potable groundwater, and 10 times the MCL or risk based concentration for sites with non-potable groundwater. Columns 6 and 10 show the fractions of the risk-based concentration that exist for each compound or hydrocarbon group. Columns 7 and 11 indicate whether the existing concentrations are within the regulatory or risk-based criteria for each compound or hydrocarbon group (a zero in the column indicates that the ADEC compliance criteria are met, and a 1 indicates that compliance criteria have not been met). Note that some compliance criteria are not risk based, for example, the MCL for benzene is 5 micrograms per liter [$\mu\text{g}/\text{L}$], while the concentration which presents an unacceptable risk is 15 $\mu\text{g}/\text{L}$. Because some MCLs are not risk based compliance criteria may not be met (the MCL may be exceeded) even though the site poses an acceptable risk. The example results show that the input water concentrations meet the regulatory standards for groundwater and also meet risk-based criteria.

Page 9, Potential Cumulative Risk Assuming All Pathways Complete. The “potential cumulative risk assuming all pathways complete” is the risk that would be present if the site was developed such that and all exposure pathways were complete. For this scenario to occur a structure (the family home or work place building) would have to be built over the contaminated soil such that the indoor air route is completed, the homes (or work place) drinking water would be from a well completed in the mixing zone at the downgradient edge of the source area, the family kids (or site workers) would have direct contact with the contaminated source area soils in the yard, and while outside, the family (or site workers) would breath outdoor air impacted by the site contaminants. Under a true risk based corrective action/risk based cleanup system the potential cumulative risk must be below an excess carcinogenic risk of 10^{-5} and the cumulative hazard quotient must be below 1 before a site may be closed. (Note that sites which are zoned industrial may be closed if the industrial risk meets the above risk criteria). Also note that the calculation of potential risks associated with the migration to indoor air route requires some assumptions about the buildings that may be built at the site.

Per ADEC guidance, the cumulative risk is calculated as the sum of the BTEX and PAH risks for all pathways. The risks associated with the GRO, DRO, and RRO compound groups are not included in the cumulative risk because the ADEC considers that the risk associated with these compounds to be represented by the BTEX and PAH data---hence the GRO, DRO and RRO cumulative risk is not displayed.

When using a four-phase solution (when NAPL is present), the risk associated with the outdoor air inhalation, indoor air inhalation and migration-to-groundwater pathways does not increase linearly with increasing concentrations. Rather in calculations preformed for other projects, the outdoor air inhalation, indoor air inhalation and migration-to-groundwater risks increase only slightly when the soil concentration is doubled and tripled. It should also be noted that soil ingestion risks do increase linearly with increasing soil concentrations and that the groundwater ingestion risks increase linearly with increasing dissolved phase concentrations.

The example calculation using the default BTEX soil cleanup levels from ADEC Table B1 and the maximum allowable GRO and DRO concentrations from Table B2 shows that the cumulative risk posed by the input soil and groundwater concentrations are within acceptable carcinogenic and noncarcinogenic risk levels. As per ADEC guidance, the cumulative risk is the sum of the BTEX and PAH risks via all exposure pathways (that is, GRO and DRO are not included in the cumulative risk calculations).

Page 10, Potential Cumulative Risk for Pathways Complete at Present Time. The “cumulative risk for the pathways complete at present time” is the risk that is present from completed exposure pathways under the current land use at the time the report is prepared. The evaluation of which exposure pathways are complete is done as part of the site characterization/site investigation work and is input to the model on page one (gold block of cells). The hydrocarbon risk calculator simply sums the risk from the completed exposure pathways. For example if a residence has contaminated soil from a heating oil tank in the backyard and under the foundation of the house, but the residence is on city water system the migration to indoor air, migration to outdoor air and soil ingestion routes would likely be considered complete, but the groundwater ingestion route would not be complete. The

hydrocarbon risk calculator would sum the risk from the complete pathways and assess if the current situation presents an acceptable or unacceptable risk. If the current site conditions present an unacceptable risk, the responsible party and regulatory agency may use hydrocarbon risk calculator data to prioritize corrective action at the site and to identify the compounds and exposure routes that drive the risk. The existing cumulative risk calculation is used primarily as a tool to allow the identification and mitigation of existing human health risk and secondarily it could be used to assign a site status. Per ADEC guidance on cumulative risk, the cumulative risk at the present time is calculated as the sum of the BTEX and PAH risks for completed pathways. The risks associated with the GRO, DRO, and RRO compound groups are not included in the existing cumulative risk because the ADEC considers that the risk associated with these compounds to be represented by the BTEX and PAH data.

In the example calculation the groundwater ingestion pathway is not complete. Hence, the fraction of risk values for all compounds in the groundwater ingestion risks column is zero. The example calculation using the default BTEX soil cleanup levels from ADEC Table B1 and the maximum allowable GRO and DRO concentrations from Table B2 shows that the cumulative risk posed by the input soil and groundwater concentrations are within acceptable carcinogenic and noncarcinogenic risk levels.

Page 11, Partitioning into Surface Water and Groundwater. This section of the hydrocarbon risk calculator assesses if contaminated soil from the site has the potential to cause groundwater to exceed MCLs or risk based concentrations or to cause surface water to exceed the ambient water quality criteria. To make these assessments the dissolved phase equilibrium concentration, or the measured groundwater concentration (depending on whether the source is in the vadose or saturated zones) is compared to the MCL or risk based groundwater concentrations and ambient water quality criteria. The information may be used to assign a site closeout status (provided human health and environmental risk criteria are met) as recommended in the technical background document on site closeout (Geosphere and CH2MHill, 2006). In the example calculation the soil from the subject site could be used as vadose zone fill at another location assuming that the default DAF applied at the new location (as indicated by the zeros in the “check for vadose zone fill” column), and/or the soil could be used as saturated zone fill (as indicated by the zeros in the “check for saturated zone fill” column). The soils from the subject site should not be used as saturated zone fill because the soils would likely cause the surface water to exceed the TAH, TAqH and surface water sheen criteria as indicated by the ones in the “check for surface water body fill” column.

Page 12, Site Status Summary. The final section of the four-phase phase cumulative risk calculator summarizes the site status as described in the SOCWG paper on proposed site closure criteria (Geosphere & CH2MHill, 2006). The summary for the hypothetical example calculation (which uses Table B1 BTEX and PAH concentrations and Table B2 maximum allowable GRO and DRO concentrations as input) shows that the hypothetical site meets the cumulative carcinogenic and non-carcinogenic risk criteria and meets the GRO, DRO and RRO risk criteria for each exposure pathway. The calculator tells us that because the human health risk criteria have been met the site can be closed provided the ecological risk criteria have been met. In addition, the calculator indicates that soils from the subject site may be used as vadose zone fill or as saturated zone fill at another site, but may not be used as fill in

a surface water body. Note that the site status categories referenced by the calculator are not officially recognized by the ADEC. However the categories are logical, quantifiable and rely on the same conceptual criteria that ADEC uses in assessing site status, so they may be useful when evaluating and negotiating site closeout and conditional closure criteria.

Summary and Recommendations

This document provides background information regarding hydrocarbon phase partitioning and describes a “hydrocarbon risk calculator”.

The phase partitioning discussion documents that fuel hydrocarbons may be present in the soil environment in four phases: dissolved in the soil moisture and groundwater; as a vapor in the air filled soil pores; adsorbed to minerals and naturally occurring organics; and as non-aqueous phase liquids (NAPL). When NAPL is not present the distribution may be described as a three-phase distribution, and when NAPL is present the distribution may be described as a four-phase distribution. When a multi-constituent NAPL is present the dissolved, vapor and adsorbed concentrations may be characterized by Raoult’s Law which indicates that the effective solubility and vapor pressure of a compound is a function of the mole fraction of that compound in the NAPL. Calculations are presented that show that GRO, DRO and RRO NAPL are present at the lowest 18 AAC 75, Table B2 levels. This indicates that four-phase calculations with Raoult’s law should be used to more accurately characterize the phase partitioning processes and human health risks associated with spilled hydrocarbons soils and groundwater at most regulated hydrocarbon spill sites in Alaska.

The “hydrocarbon risk calculator” is an Excel spreadsheet that may be used to characterize human health risks posed by fuel hydrocarbons in soil and groundwater. The hydrocarbon risk calculator performs the following functions:

- Uses the Excel add in tool “solver” to calculate the dissolved, vapor, adsorbed and NAPL concentrations in a contaminated soil source zone following the phase partitioning relationships and Raoult’s Law
- Uses the EPA and ADEC soil screening equations to calculate the soil ingestion, migration to outdoor air and groundwater ingestion risks
- Uses the Johnson & Ettinger equation to assess the vapor intrusion/migration to indoor air risks
- Presents the risk calculations for both residential and industrial sites
- Calculates cumulative risk assuming that all pathways are complete and calculates cumulative risk for pathways complete at the present time.
- Assesses if contaminated soil can be transported off-site and placed in the saturated zone, vadose zone and/or in surface water bodies without posing a potential threat to water quality.
- Uses “if- then” statements to suggest a site a status following the SOCWG document presenting a proposed “contaminated site classification system”

The hydrocarbon risk calculator has been peer reviewed by the Department of Civil & Environmental Engineering at the University of Alaska, Fairbanks and by staff from the

ADEC, and has been approved by the ADEC for use on method 3 and/or method 4 human health risk calculations.

The SOCWG recommends that the ADEC provide training for their staff on hydrocarbon phase partitioning and on the hydrocarbon risk calculator, and help facilitate the dissemination of the information in this report to responsible parties, consultants and the public.

SECTION 7

References

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Tables

Table 1 Selected Hydrocarbon Solubilities, Henry's Constant, Koc and Csat Values

Fraction	Equivalent Carbon Number	Molecular Weight	Single Component Solubility (mg/L)	H' Henry's Constant (unitless)	K _{oc} (ml/g)	Mass in Solution (mg/kg dry soil)	Mass in Vapor (mg/kg dry soil)	Mass Adsorbed (mg/kg dry soil)	Vadose Zone C _{sat} (mg/kg)	% Mass in Solution (vadose zone)	% Mass in Vapor (vadose zone)	% Mass Adsorbed (vadose zone)	Saturated Zone C _{sat} (mg/kg)		
Aromatics															
Benzene	6.50	78	1750	2.28E-01	5.89E+01	350.0	35.6	103.1	489	71.62%	7.29%	21.09%	609		
Toluene	7.58	92	526	2.72E-01	1.82E+02	105.2	12.8	95.7	214	49.23%	5.98%	44.80%	248		
Ethylbenzene	8.50	106	169	3.23E-01	2.78E+02	33.8	4.9	47.0	86	39.46%	5.69%	54.85%	96		
Xylene	8.63	106	161	2.13E-01	3.63E+02	32.2	3.1	58.4	94	34.36%	3.27%	62.37%	105		
C ₉	9.00	114	65	4.27E-01	1.58E+03	12.9	2.5	102.3	118	10.97%	2.09%	86.94%	121		
C ₁₀	10.00	122	40	2.51E-01	2.00E+03	8.0	0.9	79.4	88	9.02%	1.01%	89.97%	91		
C ₁₂	12.00	138	15	8.71E-02	3.16E+03	3.0	0.1	47.9	51	5.93%	0.23%	93.83%	52		
C ₁₄	14.00	152	5.8	3.02E-02	5.01E+03	1.2	0.0	28.8	30	3.84%	0.05%	96.11%	31		
C ₁₆	16.00	166	2.2	1.05E-02	7.94E+03	0.4	0.0	17.4	18	2.46%	0.01%	97.53%	18		
Aliphatics															
C ₆	6.00	88	16	5.25E+01	1.35E+03	3.2	74.3	21.4	99	3.21%	75.16%	21.63%	26		
C ₆ -C ₈	7.00	102	4.5	5.50E+01	3.80E+03	0.9	21.9	17.0	40	2.24%	55.08%	42.67%	18		
C ₈ -C ₁₀	9.00	130	0.35	6.03E+01	3.02E+04	0.1	1.9	10.7	13	0.56%	15.04%	84.40%	11		
C ₁₀	10.00	145	0.10	6.31E+01	85113.80	0.0	0.6	8.5	9	0.22%	6.20%	93.58%	9		
C ₁₂	12.00	172	0.007943	6.92E+01	6.76E+05	0.0	0.0	5.4	5	0.03%	0.91%	99.07%	5		
C ₁₄	14.00	200	0.000631	7.59E+01	5.37E+06	0.0	0.0	3.4	3	0.00%	0.13%	99.87%	3		
C ₁₆	16.00	228	0.000050	8.32E+01	4.27E+07	0.0	0.0	2.1	2	0.00%	0.02%	99.98%	2		
C ₂₀	20.00	283	0.0000003	1.00E+02	2.69E+09	0.0	0.0	0.9	1	0.00%	0.00%	100.00%	1		
Vadose Soil Conditions:															
porosity (n)= 0.434				foc= 0.001				na= 0.13				sp.G.= 2.65			
bulk density (g/cm ³) = 1.5				grav. soil moist.= 0.20				nw= 0.300				saturated gravimetric moisture content= 0.289308176			
Saturated Soil Conditions:															
porosity (n)= 0.434				foc= 0.001				na= 0.00							
bulk density (g/cm ³) = 1.5								nw= 0.43							

$$C_{sat} = (S \cdot n_w / p_b) + (S \cdot H' \cdot n_a / p_b) + (foc \cdot k_{oc} \cdot S)$$

Table 2 Example Dissolved BTEX Concentrations Based on COTU Fuel Analysis and 3- and 4-Phase Partitioning

Compound	Benzene	Toluene	Ethylbenzene	Xylene
Mass Fraction in COTU Arctic Diesel	0.0106	0.27	0.32	1.70
Theoretical/ Maximum Solubility (mg/L)	1750	526	169	161
3-Phase Dissolved Concentration in Soil with 5,000 mg/kg COTU Diesel (mg/L)	1.88	33.04	32.11	50.57
3-Phase Dissolved Concentration in Soil with 10,000 mg/kg COTU Diesel (mg/L)	3.76	66.09	64.22	101.14
3-Phase Dissolved Concentration in Soil with 15,000 mg/kg COTU Diesel (mg/L)	5.64	99.13	96.33	151.71
4-Phase Dissolved Concentration in Soil with 5,000 mg/kg COTU Diesel (mg/L)	0.32	2.13	0.72	3.66
4-Phase Dissolved Concentration in Soil with 10,000 mg/kg COTU Diesel (mg/L)	0.33	2.17	0.73	3.67
4-Phase Dissolved Concentration in Soil with 15,000 mg/kg COTU Diesel (mg/L)	0.33	2.18	0.76	3.68

Overestimate of Dissolved Phase Concentration When Using 3-Phase Model

3-phase model overestimate of dissolved concentration	Benzene	Toluene	Ethylbenzene	Xylene
5,000 mg/kg	5.947076604	15.51356065	44.47368943	13.81718186
10,000 mg/kg	11.47209569	30.50739739	88.56611302	27.55067155
15,000 mg/kg	17.08432915	45.47323513	126.4173377	41.22626545

All soil characteristics match ADEC default assumptions
 COTU March Sample used in calculations

Table 3	Hydrocarbon Risk Calculator	Facility Location: Example Calculation	Facility Name: Table B1 & B2 Soil Concentrations
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Version 1.3, Larry Acomb, Geosphere, Inc., October 2006	Solver solution based on work of Hun Seak Park, 1999 & 2000	Page 1	Solver Instructions & Information:
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Model Input Parameters:			Soil Properties:			FYI Unit Conversions		Climate Related Outdoor Air Inhalation and Soil Ingestion Exposure Parameters	
Chemical Concentrations in Site Soils (mg/kg):	Field Data in Yellow Highlighted Cells	Chemical Concentrations in Site Groundwater (mg/L):	Field Data in Yellow Highlighted Cells	Site Specific and/or Field Data in Yellow Highlighted Cells	ADEC Default Value (all climate zones)	bulk density conversion input (g/cm ³)	bulk density output (lbs/ft ³)	1. Set value of cell M9 to an initial value of 0001	4. By varying "M9" and "G12"
Benzene (mg/kg)	0.02	Benzene (mg/L)	0.0045	93.6	93.6	1.76	109.824	2. Select Solver from Tools menu above	6. Hit the "solve" button
Toluene (mg/kg)	5.4	Toluene (mg/L)	0.3539	2.65	2.65	K (ft/day)	K (cm/sec)	3. Select "F71" as the target cell and set value of F71=1	7. After a solution is found highlight the "keep solver solution" dot and hit the "OK" button
Ethylbenzene (mg/kg)	5.5	Ethylbenzene (mg/L)	0.1018	0.433962264	0.43	400	0.141111111	Molecular density (mol/L) initial value= 0001 0.126190495	
Xylene (mg/kg)	78.	Xylene (mg/L)	1.3748	10	10	Exposure Routes Complete at Present Time			
GRO (mg/kg)	1,400.	GRO (mg/L)	0.9512	0.0010	0.001	Exposure Routes	1 for complete, 0 for incomplete	Initial air filled porosity (used to start iterations)	
DRO (mg/kg)	12,500.	DRO (mg/L)	2.748	0.150	0.15	Soil Ingestion	1	Conservation of volume equation (should be zero)	
RRO (mg/kg)	100.	RRO (mg/L)	0.0985	0.258	0.28	Outdoor Air	1	-5.51E-12	
Total Petroleum Hydrocarbons (mg/kg)	14,000	Total Petroleum Hydrocarbons & Polar Compounds (mg/L)	3.7977	0.026	0.026	Indoor Air	1	Exposed Population estimate may be used for prioritizing sites.	
GRO Aromatics Fraction	0.2000	GRO aromatics (mg/L)	0.50	34.57%	34.57%	Groundwater Ingestion	0		
DRO Aromatics Fraction	0.2000	DRO aliphatics (mg/L)	0.40	6.03%	6.03%	Exposed Population	1		
RRO Aromatics Fraction	0.2000	DRO aromatics (mg/L)	0.40	15	25	ADEC Default Values <40" precip/yr			
Naphthalene	0.2371	Naphthalene	0.001	105	105	ADEC Default Values >40" precip/yr		Soil Ingestion & Inhalation Exposure Frequency (days/yr)	
Acenaphthene	0.2817	Acenaphthene	0.002	25.59	25.59	Residential		ADEC Default Values	
Fluorene	0.6038	Fluorene	0.0028	0.002	0.002	Industrial		arctic zone; precip <40"; precip >40"	
Anthracene	0.0467	Anthracene	4.00E-04	2.78E-03	2.78E-03	270		Res 200; 270; 330 / Indus 200; 250; 250	
Fluoranthene	0.0636	Fluoranthene	6.40E-05	32.808	32.8	Q/C for volatilization to Outdoor Air calcs.		ADEC Default Values	
Pyrene	0.2027	Pyrene	5.30E-05	32	32	Residential		arctic zone; precip <40"; precip >40"	
Benzo (a) Anthracene	0.0084	Benzo (a) Anthracene	9.50E-06	0.13	0.13	90.82		100.13; 90.82; 82.72	
Chrysene	0.0317	Chrysene	4.75E-06	0.002	0.002	Industrial			
Benzo (b) fluoranthene	0.0241	Benzo (b) fluoranthene	1.20E-05	8.77E+02	8.76E+02				
Benzo (k) fluoranthene	0.0185	Benzo (k) fluoranthene	7.50E-06	10.0	10.0				
Benzo (a) pyrene	0.0161	Benzo (a) pyrene	5.50E-06	5.5	5.5				
Indeno (1,2,3-cd) pyrene	0.0055	Indeno (1,2,3-cd) pyrene	6.50E-06	3.3	3.3				
Dibenz (a,h) anthracene	0.0032	Dibenz (a,h) anthracene	8.00E-06	10	10				
						Attenuation Factor		10 if vadose zone source, 0 for saturated zone source	
						Non Potable Aquifer?		1 for potable aquifer, 10 for non potable aquifer (based on 10x table C rule)	

Table 3	Migration to Indoor Air-- Data Entry			Example Calculation			Table B1 & B2 Soil Concentrations		Page 2			
NAPL source area soil gas concentrations calculated by the 4-phase calculator. Attenuation factor "alpha" calculated by the Johnson & Ettinger model. Incremental risk posed by NAPL source area soil gas concentrations via the migration to indoor air pathway shown here and entered into the cumulative risk calculations.												
Site Specific and/or Field Data in Yellow Highlighted Cells												
Soil Properties:	Top Layer immediately below slab (not contaminated)	Middle Layer (not contaminated)	Bottom Layer (not contaminated)	Building Properties:	input value	default input values: basement	default input values: slab on grade			Human Health Exposure Criteria		
bulk density (lbs/ft ³)	94	100	105	Lb = length of building (cm)	1000	1000	1000			Residential	Industrial	
bulk density (g/cm ³)	1.506410256	1.602564103	1.682692308	Wb = width of building (cm)	1000	1000	1000	Acrack= area of total cracks (cm ²) = Xcrack* Wcrack = Ab/n	400	TCR=	1.00E-05	1.00E-05
specific gravity of solids	2.65	2.65	2.65	Hb = height of building (cm)	366	366	244	Xcrack = floor -wall seam perimeter (cm)	4000	THQ= target hazard quotient (e.g. 1.0)	1	1
porosity	0.431543299	0.395258829	0.365021771	ER = air exchange rate (1/hr)	0.25	0.25		u = viscosity of air (g/cm-sec)	1.77E-04	ATc= averaging time carcinogen (days), (=70 years)	25,550	25,550
moisture content (% by weight)	16.11	12	14	Lf = depth below grade of bottom of floor slab or basement (cm)	200	200	15	Zcrack = crack depth below grade (cm)	200	ATnc= averaging time non-carcinogen	30	30
foc	0.00172	0.00172	0.00172	Wcrack = floor -wall seam crack width (cm)	0.1			equation 16 r crack= n /(Ab /Xcrack)	0.1	EF= exposure frequency (350 days/year)	350	250
water filled porosity	0.242682692	0.192307692	0.235576923	Lcrack = enclosed space foundation thickness or slab thickness (cm)	10	10	10	n = Acrack/Ab (0<n<=1)	0.000222222	ED= exposure duration (30 years)	30	25
air filled porosity	0.188860607	0.202951137	0.129444848	delta P = pressure differential between building and soil (g/cm-s ²)	40	40 g/cm-s ² = 4 pascals (Pa)	typical conservative values = 4 or 5 Pa; max range = 0 to 20 Pa	equation 14 Q building=building ventilation rate (cm ³ /sec) = (Lb*Wb*Hb*ER)/3,600s/h	2.54E+04	C cancer =	[(TCR*ATc)/(EF*ED *URF)]	
layer thickness (ft)	7	1	1	kv = soil vapor permeability= top soil layer (cm ²)	1.00E-08	1.00E-08		equation 14 Q building=building ventilation rate (cm ³ /sec; over ride calculated value--optional)		C non-cancer =	(TQH*Rfc*1000ug/ mg)	
layer thickness (cm)	213.36	30.48	30.48	Ab= surface area of enclosed space below grade (cm ²)	1.80E+06	=area of basement walls+ basement floor... or area of slab		equation 15 Q soil = (2* pi * delta P * kv* Xcrack)/u ln (2 Zcrack/ r crack)	6.85E+00			
Ls = Total depth from ground surface to contaminant (ft)	9	Ls soil gas reading depth (cm)	274.32	Q building =building ventilation rate (cm ³ /sec)	25416.66667			Rc (gas constant, cal/mol-degree K)	1.9872			
kv = soil vapor permeability (cm ²)	1.00E-08	1.00E-08	1.00E-08	Lr = total source-building separation distance (cm)	74.32			R (gas constant, atm-m ³ /mol-degree K)	8.2057E-05			

Table 3		Phase Partitioning Results			Example Calculation			Table B1 & B2 Soil Concentrations					
Page 3	column 1	2	3	4	5	6	7	8	9	10	11	12	13
Hydrocarbon Fractions	Median Equivalent Carbon	Distribution of DRO & GRO into Aromatic & Aliphatic Equivalent Carbon Ranges (varies by fuel type)	Soil Concentration (mg/kg)	Fraction of TPH Mass	Xi (Mole Fraction in NAPL using 4-phase model; unique solution)	Water (mg of chemical/L of pore water)	Air (mg/L pore air)	% of Hydrocarbon Mass in Dissolved Phase	% of Hydrocarbon Mass in Vapor Phase	% of Hydrocarbon Mass Adsorbed to Soils	% of Hydrocarbon Mass in NAPL	Sum of Dissolved, Vapor, Adsorbed and NAPL Phases	
Benzene C ₇ -C ₇	6.50	from analysis	0.020	0.000001	2.90E-06	5.08E-03	7.44E-04	2.539%	0.640%	1.495%	95.33%	100.00%	
Toluene C ₇ -C ₈	7.58	from analysis	5.400	0.000386	6.82E-04	3.59E-01	5.90E-02	0.664%	0.188%	1.209%	97.94%	100.00%	
Ethylbenzene C ₈ -C ₉	8.50	from analysis	5.500	0.000393	6.10E-04	1.03E-01	1.90E-02	0.188%	0.059%	0.587%	99.17%	100.00%	
Xylene C ₈ -C ₉	8.63	from analysis	78.000	0.005571	8.65E-03	1.39E+00	2.18E-01	0.179%	0.048%	0.648%	99.12%	100.00%	
Aromatic C ₉ -C ₁₀	9.50	0.6061	191.080	0.013649	1.90E-02	9.64E-01	1.23E-01	0.050%	0.011%	0.897%	99.04%	100.00%	
Aromatic C ₁₀ -C ₁₂	11.00	0.24	610.759	0.043626	5.55E-02	1.38E+00	6.80E-02	0.022%	0.002%	0.560%	99.42%	100.00%	
Aromatic C ₁₂ -C ₁₆	13.00	0.56	1392.057	0.099433	1.14E-01	1.06E+00	2.72E-02	0.008%	0.000%	0.303%	99.69%	100.00%	
Aromatic C ₁₆ -C ₂₄	17.00	0.20	497.183	0.035513	3.42E-02	4.61E-02	3.44E-04	0.001%	0.000%	0.093%	99.91%	100.00%	
Aromatic C ₂₄ -C ₃₅	25.00	1.0000	20.000	0.001429	1.07E-03	3.02E-05	1.47E-08	0.000%	0.000%	0.010%	99.99%	100.00%	
Aliphatic C ₈ -C ₈	5.50	0.00	0.000	0.000000	0.00E+00	0.00E+00	0.00E+00	0.000%	0.000%	0.000%	0.00%	0.00%	
Aliphatic C ₈ -C ₉	6.00	0.00	2.539	0.000181	3.39E-04	6.47E-03	8.49E-02	0.025%	0.575%	0.344%	99.06%	100.00%	
Aliphatic C ₉ -C ₁₀	9.00	1.00	1117.461	0.079819	1.02E-01	4.34E-02	1.29E+00	0.000%	0.020%	0.117%	99.86%	100.00%	
Aliphatic C ₁₀ -C ₁₂	11.00	0.35	3452.123	0.246580	2.59E-01	8.77E-03	3.86E-01	0.000%	0.002%	0.061%	99.94%	100.00%	
Aliphatic C ₁₂ -C ₁₆	13.00	0.56	5578.849	0.398489	3.56E-01	9.57E-04	1.09E-01	0.000%	0.000%	0.033%	99.97%	100.00%	
Aliphatic C ₁₆ -C ₂₄	17.00	0.10	969.028	0.069216	4.76E-02	8.09E-07	6.71E-04	0.000%	0.000%	0.010%	99.99%	100.00%	
Aliphatic C ₂₄ -C ₃₅	25.00	1.0000	80.000	0.005714	2.71E-03	1.83E-12	5.88E-08	0.000%	0.000%	0.001%	100.00%	100.00%	
			14000.000	100.0000%	1.00000	5.35E+00	2.39E+00						

Table 3		Soil Ingestion Level Calculations					
Page 4		Example Calculation			Table B1 & B2 Soil Concentrations		
1	2	3	4	5	6	7	8
Compounds	Sample Concentrations (mg/kg)	Soil Ingestion Level Residential Land Use	Residential Land Use Fraction of Risk Based Target Concentration (values greater than 1 exceed the risk based target)	Check for compliance with risk levels (0= in compliance; 1= not in compliance)	Soil Ingestion Level Industrial Land Use	Industrial Land Use Fraction of Risk Based Target Concentration (values greater than 1 exceed the risk based target)	Check for compliance with risk levels (0= in compliance; 1= not in compliance)
Benzene	0.02	151.	1.33E-04	0	1,041.	1.92E-05	0
Toluene	5.4	20,278.	2.66E-04	0	408,800.	1.32E-05	0
Ethylbenzene	5.5	10,139.	5.42E-04	0	204,400.	2.69E-05	0
Xylene	78.	202,778.	3.85E-04	0	4,088,000.	1.91E-05	0
GRO Aromatics	191.	20,278.	0.0094	0	408,800.	4.67E-04	0
DRO Aromatics	2,500.	4,056.	0.6164	0	81,760.	0.0306	0
RRO Aromatics	20.	3,042.	0.0066	0	61,320.	3.26E-04	0
GRO Aliphatics	1,120.	506,944.	0.0022	0	10,220,000.	1.10E-04	0
DRO Aliphatics	10,000.	10,139.	0.9863	0	204,400.	0.0489	0
RRO Aliphatics	80.	202,778.	3.95E-04	0	4,088,000.	1.96E-05	0
Naphthalene	0.2371	4,056.	5.85E-05	0	81,760.	2.90E-06	0
Acenaphthene	0.2817	6,083.	4.63E-05	0	122,640.	2.30E-06	0
Fluorene	0.6038	4,056.	1.49E-04	0	81,760.	7.39E-06	0
Anthracene	0.0467	30,417.	1.53E-06	0	613,200.	7.61E-08	0
Fluoranthene	0.0636	4,056.	1.57E-05	0	81,760.	7.78E-07	0
Pyrene	0.2027	3,042.	6.66E-05	0	61,320.	3.31E-06	0
Benzo (a) Anthracene	0.0084	11.3426	7.43E-04	0	78.4	1.08E-04	0
Chrysene	0.0317	1,134.	2.79E-05	0	7,840.	4.04E-06	0
Benzo (b) fluoranthene	0.0241	11.3426	0.0021	0	78.4	3.07E-04	0
Benzo (k) fluoranthene	0.0185	113.	1.63E-04	0	784.	2.35E-05	0
Benzo (a) pyrene	0.0161	1.1343	0.0142	0	7.84	0.0021	0
Indeno (1,2,3-cd) pyrene	0.0055	11.3426	4.87E-04	0	78.4	7.05E-05	0
Dibenz (a,h) anthracene	0.0032	1.1343	0.0028	0	7.84	4.12E-04	0
Carcinogenic Cumulative Risk			0.0207	0		0.003	0
noncarcinogenic Cumulative Risk			0.0015	0		7.59E-05	0

Values shown in the fourth and seventh columns are the normalized fraction of the risk based level, and not the carcinogenic risk level. The fraction of risk multiplied by 10⁻⁵ equals the carcinogenic risk level for the carcinogenic compounds.

Table 3		Migration to Outdoor Air Vapor Inhalation Levels					
Page 5		Example Calculation			Table B1 & B2 Soil Concentrations		
1	2	3	4	5	6	7	8
Compounds	Vapor Concentration in Sample (based on 3 or 4- phase partitioning, whichever is accurate, mg/L)	Residential Site Hypothetical Soil Vapor Concentration when HQ=1 or Target Risk =10 ⁻⁵ (mg/L; from 3-phase equation)	Fraction of Risk Based Target Concentration (values greater than 1 exceed the risk based target)	Check for compliance with risk levels (0= in compliance; 1= not in compliance)	Industrial Land Use Target Soil Vapor Concentration (Health Based Vapor Concentration Multiplied by the VF, etc.)	Fraction of Risk Based Target Concentration (values greater than 1 exceed the risk based target)	Check for compliance with risk levels (0= in compliance; 1= not in compliance)
Benzene	1.92E-04	9.748	1.97E-05	0	11.1962	1.71E-05	0
Toluene	0.0152	1,186.	1.28E-05	0	1,570.	9.69E-06	0
Ethylbenzene	0.0049	2,918.	1.68E-06	0	4,627.	1.06E-06	0
Xylene	0.0561	No Vapor Risk		0	No Vapor Risk		0
GRO Aromatics	0.0316	317.	9.98E-05	0	5,118.	6.17E-06	0
DRO Aromatics	0.0246	84.5345	2.91E-04	0	4,791.	5.14E-06	0
RRO Aromatics	3.79E-09	No Vapor Risk		0	No Vapor Risk		0
GRO Aliphatics	0.3553	51,328.	6.92E-06	0	66,803.	5.32E-06	0
DRO Aliphatics	0.1279	1,290.	9.91E-05	0	7,850.	1.63E-05	0
RRO Aliphatics	1.52E-08	No Vapor Risk			No Vapor Risk		
Naphthalene		1,1599			133.		
Acenaphthene		No Vapor Risk			No Vapor Risk		
Fluorene		No Vapor Risk			No Vapor Risk		
Anthracene		No Vapor Risk			No Vapor Risk		
Fluoranthene		No Vapor Risk			No Vapor Risk		
Pyrene		No Vapor Risk			No Vapor Risk		
Benzo (a) Anthracene		No Vapor Risk			No Vapor Risk		
Chrysene		No Vapor Risk			No Vapor Risk		
Benzo (b) fluoranthene		No Vapor Risk			No Vapor Risk		
Benzo (k) fluoranthene		No Vapor Risk			No Vapor Risk		
Benzo (a) pyrene		No Vapor Risk			No Vapor Risk		
Indeno (1,2,3-cd) pyrene		No Vapor Risk			No Vapor Risk		
Dibenz (a,h) anthracene		No Vapor Risk			No Vapor Risk		
Carcinogenic Cumulative Risk			1.97E-05	0		1.71E-05	0
noncarcinogenic Cumulative Risk			1.45E-05	0		1.07E-05	0

Values shown in the fourth and seventh columns are the normalized fraction of the risk based level, and not the carcinogenic risk level. The fraction of risk multiplied by 10⁻⁵ equals the carcinogenic risk level for the carcinogenic compounds.

Table 3		Migration to Indoor Air Vapor Inhalation Levels						
Page 6		Example Calculation			Table B1 & B2 Soil Concentrations			
1	2	3	4	5	6	7	8	9
Compounds	Vapor Concentration in Sample (ug/m ³)	Building Vapor Concentration given site conditions (ug/m ³)	Residential Land Use Target Building Vapor Concentration when HQ=1 or Target Risk =10 ⁻⁵ (ug/m ³)	Residential Land Use Hazard Quotient or Fraction of Risk Based Target Concentration (values greater than 1 exceed the risk based target)	Residential Land Use check for compliance with risk levels (0= in compliance; 1= not in compliance)	Industrial Land Use Target Building Vapor Concentration when HQ=1 or Target Risk =10 ⁻⁵ (ug/m ³)	Industrial Land Use Hazard Quotient or Fraction of Risk Based Target Concentration (values greater than 1 exceed the risk based target)	Industrial Land Use check for compliance with risk levels (0= in compliance; 1= not in compliance)
Benzene	744.	0.1634	3.1197	0.05238	0	5.24103	0.0312	0
Toluene	59,014.	12.9278	417.	0.03099	0	700.8.	0.0184	0
Ethylbenzene	19,031.	4.0477	22.1212	0.18298	0	37.16364	0.1089	0
Xylene	217,735.	45.6307	7,300.	0.00625	0	12,264.0.	0.0037	0
GRO Aromatics	122,516.	27.5127	417.	0.06596	0	700.8.	0.0393	0
DRO Aromatics	95,508.	21.4716	209.	0.10295	0	350.4.	0.0613	0
RRO Aromatics	0.0147	3.59E-06	NA	NA	0	NA	NA	0
GRO Aliphatics	1,378,322.	309.	19,189.	0.01612	0	32,236.8.	0.0096	0
DRO Aliphatics	496,205.	111.	1,043.	0.10677	0	1,752.0.	0.0636	0
RRO Aliphatics	0.0588	1.32E-05	NA	NA	0	NA	NA	0
Naphthalene	2,9085	6.59E-04	3.1286	2.105E-04	0	5.256	1.25E-04	0
Acenaphthene	0.1045	2.41E-05	219.	1.103E-07	0	367.9.	6.56E-08	0
Fluorene	0.0396	9.40E-06	146.	6.438E-08	0	245.3.	3.83E-08	0
Anthracene	5.65E-05	1.35E-08	1,147.	1.173E-11	0	1,927.2.	6.98E-12	0
Fluoranthene	7.20E-05	1.81E-08	146.	1.243E-10	0	245.3.	7.40E-11	0
Pyrene	9.91E-05	2.53E-08	115.	2.209E-10	0	192.7.	1.31E-10	0
Benzo (a) Anthracene	6.77E-08	1.77E-11	0.1159	1.529E-10	0	0.19467	9.10E-11	0
Chrysene	1.12E-06	2.41E-10	11.5873	2.082E-11	0	19.46667	1.24E-11	0
Benzo (b) fluoranthene	7.95E-07	1.67E-10	0.1159	1.439E-09	0	0.19467	8.57E-10	0
Benzo (k) fluoranthene	2.20E-09	6.12E-13	1.1587	5.281E-13	0	1.94667	3.14E-13	0
Benzo (a) pyrene	4.92E-09	1.32E-12	1.62E-04	8.148E-09	0	2.725E-04	4.85E-09	0
Indeno (1,2,3-cd) pyrene	2.78E-11	7.44E-15	0.1159	6.420E-14	0	0.19467	3.82E-14	0
Dibenz (a,h) anthracene	6.39E-12	1.03E-13	0.0116	8.872E-12	0	0.01947	5.28E-12	0
Carcinogenic Cumulative Risk			ethylbenzene as carcinoger	0.2354	0		0.1401	0
noncarcinogenic Cumulative Risk				0.0375	0		0.0223	0

columns are the normalized fraction of the risk based level, and not the

Table 3										
Calculated Migration to Groundwater Levels										
Page 7	Example Calculation				Table B1 & B2 Soil Concentrations					
1	2	3	4	5	6	7	8	9	10	11
Compounds	Dissolved Concentration in Soil Sample (based on 3 or 4 phase partitioning, whichever is accurate, mg/l)	Maximum Contaminant Level (mg/L)	Residential Land Human Health Risk Based Drinking Water Concentration (mg/l)	Residential Land Soil Moisture Target Concentration (MCL or Risk Based Concentration Multiplied by the DAF.....MCLs values used for compounds with MCLs)	FYI Fraction of Risk Based Target Concentration (values greater than 1 exceed the risk based target; MCLs not used)	Check for compliance with regulatory levels (MCLs used for compounds with MCLs: 0= in compliance; 1= not in compliance)	Industrial Land Human Health Risk Based Drinking Water Concentration (mg/l)	Industrial Land Soil Moisture Target Concentration (MCL or Risk Based Concentration Multiplied by the DAF.....MCLs values used for compounds with MCLs)	FYI Fraction of Risk Based Target Concentration (values greater than 1 exceed the risk based target; MCLs not used)	Check for compliance with regulatory levels (MCLs used for compounds with MCLs: 0= in compliance; 1= not in compliance)
Benzene	0.0051	0.005	0.0155	0.0666	0.0246	0	0.026	0.0666	0.0147	0
Toluene	0.3586	1.	7.3	13.3176	0.0037	0	10.22	13.3176	0.0026	0
Ethylbenzene	0.1032	0.7	3.65	9.3224	0.0021	0	5.11	9.3224	0.0015	0
Xylene	1.3933	10.	73.	133.	0.0014	0	102.	133.	0.001	0
GRO Aromatics	0.964		7.3	97.2188	0.0099	0	10.22	136.	0.0071	0
DRO Aromatics	2.4687		1.46	19.4438	0.127	0	2.044	27.2213	0.0907	0
RRO Aromatics	3.02E-05		1.095	14.5828	2.07E-06	0	1.533	20.416	1.48E-06	0
GRO Aliphatics	0.0498		183.	2.430.	2.05E-05	0	256.	3.403.	1.46E-05	0
DRO Aliphatics	0.0097		3.65	48.6094	2.00E-04	0	5.11	68.0532	1.43E-04	0
RRO Aliphatics	1.83E-12		73.	972.	1.88E-15	0	102.	1.361.	1.34E-15	0
Naphthalene	3.02E-04		1.46	19.4438	1.56E-05	0	2.044	27.2213	1.11E-05	0
Acenaphthene	4.09E-05		2.19	29.1656	1.40E-06	0	3.066	40.8319	1.00E-06	0
Fluorene	3.80E-05		1.46	19.4438	1.95E-06	0	2.044	27.2213	1.39E-06	0
Anthracene	5.99E-08		10.95	146.	4.11E-10	0	15.33	204.	2.94E-10	0
Fluoranthene	3.42E-07		1.46	19.4438	1.76E-08	0	2.044	27.2213	1.26E-08	0
Pyrene	7.14E-07		1.095	14.5828	4.89E-08	0	1.533	20.416	3.50E-08	0
Benzo (a) Anthracene	1.83E-09	0.001	0.0012	0.0133	1.18E-07	0	0.002	0.0133	7.01E-08	0
Chrysene	1.17E-09	0.1	0.1167	1.3318	7.53E-10	0	0.196	1.3318	4.48E-10	0
Benzo (b) fluoranthene	7.54E-10	0.001	0.0012	0.0133	4.85E-08	0	0.002	0.0133	2.89E-08	0
Benzo (k) fluoranthene	3.09E-10	0.001	0.0117	0.0133	1.99E-09	0	0.0196	0.0133	1.18E-09	0
Benzo (a) pyrene	5.46E-10	2.00E-04	1.17E-04	0.0016	3.52E-07	0	1.96E-04	0.0026	2.09E-07	0
Indeno (1,2,3-cd) pyrene	2.32E-12	0.001	0.0012	0.0133	1.49E-10	0	0.002	0.0133	8.90E-11	0
Dibenz (a,h) anthracene	1.52E-10	1.00E-04	1.17E-04	0.0013	9.81E-08	0	1.96E-04	0.0013	5.84E-08	0
Carcinogenic Cumulative Risk					0.0246	0			0.0147	0
noncarcinogenic Cumulative Risk					0.0073	0			0.0052	0

Values shown in the sixth and tenth columns are the normalized fraction of the risk based level, and not the carcinogenic risk level. The fraction of risk multiplied by 10⁻⁵ equals the carcinogenic risk level for the carcinogenic compounds.
PAH dissolved concentrations estimated by assuming all measured PAH mass is in the NAPL phase

Table 3		Measured Groundwater Concentrations								
Page 8		Example Calculation			Table B1 & B2 Soil Concentrations					
1	2	3	4	5	6	7	8	9	10	11
Compounds	Dissolved Concentration Measured in Water Sample (mg/L)	Maximum Contaminant Level (mg/L)	Residential Land Use Human Health Risk Based Water Concentration (mg/l)	Groundwater Compliance Concentration (MCL or Residential Land Use Health Based Water Concentration at down gradient edge of source area multiplied by 1 for potable water & 10 for nonpotable water; mg/l)	FYI Fraction of Risk Based Target Concentration (values greater than 1 exceed the risk based target; MCLs not used)	Check for compliance with regulatory levels (MCLs used for compounds with MCLs: 0= in compliance; 1= not in compliance)	Industrial Land Use Human Health Based Water Concentration (mg/l)	Groundwater Compliance Concentration (MCL or Industrial Land Use Health Based Water Concentration at down gradient edge of source area multiplied by 1 for potable water & 10 for nonpotable water; mg/l)	FYI Fraction of Risk Based Target Concentration (values greater than 1 exceed the risk based target; MCLs not used)	Check for compliance with regulatory levels (MCLs used for compounds with MCLs: 0= in compliance; 1= not in compliance)
Benzene	0.0045	0.005	0.0155	0.005	0.2906	0	0.026	0.005	0.173	0
Toluene	0.3539	1.	7.3	1.	0.0485	0	10.22	10.22	0.0346	0
Ethylbenzene	0.1018	0.7	3.65	0.7	0.0279	0	5.11	5.11	0.0199	0
Xylene	1.3748	10.	73.	10.	0.0188	0	102.	102.	0.0135	0
GRO Aromatics	0.9512		7.3	7.3	0.1303	0	10.22	10.22	0.0931	0
DRO Aromatics	0.878		1.46	1.46	0.6014	0	2.044	2.044	0.4295	0
RRO Aromatics	0.0985		1.095	1.095	0.09	0	1.533	1.533	0.0643	0
GRO Aliphatics	0.00E+00		183.	183.	0.00E+00	0	256.	256.	0.00E+00	0
DRO Aliphatics	1.87		3.65	3.65	0.5123	0	5.11	5.11	0.3659	0
RRO Aliphatics	0.0493		73.	73.	6.75E-04	0	102.	102.	4.82E-04	0
Naphthalene	0.001		1.46	1.46	6.85E-04	0	2.044	2.044	4.89E-04	0
Acenaphthene	0.002		2.19	2.19	9.13E-04	0	3.066	3.066	6.52E-04	0
Fluorene	0.0028		1.46	1.46	0.0019	0	2.044	2.044	0.0014	0
Anthracene	4.00E-04		10.95	10.95	3.65E-05	0	15.33	15.33	2.61E-05	0
Fluoranthene	6.40E-05		1.46	1.46	4.38E-05	0	2.044	2.044	3.13E-05	0
Pyrene	5.30E-05		1.095	1.095	4.84E-05	0	1.533	1.533	3.46E-05	0
Benzo (a) Anthracene	9.50E-06	0.001	0.0012	0.001	0.0081	0	0.002	0.002	0.0048	0
Chrysene	4.75E-06	0.1	0.1167	0.1	4.07E-05	0	0.196	0.196	2.42E-05	0
Benzo (b) fluoranthene	1.20E-05	0.001	0.0012	0.001	0.0103	0	0.002	0.002	0.0061	0
Benzo (k) fluoranthene	7.50E-06	0.001	0.0117	0.001	6.43E-04	0	0.0196	0.0196	3.83E-04	0
Benzo (a) pyrene	5.50E-06	2.00E-04	1.17E-04	1.17E-04	0.0471	0	1.96E-04	1.96E-04	0.0281	0
Indeno (1,2,3-cd) pyrene	6.50E-06	0.001	0.0012	0.001	0.0056	0	0.002	0.002	0.0033	0
Dibenz (a,h) anthracene	8.00E-06	1.00E-04	1.17E-04	1.00E-04	0.0686	0	1.96E-04	1.96E-04	0.0408	0
Carcinogenic Cumulative Risk					0.431	0			0.2566	0
noncarcinogenic Cumulative Risk					0.0988	0			0.0706	0
Values shown in the seventh and eleventh columns are the normalized fraction of the risk based level, and not the carcinogenic risk level. The fraction of risk multiplied by 10 ⁻⁵ equals the carcinogenic risk level for the carcinogenic compounds.										
If the 10x rule is used the groundwater is not a drinking water source and the groundwater ingestion risk is zero.										

Table 3		Potential Cumulative Risk Assuming All Pathways Complete							DRO, GRO and RRO not included in cumulative risk calculations				
Page 9		Example Calculation				Table B1 & B2 Soil Concentrations							
1	2	3	4	5	6	7	8	9	10	11	12	13	
Compounds	Fraction of Target Soil Ingestion Risk, Residential Site	Fraction of Target Outdoor Air Inhalation Risk, Residential Site	Fraction of Target Indoor Air Inhalation Risk, Residential Site	Fraction of Target Groundwater Ingestion Risk, Residential Site	Sum of Risks for Residential Site	Residential Site Check for compliance with risk levels (0= in compliance; 1= not in compliance)	Fraction of Target Soil Ingestion Risk, Industrial Site	Fraction of Target Outdoor Air Inhalation Risk, Industrial Site	Fraction of Target Indoor Air Inhalation Risk, Industrial Site	Fraction of Target Groundwater Ingestion Risk, Industrial Site	Sum of Risks for Industrial Site	Industrial Site Check for compliance with risk levels (0= in compliance; 1= not in compliance)	
Benzene	1.33E-04	1.97E-05	0.0524	0.2906	0.3431	0	1.92E-05	1.71E-05	0.0312	0.173	0.2042	0	
Toluene	2.66E-04	1.28E-05	0.031	0.0485	0.0797	0	1.32E-05	9.69E-06	0.0184	0.0346	0.0531	0	
Ethylbenzene	5.42E-04	1.68E-06	0.183	0.0279	0.2114	0	2.69E-05	1.06E-06	0.1089	0.0199	0.1289	0	
Xylene	3.85E-04	0.00E+00	0.0063	0.0188	0.0255	0	1.91E-05	0.00E+00	0.0037	0.0135	0.0172	0	
GRO Aromatics													
DRO Aromatics													
RRO Aromatics													
GRO Aliphatics													
DRO Aliphatics													
RRO Aliphatics													
Naphthalene	5.85E-05	0.00E+00	2.11E-04	6.85E-04	9.54E-04	0	2.90E-06	0.00E+00	1.25E-04	4.89E-04	6.17E-04	0	
Acenaphthene	4.63E-05	0.00E+00	1.10E-07	9.13E-04	9.60E-04	0	2.30E-06	0.00E+00	6.56E-08	6.52E-04	6.55E-04	0	
Fluorene	1.49E-04	0.00E+00	6.44E-08	0.0019	0.0021	0	7.39E-06	0.00E+00	3.83E-08	0.0014	0.0014	0	
Anthracene	1.53E-06	0.00E+00	1.17E-11	3.65E-05	3.81E-05	0	7.61E-08	0.00E+00	6.98E-12	2.61E-05	2.62E-05	0	
Fluoranthene	1.57E-05	0.00E+00	1.24E-10	4.38E-05	5.95E-05	0	7.78E-07	0.00E+00	7.40E-11	3.13E-05	3.21E-05	0	
Pyrene	6.66E-05	0.00E+00	2.21E-10	4.84E-05	1.15E-04	0	3.31E-06	0.00E+00	1.31E-10	3.46E-05	3.79E-05	0	
Benzo (a) Anthracene	7.43E-04	0.00E+00	1.53E-10	0.0081	0.0089	0	1.08E-04	0.00E+00	9.10E-11	0.0048	0.005	0	
Chrysene	2.79E-05	0.00E+00	2.08E-11	4.07E-05	6.86E-05	0	4.04E-06	0.00E+00	1.24E-11	2.42E-05	2.83E-05	0	
Benzo (b) fluoranthene	0.0021	0.00E+00	1.44E-09	0.0103	0.0124	0	3.07E-04	0.00E+00	8.57E-10	0.0061	0.0064	0	
Benzo (k) fluoranthene	1.63E-04	0.00E+00	5.28E-13	6.43E-04	8.06E-04	0	2.35E-05	0.00E+00	3.14E-13	3.83E-04	4.06E-04	0	
Benzo (a) pyrene	0.0142	0.00E+00	8.15E-09	0.0471	0.0614	0	0.0021	0.00E+00	4.85E-09	0.0281	0.0301	0	
Indeno (1,2,3-cd) pyrene	4.87E-04	0.00E+00	6.42E-14	0.0056	0.0061	0	7.05E-05	0.00E+00	3.82E-14	0.0033	0.0034	0	
Dibenz (a,h) anthracene	0.0028	0.00E+00	8.87E-12	0.0686	0.0714	0	4.12E-04	0.00E+00	5.28E-12	0.0408	0.0412	0	
Carcinogenic Cumulative Risk					0.5041	0					0.2907	0	
noncarcinogenic Cumulative Risk					0.3208	0					0.2019	0	

Values shown in the second through sixth and eighth through twelfth columns are the normalized fraction of the risk based level, and not the carcinogenic risk level. The fraction of risk multiplied by 10⁻⁵ equals the carcinogenic risk level for the carcinogenic compounds.

Table 3		Cumulative Risk for Pathways Complete at Present Time							DRO, GRO and RRO not included in cumulative risk calculations			
Page 10		Example Calculation			Table B1 & B2 Soil Concentrations							
1	2	3	4	5	6	7	8	9	10	11	12	13
Compounds	Fraction of Target Soil Ingestion Risk, Residential Site	Fraction of Target Outdoor Air Inhalation Risk, Residential Site	Fraction of Target Indoor Air Inhalation Risk, Residential Site	Fraction of Target Groundwater Ingestion Risk, Residential Site	Sum of Risks for Residential Site	Residential Site Check for compliance with risk levels (0= in compliance; 1= not in compliance)	Fraction of Target Soil Ingestion Risk, Industrial Site	Fraction of Target Outdoor Air Inhalation Risk, Industrial Site	Fraction of Target Indoor Air Inhalation Risk, Industrial Site	Fraction of Target Groundwater Ingestion Risk, Industrial Site	Sum of Risks for Industrial Site	Industrial Site Check for compliance with risk levels (0= in compliance; 1= not in compliance)
Benzene	1.33E-04	1.97E-05	0.0524	0.00E+00	0.0525	0	1.92E-05	1.71E-05	0.0312	0.00E+00	0.0312	0
Toluene	2.66E-04	1.28E-05	0.031	0.00E+00	0.0313	0	1.32E-05	9.69E-06	0.0184	0.00E+00	0.0185	0
Ethylbenzene	5.42E-04	1.68E-06	0.183	0.00E+00	0.1835	0	2.69E-05	1.06E-06	0.1089	0.00E+00	0.1089	0
Xylene	3.85E-04	0.00E+00	0.0063	0.00E+00	0.0066	0	1.91E-05	0.00E+00	0.0037	0.00E+00	0.0037	0
GRO Aromatics												
DRO Aromatics												
RRO Aromatics												
GRO Aliphatics												
DRO Aliphatics												
RRO Aliphatics												
Naphthalene	5.85E-05	0.00E+00	2.11E-04	0.00E+00	2.69E-04	0	2.90E-06	0.00E+00	1.25E-04	0.00E+00	1.28E-04	0
Acenaphthene	4.63E-05	0.00E+00	1.10E-07	0.00E+00	4.64E-05	0	2.30E-06	0.00E+00	6.56E-08	0.00E+00	2.36E-06	0
Fluorene	1.49E-04	0.00E+00	6.44E-08	0.00E+00	1.49E-04	0	7.39E-06	0.00E+00	3.83E-08	0.00E+00	7.42E-06	0
Anthracene	1.53E-06	0.00E+00	1.17E-11	0.00E+00	1.53E-06	0	7.61E-08	0.00E+00	6.98E-12	0.00E+00	7.61E-08	0
Fluoranthene	1.57E-05	0.00E+00	1.24E-10	0.00E+00	1.57E-05	0	7.78E-07	0.00E+00	7.40E-11	0.00E+00	7.78E-07	0
Pyrene	6.66E-05	0.00E+00	2.21E-10	0.00E+00	6.66E-05	0	3.31E-06	0.00E+00	1.31E-10	0.00E+00	3.31E-06	0
Benzo (a) Anthracene	7.43E-04	0.00E+00	1.53E-10	0.00E+00	7.43E-04	0	1.08E-04	0.00E+00	9.10E-11	0.00E+00	1.08E-04	0
Chrysene	2.79E-05	0.00E+00	2.08E-11	0.00E+00	2.79E-05	0	4.04E-06	0.00E+00	1.24E-11	0.00E+00	4.04E-06	0
Benzo (b) fluoranthene	0.0021	0.00E+00	1.44E-09	0.00E+00	0.0021	0	3.07E-04	0.00E+00	8.57E-10	0.00E+00	3.07E-04	0
Benzo (k) fluoranthene	1.63E-04	0.00E+00	5.28E-13	0.00E+00	1.63E-04	0	2.35E-05	0.00E+00	3.14E-13	0.00E+00	2.35E-05	0
Benzo (a) pyrene	0.0142	0.00E+00	8.15E-09	0.00E+00	0.0142	0	0.0021	0.00E+00	4.85E-09	0.00E+00	0.0021	0
Indeno (1,2,3-cd) pyrene	4.87E-04	0.00E+00	6.42E-14	0.00E+00	4.87E-04	0	7.05E-05	0.00E+00	3.82E-14	0.00E+00	7.05E-05	0
Dibenz (a,h) anthracene	0.0028	0.00E+00	8.87E-12	0.00E+00	0.0028	0	4.12E-04	0.00E+00	5.28E-12	0.00E+00	4.12E-04	0
Carcinogenic Cumulative Risk					0.0731	0					0.0342	0
noncarcinogenic Cumulative Risk					0.222	0					0.1313	0

Values shown in the second through sixth and eighth through twelfth columns are the normalized fraction of the risk based level, and not the carcinogenic risk level. The fraction of risk multiplied by 10⁻⁵ equals the carcinogenic risk level for the carcinogenic compounds.

Table 3		Partitioning into Groundwater & Surface Water					
Page 11		Example Calculation			Table B1 & B2 Soil Concentrations		
1	2	3	4	5	6	7	8
Compounds	Calculated Equilibrium Conc. (from soil data & solver) (mg/L)	Measured Dissolved Phase Conc. (mg/L)	Groundwater Compliance Concentration (MCL or Residential Land Use Health Based Water Concentration at down gradient edge of source area multiplied by 1 for potable water & 10 for nonpotable water; mg/l)	check for vadose zone fill potential (0 yes; 1 no)	check for saturated zone fill potential (0 yes; 1 no)	AWQC (mg/L)	check for surface water body fill potential (0 yes; 1 no)
Benzene	0.0051	0.0045	0.005	0	0	0.005	0
Toluene	0.3586	0.3539	1.	0	0		
Ethylbenzene	0.1032	0.1018	0.7	0	0		
Xylene	1.3933	1.3748	10.	0	0		
GRO Aromatics	0.964	0.9512	7.3	0	0		
DRO Aromatics	2.4687	0.878	1.46	0	0		
RRO Aromatics	3.02E-05	0.0985	1.095	0	0		
GRO Aliphatics	0.0498	0.00E+00	183.	0	0		
DRO Aliphatics	0.0097	1.87	3.65	0	0		
RRO Aliphatics	1.83E-12	0.0493	73.	0	0		
Naphthalene	3.02E-04	0.001	1.46	0	0		
Acenaphthene	4.09E-05	0.002	2.19	0	0		
Fluorene	3.80E-05	0.0028	1.46	0	0		
Anthracene	5.99E-08	4.00E-04	10.95	0	0		
Fluoranthene	3.42E-07	6.40E-05	1.46	0	0		
Pyrene	7.14E-07	5.30E-05	1.095	0	0		
Benzo (a) Anthracene	1.83E-09	9.50E-06	0.001	0	0		
Chrysene	1.17E-09	4.75E-06	0.1	0	0		
Benzo (b) fluoranthene	7.54E-10	1.20E-05	0.001	0	0		
Benzo (k) fluoranthene	3.09E-10	7.50E-06	0.001	0	0		
Benzo (a) pyrene	5.46E-10	5.50E-06	1.17E-04	0	0		
Indeno (1,2,3-cd) pyrene	2.32E-12	6.50E-06	0.001	0	0		
Dibenz (a,h) anthracene	1.52E-10	8.00E-06	1.00E-04	0	0		
TAH	1.8602	1.835				0.01	1
TAqH	1.8606	1.8414				0.015	1
DRO sheen (mg/kg)						230	1
			sum	0	0	sum	3

Table 3		Site Status Summary				
Page 12		Example Calculation			Table B1 & B2 Soil Concentrations	
1	2	3	4	5	6	7
	Cumulative Risks for Residential Site	soil ingestion check for compliance with risk levels (0= in compliance; 1= not in compliance)	groundwater ingestion check for compliance with clean up levels (0= in compliance; 1= not in compliance)	migration to outdoor air check for compliance with clean up levels (0= in compliance; 1= not in compliance)	migration to indoor air check for compliance with clean up levels (0= in compliance; 1= not in compliance)	
Potential Carcinogenic Cumulative Fraction of Risk	0.5041					
Potential noncarcinogenic Cumulative Risk	0.3208					
Existing Carcinogenic Cumulative Fraction of Risk	0.0731					
Existing noncarcinogenic Cumulative Risk	0.222					
Site ranking score= existing carcinogenic cumulative risk * population	0.0731					
Site ranking score= existing noncarcinogenic cumulative risk * population	0.222					
GRO Aromatics		0	0	0	0	
DRO Aromatics		0	0	0	0	
RRO Aromatics		0	0	0	0	
GRO Aliphatics		0	0	0	0	
DRO Aliphatics		0	0	0	0	
RRO Aliphatics		0	0	0	0	
check for ultimate GRO, DRO, RRO compliance		0				
Acceptable human health risk levels met--site may be closed provided ecological risk criteria met						
Site soils may be used as vadose zone fill--eligible for closeout level C						
Site soils may be used as saturated zone fill--- --eligible for closeout level B						
Site soils cannot be used as wetlands or surface water fill						

Figures

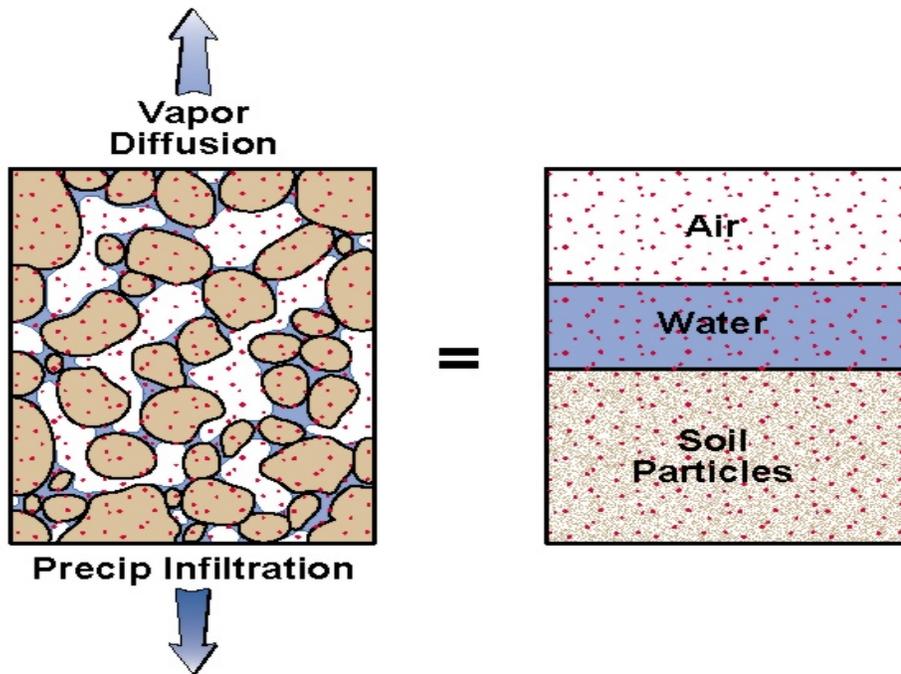


FIGURE 1
 Block Diagram of a Soil Containing Dissolved, Vapor and Adsorbed Hydrocarbon Phases
Phase Partitioning Technical Background Report

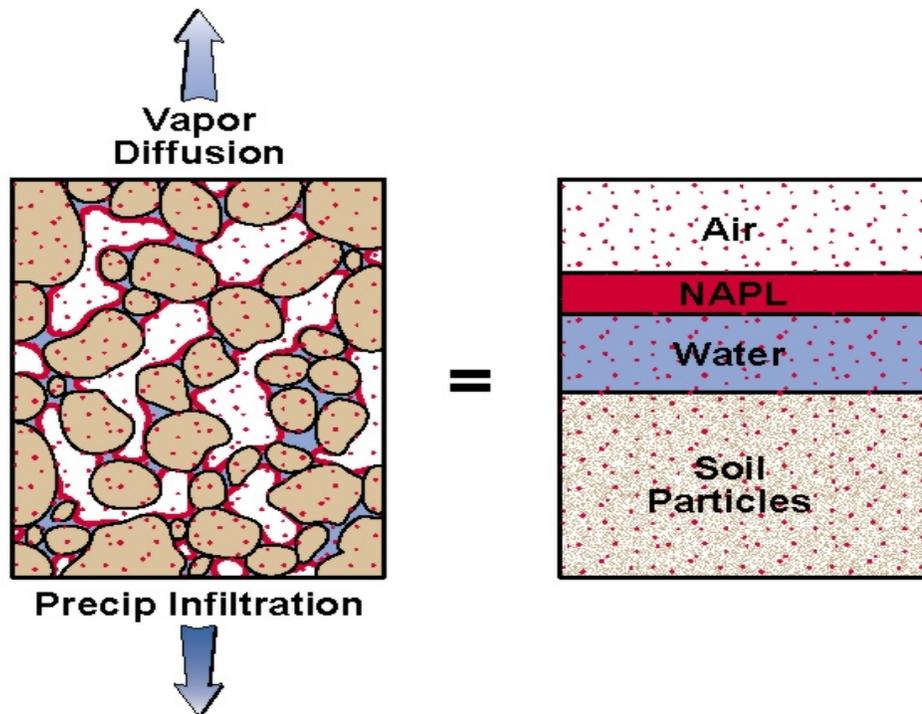


FIGURE 2
 Block Diagram of a Soil Containing Dissolved, Vapor, Adsorbed Hydrocarbons and NAPL
Phase Partitioning Technical Background Report

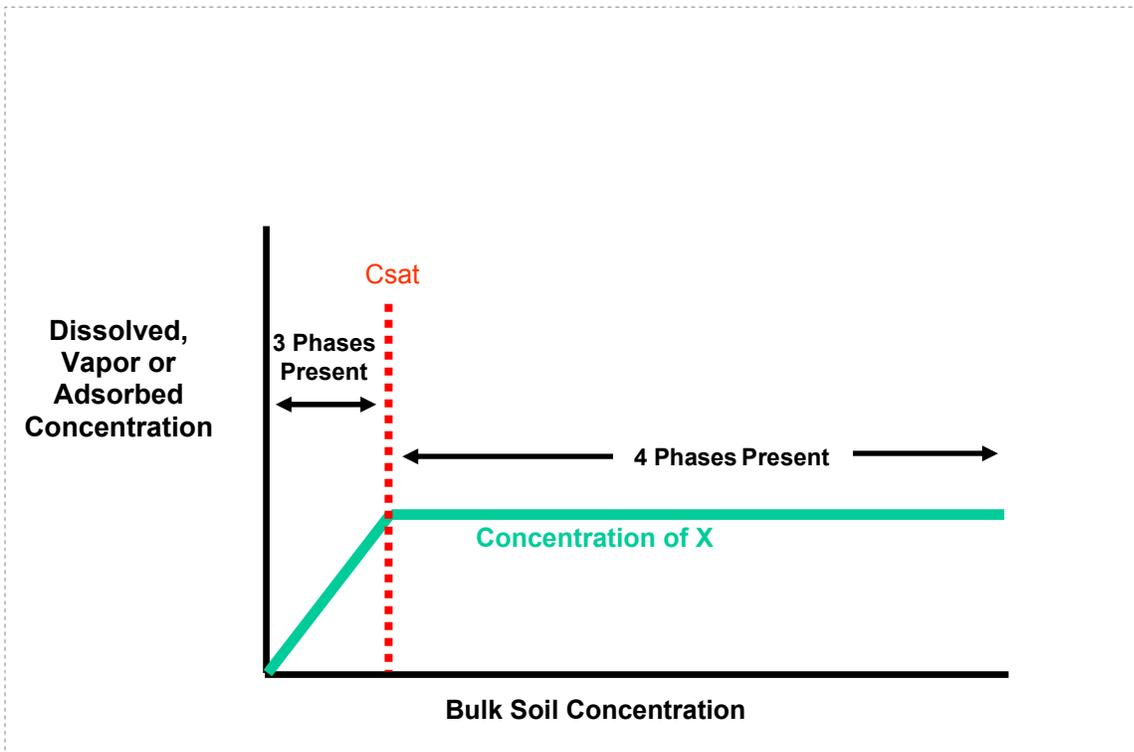


FIGURE 3
 Dissolved, Adsorbed and Vapor Phase Concentrations Increase Linearly with Increasing Bulk Soil Concentration Up to C_{sat} (the Soil Saturation Concentration) Where They Reach Their Maximum Values
Phase Partitioning Technical Background Report

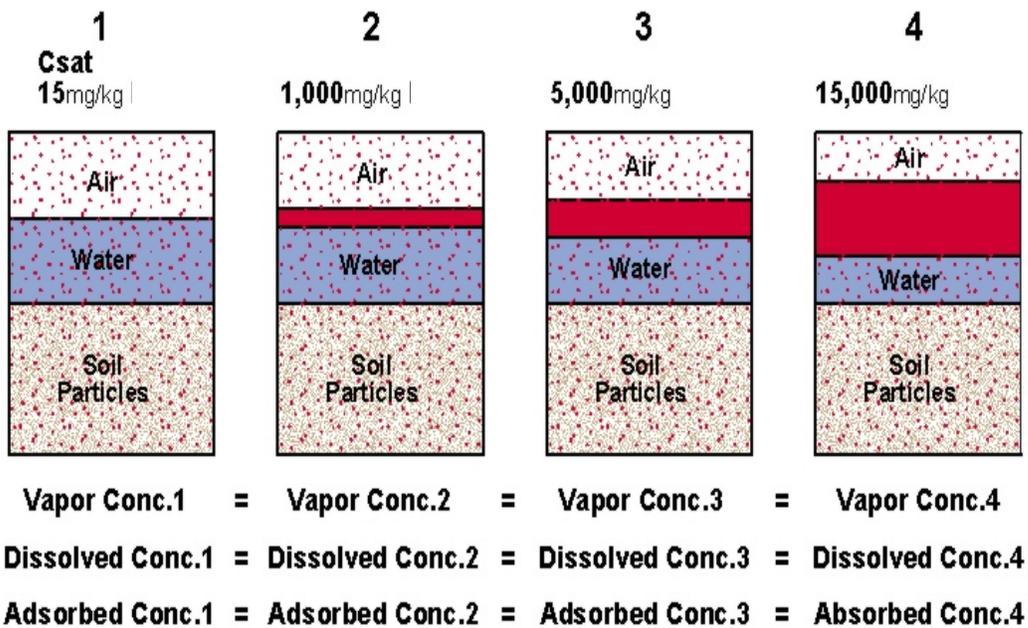


FIGURE 4
 Block Diagrams Showing That the Dissolved, Vapor, and Adsorbed Concentrations in Soil do Not Increase as the NAPL Concentration Increases
Phase Partitioning Technical Background Report

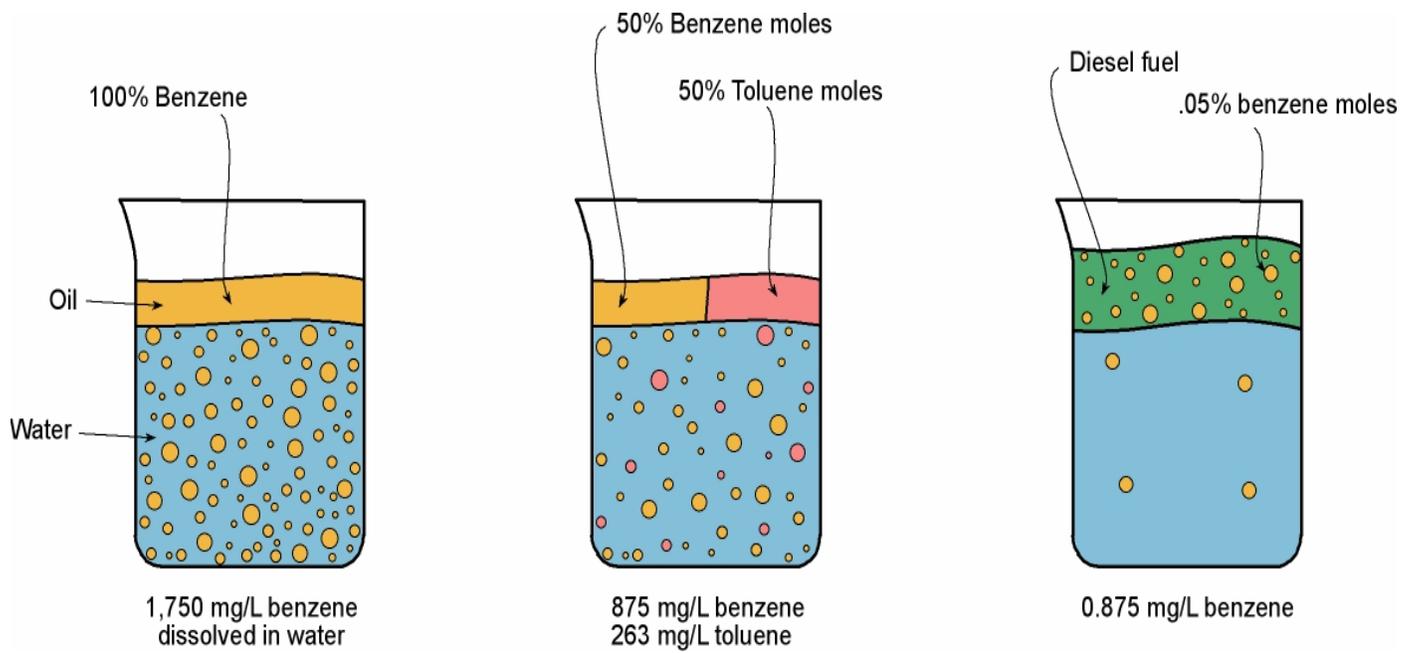
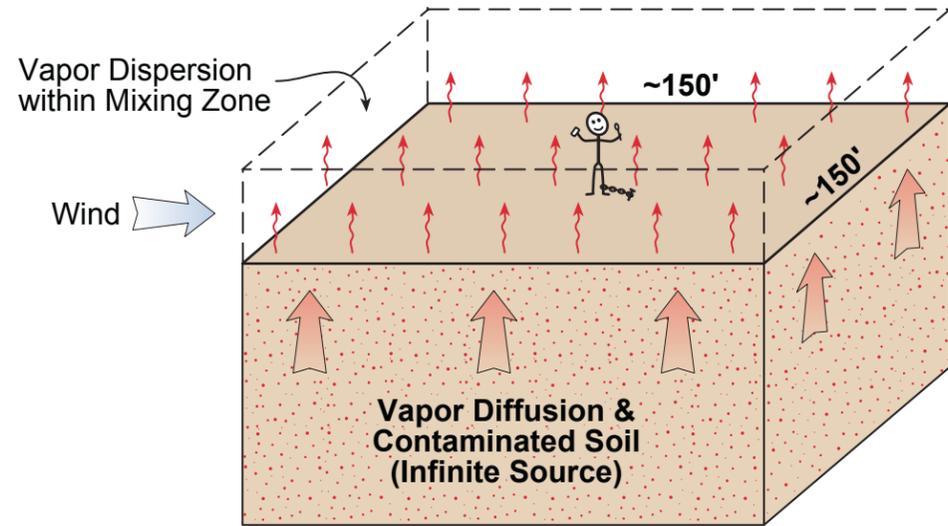


FIGURE 5
 Beakers of Water with Floating Hydrocarbon NAPL Layers Illustrating the Effect of Raoult's Law on the Solubility of Benzene
Phase Partitioning Technical Background Report

Vapor Inhalation Conceptual Site Model



- Q/C = dispersion or mining factor
- Value depends on climate/average wind speed; Higher wind = higher Q/C value
 - Value varies with size of site; Larger site = smaller Q/C value
 - Square site
 - Seattle, Minneapolis, and Casper Values used for >40°, <40° and Arctic zones

- DA = Effective Diffusion Coefficient
- Calculates vapor emission rate to atmosphere
 - Assumes diffusion through soil vapor and soil moisture
 - Uses "Jury" model with "Millington & Quirk" effective diffusion calculation
 - Vapor phase diffusion >> aqueous phase diffusion

Equation 6. Equation 6: Soil Cleanup Level Equation for Direct Inhalation of Carcinogenic Volatile Contaminants in Soil¹

$\text{Cleanup Level (mg/kg)} = \frac{\text{TR} \times \text{AT} \times 365 \text{ d/yr}}{\text{URF} \times 1000 \Phi \text{g/mg} \times \text{EF} \times \text{ED} \times [1/\text{VF}]}$		
Parameter/Definition (units)	Default	
TR/target cancer risk (unitless)	10 ⁻⁵	
AT/averaging time (yr)	70	
URF/inhalation unit risk factor (Φg/m ³) ⁻¹	chemical-specific (See Appendix C)	
EF/exposure frequency (d/yr)	Arctic Zone	200 d/yr
	Under 40 Inch Zone	270 d/yr
	Over 40 Inch Zone	330 d/yr
ED/exposure duration (yr)	30	
VF/soil-to-air volatilization factor (m ³ /kg)	chemical-specific (See Appendix C)	

Equation 7. Soil Cleanup Level Equation for Direct Inhalation of Noncarcinogenic Contaminants in Soil¹

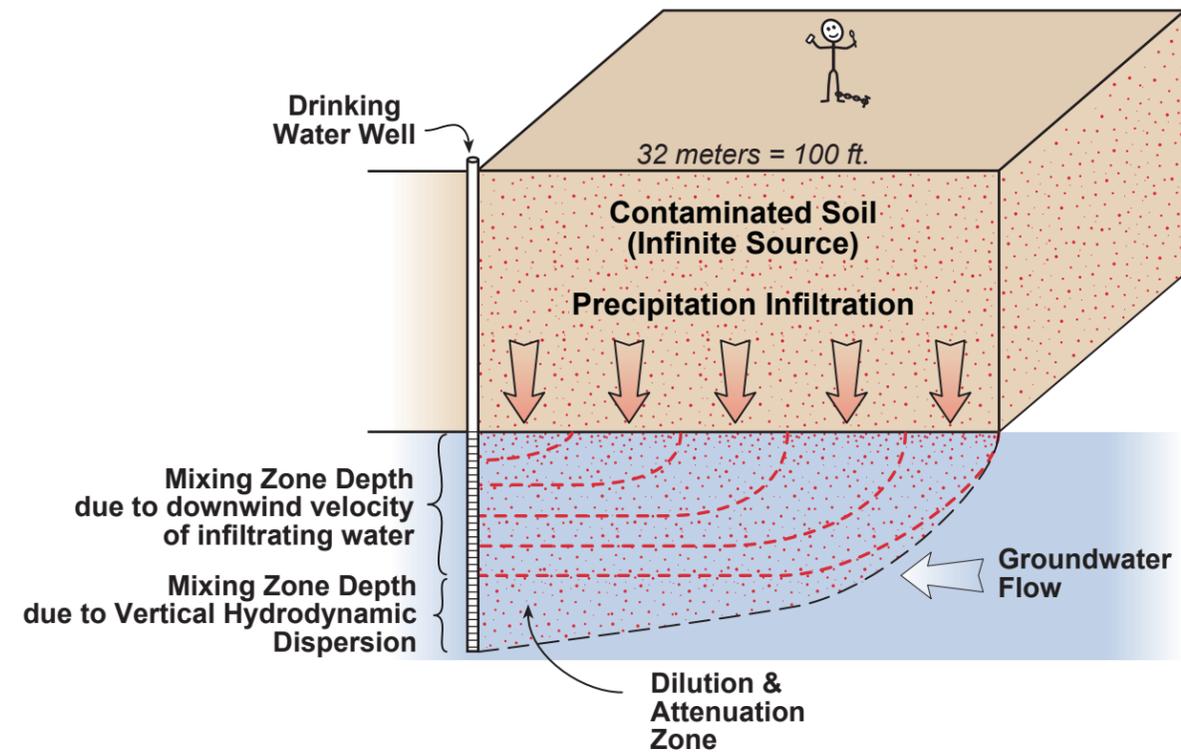
$\text{Cleanup Level (mg/kg)} = \frac{\text{THQ} \times \text{AT} \times 365 \text{ d/yr}}{\text{EF} \times \text{ED} \times [(1/\text{RfC}) \times (1/\text{VF})]}$		
Parameter/Definition (units)	Default	
THQ/target hazard quotient (unitless)	1	
AT/averaging time (yr)	30	
EF/exposure frequency (d/yr)	Arctic Zone	= 200 d/yr
	Under 40 Inch Zone	= 270 d/yr
	Over 40 Inch Zone	= 330 d/yr
ED/exposure duration (yr)	30	
RfC/inhalation reference concentration (mg/m ³)	chemical-specific (See Appendix C)	
VF/soil-to-air volatilization factor (m ³ /kg)	chemical-specific (See Equation 8)	

Equation 8. Derivation of the Volatilization Factor¹

$\text{VF (m}^3/\text{kg)} = \frac{\text{Q/C} \times (3.14 \times \text{D}_A \times \text{T})^{1/2} \times 10^{-4} \text{m}^2/\text{cm}^2}{(2 \times \rho_b \times \text{D}_A)}$		
<p>where $\text{D}_A = \frac{[(\theta_a^{10/3} \text{D}_i \text{H}' + \theta_w^{10/3} \text{D}_w)/n^2]}{\rho_b \text{K}_d + \theta_w + \theta_a \text{H}'}$</p>		
Parameter/Definition (units)	Default	
VF/volatilization factor (m ³ /kg)	---	
Q/C/inverse of the mean conc. at the center of a 0.5 acre square source (g/m ² -s per kg/m ³)	Arctic Zone	=100.13
	Under 40 Inch Zone	=90.80
	Over 40 Inch Zone	=82.72
T/exposure interval (s)	9.5 x 10 ⁸ s	
ρ _b /dry soil bulk density (g/cm ³)	1.5	
ρ _s /soil particle density (g/cm ³)	2.65	
n/total soil porosity (L _{pore} /L _{soil})	0.434 or 1 - (ρ _b /ρ _s)	
θ _w /water-filled soil porosity (L _{water} /L _{soil})	0.15 or wρ _b	
θ _a /air-filled soil porosity (L _{air} /L _{soil})	0.284 or n - wρ _b	
D _i /diffusivity in air (cm ² /s)	chemical-specific (See Appendix C)	
H'/dimensionless Henry's law constant	chemical-specific (See Appendix C)	
w/average soil moisture content (g _{water} /g _{soil} or cm ³ _{water} /g _{soil})	0.1 (10%)	
D _w /diffusivity in water (cm ² /s)	chemical-specific (See Appendix C)	
K _d /soil-water partition coefficient (cm ³ /g)	K _{oc} x f _{oc} (organics)	
K _{oc} /organic carbon partition coefficient (cm ³ /g)	chemical-specific (See Appendix C)	
f _{oc} /organic carbon content of soil (g/g)	0.001 (0.1%)	

Figure 6
Conceptual Model and Equations for the Vapor Inhalation Pathway

Migration to Groundwater Conceptual Site Model



Equation 11. Organic Contaminants-- Soil-Water Partitioning Equation for Migration to Groundwater¹

$$\text{Soil cleanup level (mg/kg)} = C_w \{ (K_{oc} f_{oc}) + ((\theta_w + \theta_a H) / \rho_b) \}$$

Note: For ionizing organics, the cleanup standards are pH dependant. As site pH deviates from 6.8, K_{oc} should be modified according to Part 5 of EPA's Soil Screening Levels Guidance in Reference 1 and the soil cleanup values must be recalculated for the site.

Parameter/Definition (units)	Default
C_w /target soil leachate concentration (mg/L)	Groundwater Cleanup Level x (10 + DF), 10 is attenuation factor
K_{oc} /soil organic carbon/water partition coefficient (L/kg)	chemical-specific and pH dependant (See Appendix C)
f_{oc} /fraction organic carbon in soil (g/g)	0.001 (0.1%)
ρ_b /dry soil bulk density (kg/L)	1.5
ρ_s /soil particle density (kg/L)	2.65
n /total soil porosity (L_{pore}/L_{soil})	0.434 or $(1 - \rho_b/\rho_s)$
θ_w /water-filled soil porosity (L_{water}/L_{soil})	0.3 (30%) or $w\rho_b$
θ_a /air-filled soil porosity (L_{air}/L_{soil})	0.13 or $n - w\rho_b$
w /average soil moisture content (kg_{water}/kg_{soil} or L_{water}/kg_{soil})	0.2 (20%)
H /Henry's law constant (unitless)	Chemical Specific (assume to be zero for inorganic contaminants except mercury) (See Appendix C)

Two Terms in Equation 11

Hydrodynamic Dispersion mixing depth, d & $v = (0.0112L)$
 • Increases as source length increases

Infiltration Velocity Mixing Depth, $d_{lv} = d(1 - \exp(-LI)/(Kida))^{0.5}$
 • increases as infiltration rate increases
 • increases as source length increases
 • decreases as groundwater velocity increases
 • decreases as aquifer depth increases
 • dilution factor applies to "Mixing Zone"
 • most monitoring wells do not penetrate Mixing Depth

Equation 12. Derivation of Dilution Factor¹

$$DF = 1 + (K_{id} / IL)$$

Parameter/Definition (units)	Default
DF/dilution factor (unitless)	---
K /aquifer hydraulic conductivity (m/yr)	876 m/yr
i /hydraulic gradient (m/m)	0.002 m/m
d /mixing zone depth (m)	(See Equation 13 below)
I /infiltration rate (m/yr)(calculated as $1/5 * (\text{mean plus one standard deviation of yearly rainfall})$)	Over 40 Inch Zone = 0.6 m/yr Under 40 Inch Zone = 0.13 m/yr
L /source length parallel to groundwater flow (m)	32 m

The standard default dilution factors used to determine the cleanup standards are $DF = 1.9$ for the Over 40 Inch Zone; and $DF = 3.3$ for the Under 40 Inch Zone.

Equation 13. Estimation of Mixing Zone Depth¹

$$d = (0.0112L^2)^{0.5} + d_a \{1 - \exp[-LI/(Kida)]\}$$

Parameter/Definition (units)	Default
d /mixing zone depth (m)	---
L /source length parallel to groundwater flow (m)	32 m
I /infiltration rate (m/yr)(calculated as $1/5 * (\text{mean plus one standard deviation of yearly rainfall})$)	Over 40 Inch Zone = 0.6 m/yr Under 40 Inch Zone = 0.13 m/yr
K /aquifer hydraulic conductivity (m/yr)	876 m/yr
i /hydraulic gradient (m/m)	0.002
d_a /aquifer thickness (m)	10 m

The standard default mixing zone depths used to determine the cleanup standards are: $d = 10.0$ for the Over 40 Inch Zone; and $d = 5.5$ for the Under 40 Inch Zone.

Figure 7
Conceptual Model and Equations for the Migration to Groundwater Pathway