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Evaluation of the Total Petroleum Hydrocarbon (TPH) Standard for JP-4 Jet Fuel

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ABSTRACT: The potential for use of alternatives to total petroleum hydrocarbons (TPH) for remediation purposes was examined specifically for JP-4 fuel. The study objective was to determine the scientific basis for use of fuel constituents other than TPH in establishing soil cleanup standards at JP-4-contaminated sites. The general bases for TPH soil cleanup standards or goals were characterized. Problems with the use of TPH for cleanup included its lack of specificity (e.g., method-, medium-, and time-from-spill-dependency) as well as the lack of toxicological relevance. JP-4 fuel constituents (alkanes, BTEX [i.e., benzene, toluene, ethylbenzene, xylenes], polycyclic aromatic hydrocarbons [PAHs, i.e., chrysene], and naphthalenes) were identified as potential TPH alternatives. A series of criteria were applied to assess the viability of the use of specific JP-4 constituents as TPH alternatives, and to select the most appropriate alternative. Criteria included chemical fate and transport, toxicity, and regulatory standards for relevant media of concern. Consideration of these criteria ultimately resulted in selection of benzene as the JP-4 indicator of choice. The potential for altering risk-based benzene soil cleanup concentrations (preliminary remediation goals, PRGs) was examined, and encompassed the basis for the existing benzene cancer slope factor (SF) as well as the role of distributional analysis of exposure parameters (Monte Carlo) that might be employed at JP-4 spill sites. Results and conclusions are presented, and the implications for fuels other than JP-4 are also discussed.

KEY WORDS: risk assessment, remediation, indicator, groundwater quality, Monte Carlo.

I. INTRODUCTION

Historically, there are numerous sites at which jet fuel spills or leaks have occurred or can be anticipated to occur. Fuel storage tanks, pumphouses, and fuel lines can be typical sources of unexpected releases of fuels to the environment. As part of the Installation Restoration Program (IRP), military installations are required to

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delineate and remediate contaminants in site media whose concentrations exceed existing standards or guidance concentrations. Sources of controversy and uncertainty regarding the extent of remediation required at a site can sometimes stem from the lack of a sound, scientific basis for establishing the applicable standards or guidance criteria. This study explores the bases (scientific, technological, or otherwise) for setting soil cleanup concentrations or guidance criteria specifically for fuel spill-related compounds, with a focus on constituents of JP-4 jet fuel.

Typically, soil or water samples taken from fuel spill sites have been analyzed for total petroleum hydrocarbons (TPH). Several methods for analyzing TPH exist (EPA Methods 418.1 and 8015 'Modified' are the most widely used for soil), each delivering a single analytical result per sample for what is certainly a mixture of compounds. Contrary to the analytical name, these methods do not measure all hydrocarbons in a sample, nor do they measure identical subsets of hydrocarbons when methods are compared (Baugh and Lovegreen, 1990). In this sense, the reported TPH concentration becomes a method-dependent entity in all media. In addition to method specificity, a soil analysis for TPH will not be particularly comparable to a TPH analysis of a water sample because, in the absence of floating free product, the water-miscible fuel components present in a water sample will not necessarily parallel those fuel components associated with soil. Therefore, TPH becomes a medium-specific entity as well. Due to differential volatilization and dissolution of petroleum constituents, the results of TPH analyses may be expected to be dependent on the elapsed time since spill as well as the fuel type. In light of these limitations, alternatives to TPH as a measurement of residual fuels are being sought.

In addition to TPH, measurements of the individual benzene, toluene, ethylbenzene, and xylene (BTEX) compounds are routinely made for purposes of defining the nature and extent of fuel spills.

Several approaches to handling complex chemical mixtures (such as fuels) for purposes of characterization and determining representative properties have been proposed (Custance *et al.*, 1993). These include selection of indicator compounds, surrogates, and consideration of the whole mixture. An indicator approach essentially adheres to the concept that a specific chemical or subset of the chemical mixture can be viewed as representative of the overall mixture, with respect to considerations such as mobility and toxicity, from a worst-case perspective. A surrogate approach involves identifying a constituent or subset of constituents that can be used to characterize or define the entire mixture. Surrogates would, by default, have to exhibit the same properties as the parent mixture, and for purposes of analytical measurement, have to yield measurements either in parallel to or in constant proportion to measurements of the parent mixtures. A whole mixture approach entails examining and treating the mixture as a single unit, on the assumption that all constituents will have similar mobility and toxicity. As part of the process of defining potential alternates to TPH, an indicator approach evolved as the approach of choice for JP-4 fuel.

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A rigorous evaluation of TPH and other potential cleanup standards for hydrocarbon-contaminated sites is presented in this paper. The general approaches to and bases for regulating TPH or other potential indicators were determined, and the degree to which they were based on scientific principles assessed. In addition, the relative merits of other standards were compared to the TPH standard. An assumption was made that uncertainty associated with an indicator-based standard could be approximated or given context within a risk-based approach to soil cleanup.

II. APPROACHES TO ESTABLISHING SOIL CLEANUP CONCENTRATIONS FOR JET FUELS

A. Jet Fuel (JP-4), As TPH and/or BTEX, For Pursuing Soil Cleanup

General assumptions underlying sampling plans for fuel-contaminated sites are that analyses for BTEX compounds will quantify individual small, volatile fuel components, while TPH measurements will provide gross information on various size ranges of hydrocarbons (i.e., semivolatile to nonvolatile fuel components, as well as BTEX), depending on the method employed and the fuel type. Soil remediation of fuels has been primarily based on the presence of measurable amounts of the four BTEX compounds, TPH, or both. Precedents exist at U.S. Air Force sites (and others), for enforcing soil remediation based on these fuel components. Therefore, a determination of the approaches to using TPH and BTEX for soil remediation purposes was undertaken.

B. General Bases for Soil Cleanup Concentrations for TPH and BTEX

Because remediation efforts at National Priority List (NPL) sites are dictated by compliance with federal and state mandates, the ranges of federal and state regulatory approaches for establishing fuel-related cleanup concentrations were sought.

1. Federal Approach to TPH and BTEX Cleanup Standards

The U.S. Environmental Protection Agency (USEPA) has not proposed federal standards for soil remediation of TPH or BTEX compounds. Two USPEPA programs are involved in fuel-related cleanup activities, but each proposes a separate approach for remediation goals.

The USEPA's underground storage tank (UST) program has decided not to develop federal guidelines for the cleanup of soils contaminated with TPH/BTEX, but rather to leave the selection of TPH/BTEX soil cleanup levels to the discretion

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of individual states (Heffelfinger, personal communication, 1993). The UST program funded an effort to summarize state activities related to TPH/BTEX soil cleanup (Tremblay, personal communication, 1993), the results of which (Oliver *et al.*, 1993) are utilized in a subsequent section of this article.

A work group sponsored by the USEPA's Office of Solid Waste and the Superfund Office has proposed development of a tiered approach for establishing soil screening levels for 30 chemicals, including BTEX, for use at NPL sites Henning, personal communication, 1993). Exceeding the screening level would warrant further investigation and characterization of the site. The first tier would involve estimating a generic, conservative soil screening concentration (one that would not result in the exceeding of any groundwater standards), using partitioning/dilution/attenuation factor equations and default values. The second tier soil screening concentration might use the same equation, but with site-specific information. Third and fourth tiers could include a soil leachate test and a full site-specific characterization, respectively. Successively higher tiers will presumably yield progressively less conservative (i.e., higher) soil cleanup concentrations.

2. State Approaches to TPH and BTEX Soil Cleanup Standards

The bases for existing state cleanup standards were obtained from literature sources, state guidance documents, and personal communications. A preliminary screening of cleanup concentrations in all 50 states was done using a national survey (Bell *et al.*, 1991). This screening enabled the identification and targeting of a subset of 26 states for more in-depth classification, and encompassed states with the highest, lowest, and midpoint cleanup criteria, in addition to states that historically have exhibited environmental leadership, innovation, or conservative environmental policy. Guidance documentation was sought from all target states, and personal contacts with state officials were made in cases where documentation was unobtainable or further validation was necessary. These efforts were supplemented by a more recent national survey (Oliver *et al.*, 1993) of state cleanup criteria. State-specific approaches for TPH are shown in Table 1, and for BTEX in Table 2 (cleanup concentrations were not listed for states that advocate development of site-specific cleanup concentrations, unless defined criteria existed as well).

Several broad categorizations of the bases for state-specific TPH and BTEX cleanup concentration were made: application of *scientifically based* rationales (e.g., human health risk assessment, fate-and-transport computer modeling), use of *technology-driven* criteria (e.g., best available technology [BAT] remediation, detection limits, monitoring programs), or use or consideration of *other* approaches (e.g., comparison to other states, "cleanup to background" policy, use of generic migration and attenuation assumptions). More than one approach may be employed within a single state in some instances, based on the classification of a particular site within one of several alternate schemes.

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TABLE 1
Derivation Methodologies for TPH Soil Cleanup Levels For 26 Target States

	Aesthetics	Remediation Technology	Analyzed Other States	Attenuation Factor	Background/ Detection Limit	Fate and Transport Modeling	Human Health Risk	Completely Site-Specific	Regulatory Goal	Type of Level	Level (ppm)	Remarks
CA						*		*	GW	RG	Site-specific	Use of SESOIL/ AT123D. Derived from BTEX levels
CO			*						GW	RG	100-500	Emphasis on ground water potability
DE								*	GW	RG	Site-specific	Levels derived for 3 site classes (high, medium, low). Emphasis on ground-water and land use.
FL				*					GW	RG	10 as TRPH [1]	Applies attenuation factor (2) to ground-water cleanup goal
GA			*		*				GW,SW	CS	100-500	In-stream water quality drives cleanup levels; considers distance from groundwater withdrawal site
HI											None	Regulate BTEX only, in absence of water quality standards
ID			*						GW	RG	100-1000	Based on Oregon's approach
IL											None	Regulate BTEX only
KS	*				*				GW	CAL	100	Cleanup level is flexible, based on professional judgement of regulator
LA								*	GW	RG	Site-specific; < 300	Derivation encouraged
MA						*			GW,HH	RG	500-5000	Use of SESOIL/ AT123D. Derived from BTEX levels
MD		*							GW	RG	Site-specific	Site remediated until GW concentrations stabilize
MI											None	Regulate BTEX only

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Table 1, Continued

	Aesthetics	Remediation Technology	Analyzed Other States	Attenuation Factor	Background/ Detection Limit	Fate and Transport Modeling	Human Health Risk	Completely Site-Specific	Regulatory Goal	Type of Level	Level (ppm)	Remarks
MN						*	*	*	GW,SW	RG	Site-specific	Derivation encouraged; Typically fate/transport based
MO			*						GW	RG	Site-specific; 50-500	Importance of ground water potability, for soil use cleanup scenario
NH						*		*	GW	RG	Site-specific[2]	Based on CA LUFT procedure, using state's input parameters
NJ											None	Regulate BTEX only
NY											None	Regulate BTEX only
OH			*	*			*		GW,HH	RG, CAL	105-1156	Importance of drinking water quality
OR				*					GW,HH	CS	40-1000	Use of attenuation factor of 100 (USEPA standard factor)
SD			*	*					GW	RG, CAL	10-100	Use conservative attenuation factor from 1-10
TN			*	*				*	GW	CS	100-1000	Levels applied by site class. Can use state's levels or derive levels
TX						*	*	*	GW,HH	RG	Site-specific	Use of computer model (API) with site data
UT								*	GW	RG	Site-specific; considers action levels: 30-100	Established on a case-by-case basis
WA			*				*	*	GW,HH	RG	100-200	Choice of state's levels or risk assessment; 3 site classes for cleanup

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Table 1, Continued

	Aesthetics	Remediation Technology	Analyzed Other States	Attenuation Factor	Background/ Detection Limit	Fate and Transport Modeling	Human Health Risk	Completely Site-Specific	Regulatory Goal	Type of Level	Level (ppm)	Remarks
WI								*	GW,HH	RG	Site-specific	Derivation encouraged. Action level triggers are MDL. Accept fate and transport, detection limits, remediation-based cleanup

(1) TRPH - Total Recoverable Petroleum Hydrocarbon
(2) In the future, NH intends to eliminate regulation of TPH

Aesthetics: Aesthetic qualities are important considerations for "clean" soil
Remediation Technology: Soil considered "clean" when ground water concentrations achieve asymptotic levels
Analyzed Other States: Cleanup levels used by other states were considered or used
Attenuation Factor: Soil cleanup concentrations were determined by multiplying "acceptable" ground water concentrations by an attenuation factor (e.g., often 20)
Background/Detection Limit: Remediation goal equals background levels (in literature or via sampling) or designated MDL (Method Detection Limit)
Fate/Transport: Computer modeling was used to calculate soil concentrations corresponding to acceptable ground water concentrations
Human Health Risk: *=Risk-based remediation goals (i.e., PRGs, or preliminary remediation goals) established through use of a structured risk assessment methodology
Site-Specific: Remediation goals established on a case-by-case basis, using various scientific methods
Regulatory Goal: GW=Goal of cleanup level is protection of ground water; HH = Human Health; SW = Surface Water
Type of Level: RG=Remediation Goal; CS=Cleanup Standard (Law); CAL=Corrective Action Level
Level: Fixed or Site-specific cleanup levels; Cleanup range is listed if one exists.

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TABLE 2
Derivation Methodologies for BTEX Soil Cleanup Levels for 26 Target States

	Aesthetics	Remediation Technology	Analyzed Other States	Attenuation Factor	Background/ Detection Limit	Fate and Transport Modeling	Human Health Risk	Completely Site-Specific	Regulatory Goal	Type of Level	Level (ppm)	Remarks
CA						*	**	*	GW,HH	RG	Site-specific; 0.3-1 B, 0.3-50 T, 1-50 E, 1-50 X (ranges)	Use of SESOIL/ AT123D; cleanup ranges based on site classification; considers depth to GW and annual rainfall
CO			*				**		GW,HH	RG	20-100 total BTEX	Importance of ground water pot-ability
DE							**	*	GW,HH	RG	Site-Specific; Site-classification drives levels	Levels derived for 3 site classes (high, medium, low). Emphasis on ground-water and land use.
FL							*		HH	RG	0.1 total VOA (Volatile organics)	Assumes conservative residential exposure scenario
GA			*		*				GW,SW	CS	20-100 total BTEX	In-stream water quality criteria drive cleanup levels; considers distance from GW with-drawal site
HI				*			**		GW,HH, SW	RG	1.7 B; 21 T; 1.4 E for diesel/jet fuel/ kerosene; (Options include site-specific PRG or monitoring)	Cleanup driven by state water quality criteria (drinking or surface), based on GW use
ID			*				**		GW,HH	RG	1 B, 1 T, 1 E, 1 X	Looked at Oregon's approach
IL						*	**		GW	CAL	Dual site classes (Type A/B): BTEX 11.7/13.5 B 0.005/0.025	Apply to USTs only; site class considers soil type and GW use; non-gas fuels regulated for 5 PAHs and naphthalene
KS				*			**		GW,HH	CAL	1.4 B	Cleanup level flexible; also regulate 1,2-dichloroethane (8 ppm)

Table 2, Continued

	Aesthetics	Remediation Technology	Analyzed Other States	Attenuation Factor	Background/ Detection Limit	Fate and Transport Modeling	Human Health Risk	Completely Site-Specific	Regulatory Goal	Type of Level	Level (ppm)	Remarks
LA								*	GW	RG	Site-Specific; < 100	Derivation encouraged; currently working towards risk-based approach
MA				*		*	*		GW,HH	RG	B 10-200; T 90-2500; E 80-500; X 500-2500 (applying attentuation factor/cleanup matrix approach)	Use of SESOIL/ AT123D; allows site-specific risk assessment and PRGs. [Regulates diesel for naphthalene, phenathrene and benzene]
MD		*							GW	RG	Site-Specific; considers land and GW uses, and receptors	Site remediated until GW concentrations stabilize (monitoring)
MI					*		*	*	GW,HH	CAL	0.024 B, 16 T, 1.5 E, 5.6 X (gas)	Allows for choice of 3 approaches: cleanup to background/detect-ion limit, PRGs, or site-specific risk assessment
MN						*	*	*	GW,HH	RG	Site-specific	Typically risk or fate/ transport based
MO			*				**		GW,HH	RG	1.0 total BTEX; 0.5 B	For USTs only; stress importance of ground water potability
NH						*	**	*	GW,HH	RG	Site-specific; Based on CA LUFT manual	CA method, with NH input parameters
NJ							*		HH	RG	Residential/non-residential: 3/13 B; 1000/1000 T; 1000/1000 E; <110-1000 X	Stress GW impact; 2 cleanup levels: residential/non-residential land use; also regulate naphthalene, benzo-(a)pyrene, anthracene, lead
NY	*			*			*		GW,HH	AL	Site-specific; for Gas/ Diesel: 0.014/0.2 B; 0.1/1.0 T; 0.1/1.0 E; 0.1/1.0 X	Must satisfy both GW and HH state criteria; regulate other compounds, too.

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Table 2, Continued

	Aesthetics	Remediation Technology	Analyzed Other States	Attenuation Factor	Background/ Detection Limit	Fate and Transport Modeling	Human Health Risk	Completely Site-Specific	Regulatory Goal	Type of Level	Level (ppm)	Remarks
OH			*	*			*		GW,HH	AL-based	Site-specific; 0.006-0.5 B; 4-12 T; 6-18 E; 28-85 X	Stress importance of drinking water quality; considers soil type, distance to drinking water
OR						*	*		GW,HH	CS	Site-specific matrix; 0.1 B; 80 T; 100 E; 800 X	Use of SESOIL/ AT123D; generates a site score-based cleanup matrix
SD											None	Regulate TPH only
TN			*	*			**	*	GW,HH, SW	CS	10-500 total BTEX (based on site classification)	Choice of state's levels or site-based derived levels; considers soil permeability, GW and SW uses
TX						*	*	*	GW,HH	RG	Site-specific	Use of computer model (API) with site data
UT							**	*	GW,HH	RG	Site-specific; Considers action levels of 0.2 B, 100 T, 70 E, 1000 X	Developed on a site-by-site basis; advocate GW monitoring program
WA			*				*	*	HH,GW	RG	0.5 B, 40 T, 20 E, 20 X	Choice of state's levels or risk assessment; 3 site classes for cleanup
WI								*	GW,HH	RG	Site-specific	Derivation allowed; action level triggers are MDL; accept fate and transport, detection limits, remediation-based cleanup

Aesthetics: Aesthetic qualities are important considerations for "clean" soil
Remediation Technology: Soil considered "clean" when ground water concentrations achieve asymptotic levels
Analyzed Other States: Cleanup levels used by other states were considered or used
Attenuation Factor: Soil cleanup concentrations were determined by multiplying "acceptable" ground water concentrations by an attenuation factor (e.g., often 20)
Background/Detection Limit: Remediation goal equals background levels (in literature or via sampling) or designated MDL (Method Detection Limit)
Fate/Transport: Computer modeling was used to calculate soil concentrations corresponding to acceptable ground water concentrations
Human Health Risk: *=Risk-based remediation goals (i.e., PRGs, or preliminary remediation goals) established through use of a structured risk assessment methodology

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Table 2, Continued

**=Level is protective of human health via protection of ground water to a drinking water standard
Site-Specific: Remediation goals established on a case-by-case basis, using various scientific methods
Regulatory Goal: GW=Goal of cleanup level is protection of ground water, HH = Human Health, SW = Surface Water
Type of Level: RG=Remediation Goal; CS=Cleanup Standard (Law); CAL=Corrective Action Level
Level: Fixed or Site-specific cleanup levels; Cleanup range is listed if one exists.

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Of the 20 states that have developed soil cleanup concentrations for TPH (one state, Florida, has levels for total recoverable petroleum hydrocarbons, and not TPH per se), 12 use indirect, partially scientific bases for their derivation (e.g., such as extrapolation from BTEX cleanup concentrations using fuel-specific compositional assumptions of BTEX content) (California, Delaware, Louisiana, Massachusetts, Minnesota, New Hampshire, Ohio, Tennessee, Texas, Utah, Washington, and Wisconsin); three use technology-driven cleanup criteria (Georgia, Kansas, and Maryland), and five states (Colorado, Idaho, Missouri, Oregon, and South Dakota) fall into the category of other approaches. The remaining five states (Hawaii, Illinois, Michigan, New Jersey, and New York) do not currently consider TPH for remediation purposes. New Hampshire intends to eliminate the use of TPH as a remediation parameter in the future.

Of the 24 states that have developed soil cleanup concentrations for BTEX (one state, Florida, has levels for volatile organics [VOA], and not BTEX per se), 17 allow for scientifically based approaches in their derivations (California, Delaware, Illinois, Louisiana, Massachusetts, Michigan, Minnesota, New Hampshire, New Jersey, New York, Ohio, Oregon, Tennessee, Texas, Utah, Washington, and Wisconsin), one uses technology-driven cleanup criteria (Maryland), while one allows for its use (Michigan), and six states use other approaches exclusively (Colorado, Georgia, Hawaii, Idaho, Kansas, and Missouri), while three also allow for the use of other approaches (New York, Ohio, and Tennessee).

3. ***Focus of State Cleanup Efforts: Protection of Human Health and Groundwater***

There are four overriding trends noted following examination of the target state approaches to establishing soil cleanup concentrations. (1) States acknowledged the limitations of using a TPH cleanup concentration. Five states do not regulate TPH at all, while two use TPH levels for screening or qualitative estimation of the degree of contamination, and one state plans to phase out TPH. (2) Most states seek to protect the quality of groundwater. Whether via fate-and-transport modeling, "generic" attenuation factors, application of background levels, or technology-based cleanup plans, soil standards are meant to ensure compliance with some existing groundwater quality standard. (3) The underlying goal for most states is the protection of human health. Groundwater standards are drinking water standards when potable water was impacted (the federal maximum contaminant level [MCL] under the Safe Drinking Water Act [SDWA] or a state-specific drinking water standard). (4) The primary trend in methodology for establishing soil cleanup concentrations is toward use of site-specific, quantitative, scientifically defensible approaches, with quantitative human health risk assessment playing an increasingly important role. Regardless of the exact nature of the methods, the overriding concerns were centered on human health protection, particularly by achieving relevant groundwater standards.

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III. SELECTION OF POTENTIAL JET FUEL INDICATOR COMPOUNDS

A. Criteria for Assessing and Selecting Jet Fuel Indicators

The potential for specific constituents of JP-4 fuel to serve as TPH alternatives was investigated using a three-pronged approach: (1) consideration of fate and transport properties, (2) assessment of toxicity, and (3) determination of regulatory standards for the media of concern. Fate and transport considerations included the relative proportions of constituents in JP-4, their physicochemical properties, temporal variations in soil-related distributions of constituents, and the implications for human routes of exposure. Toxicity assessment involved examining constituent-specific toxic effects coupled with the availability of relevant toxicity information, as well as the availability of established toxicity values (i.e., USEPA). Regulatory standards for relevant media of concern (i.e., groundwater and soil) were identified (i.e., MCLs for potable groundwater).

1. Fate and Transport

Two primary fate and transport-related considerations influence the selection of potential TPH alternative(s) for determining soil cleanup levels: (1) presence in JP-4 fuels in a quantity sufficient to ensure detection in environmental media and (2) physicochemical properties that promote migration through subsurface strata.

a. Amounts of Potential TPH Alternatives in JP-4 or Related Fuels

JP-4 is a broad cut, naphtha jet fuel, similar to fuel oil no. 1 (kerosene), whose composition has been described as a mixture of approximately 65% gasoline and 35% light petroleum distillates (Curl and O'Connell, 1977). The blending of JP-4 fuel is designed to produce a product with a composition that broadly segregates (by weight) as 32% *n*-alkanes, 31% branched alkanes, 16% cycloalkanes, 18% benzenes and alkylbenzenes, and 3% naphthalenes* (IARC, 1989; Air Force, 1989). Weight percents of fuel constituents are representative estimates only, given the variation in precursor crude oils as well as in the refining process of fuel manufacturers (Air Force, 1989; Curl and O'Connell, 1977; NRC, 1985). In addition to these broad classes of components stated above, jet fuels such as JP-4 contain polycyclic aromatic hydrocarbons (PAHs), although their combined weight fraction is typically less than the naphthalenes (USEPA, 1980; IARC, 1989). PAHs

* For purposes of this report, naphthalenes are defined as a group of compounds, substituted and unsubstituted, that have two fused aromatic rings. While naphthalenes may sometimes be categorized as polycyclic aromatic hydrocarbons (PAHs), they were considered to be distinct entities in this report.

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found in jet fuels tend to be those within the relatively low molecular weight range for PAHs (USEPA, 1980). Ranges of concentrations for fuel constituents have been generated based on available compositional information for various jet fuels or similar fuel types.

Table 3 identifies the relative concentrations of the BTEX compounds within JP-4 or similar fuels. Similar information for other primary components of JP-4-related fuels that could potentially serve as TPH alternatives (e.g., alkanes, naphthalenes, and PAHs) is shown in Table 4. Fuels chosen to approximate some of the constituents of JP-4 included low-sulphur Jet fuel A, high-sulfur Jet fuel A, and a more generic jet fuel. The composition of fuel oil no. 1 (kerosene) was used as the source of information for select compounds when jet fuel-specific data were not available. The consideration of Jet fuel A constituents in lieu of bona fide JP-4 constituents adds qualitative as well as quantitative uncertainty to the identification of potential TPH alternatives. However, it is believed that differences between JP-4 and Jet A would not affect the identification of gross classes of potential TPH alternatives (e.g., BTEX, alkanes, napthalenes, and PAHs), unless in a manner that errs on the conservative side from a health perspective. Ultimately, selection of specific TPH alternatives from within these classes will be sufficiently conservative with respect to their *known* potential for adverse health effects (i.e., the existing toxicological database) to minimize uncertainty and to not substantially alter forthcoming conclusions.

TABLE 3
Concentrations of BTEX Compounds in JP-4 and Similar Fuels

Compound	Kerosene (ppm or mg/L)[a]	Jet A Fuel (ppm) [b]	JP-4 (ppm)[c]
Benzene	<1681	2521	3750
Toluene	2773	11765	9975
Ethylbenzene	3109	2521	2775
Xylenes (total *o-*,*m-*,*p-*)	8067	7563	17,400

(a) In: *Development of a Standard Pure-Compound Base Gasoline Mixture for Use as a Reference in Field and Laboratory Experiments*. 1990. Kreamer and Stetzenbach. Values were converted from a range of weight percents to ppm (mg/L) by using the midpoint value of the weight percent range in combination with the midpoint value for the density of kerosene. [{weight percent (g/kg) × 1 kg kerosene/1.19 L} × 1000 (mg/g) = ppm (mg/L)]

(b) In: *Soluble Hydrocarbons Analysis From Kerosene/Diesel Type Hydrocarbons.* Dunlap and Beckmann. Values were converted from weight percents in manner analogous to that described in footnote (a).

(c) In: *Variability of Major Organic Compounds in Aircraft Fuels.* 1984. Hughes *et al.* Values were converted from a range of weight percents to ppm (mg/L) by using the weight percent in combination with the density of JP-4. [{weight percent (g/kg) × 0.75 kg JP-4/ L} × 1000 (mg/g) = ppm (mg/L)] The value for xylenes was based on the average weight percent for the o-,m- and p- isomers.

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TABLE 4
Concentrations of Potential TPH Alternatives in Fuels Similar to JP-4

Compound	Jet A Fuel (low sulfur) (ppb) [a]	Jet A Fuel (high sulfur) (ppb) [a]	Jet fuel (ppb) [b]	Fuel oil no. 1 (Kerosene) (ppm) [c]
Polycyclicaromatic hydrocarbons (PAHs):				
Phenanthrene	1800	2200		210
Anthracene	140	200		0.84
Fluoranthene	12	48		
Pyrene	18	76		
Triphenylene	3.6	7.2		
Chrysene	2.8	3.2		
Benzo(*e*)pyrene	1.6	11.4		
Benzo(*a*)anthracene	ND	ND		
Benzo(*a*)pyrene	ND	ND		
Benzo(*g,h,i*)perylene	ND	ND		
Anthanthrene	ND	ND		
Corenene	ND	ND		
Fluorene	ND	ND		
Total PAHs	1978	2546	150	151
Naphthalene				
Total Naphthalenes	5882 ppm [d] 22790 ppm [e]			3781
Alkanes:		NR	NR	NR
n-pentane, *n*-Hexane	NR			
Cyclohexane	NR			
Total Alkanes (n- and branched)	423099 ppm[e]			
Total Cycloalkanes	5506 ppm[e]			

ND = Not Detected; NR = Not Reported

(a) In: *Quantitative Analysis of Polynuclear Aromatic Hydrocarbons in Liquid Fuels*. 1980. USEPA, Environmental Sciences Research Laboratory, Reserach Triangle Park, NC. EPA-600/2-80-069. Values represent the average concentration for two samples.

(b) In: *Soil Cleanup Criteria For Selected Petroleum Products*. 1986. Stokman and Dime.

(c) In: *Development of a Standard Pure-Compound Base Gasoline Mixture for Use as a Reference in Field and Laboratory Experiments*. 1990. Kreamer and Stetzenbach. Values were converted from a range of weight percents to ppm (mg/L) by using the midpoint value of the weight percent range in combination with the midpoint value for the density of kerosene. [

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{weight percent (g/kg) x 1 kg kerosene/1.19 L} x 1000 (mg/g) = ppm (mg/L)]

(d) In: *Soluble Hydrocarbons Analysis From Kerosene/Diesel Type Hydrocarbons.* Dunlap and Beckmann. Values were converted from weight percents in manner analogous to that described in footnote (c).

(e) In: *TPH in Soil Primer.* 1993. E.M. Schwerko, BP Oil Environmental Technology Branch. Values are for Jet A, unknown sulfur type, and were derived from volume percents using the density of the individual naphthalene constituents [volume percent (ml/100 ml) x 1000 (ml/L) x density (g/ml) x 1000 (mg/g) = ppm (mg/L)]

b. ***Physicochemical Properties of Potential TPH Alternatives***

Physicochemical factors that influence the fate and transport of compounds include the potential for volatilization and the potential to migrate through soil. Compounds expected to exhibit high soil mobility typically include those with low molecular weights, low boiling points, low octanol-water partition coefficients, low organic-carbon partition coefficients, high vapor pressures, high water solubility, and high Henry's law constants. Physicochemical properties for potential TPH alternatives (BTEX and others) are listed in Table 5.

c. ***Fate and Transport of Potential TPH Alternatives***

i. **BTEX**

Based on their relatively high vapor pressures and moderate to high water solubilities (Table 5), the BTEX compounds typically exhibit high mobility in soils. They volatilize extensively to air following a surface spill, and from surface water following a spill and subsequent transport processes (Air Force, 1981a, 1987, 1988; USEPA, 1985a). The relatively low K_{oc}s indicate minimal to moderate association with organic carbon in soils, especially in light of their water solubilities. Trends toward decreased leaching (soil migration) with increasing soil organic carbon fraction have been observed for toluene and the xylenes (ATSDR, 1992, 1989a). All BTEX compounds undergo biodegradation in soil or water, to moderate extents, although benzene biodegradation in soil is minimal (ATSDR, 1991). The nature and extent of biodegradation appears to be highly influenced by the degree of oxygenation of the soils, as well as other site-specific parameters. BTEX compounds have been found in association with groundwater, although toluene is not typically encountered to any significant extent (ATSDR, 1989a, 1991, 1992).

ii. **Alkanes**

The physicochemical properties of low-molecular-weight alkanes (Table 5) such as pentane, hexane, heptane, and cyclohexane indicate that they are fairly volatile compounds, and therefore will tend to vaporize following spills. However, unlike the BTEX compounds, their hydrophobic nature and affinity for organic carbon (CRC, 1986) does not indicate a great tendency to leach and migrate into subsurface soils or groundwater.

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TABLE 5
Physical-Chemical Properties of Potential TPH Alternatives

Chemical	Molecular Weight	Boiling Point (°C)	Vapor Pressure (mm Hg)	Henry's Law Constant (atm-m^3/mole)	Water Solubility (mg/L)	Organic Carbon Partition Coefficient (K_{oc})	Octanol Water Partition Coefficient (K_{ow})
Range of Values (Bold values indicate higher soil mobility)	**78.1** to 252.3	**69** to 448	5.6×10^{-9} to **400**	4.9×10^{-7} to **3.21**	3.8×10^{-9} to **1780**	**48** to 5.5×10^{6}	**135** to 1.55×10^{6}
BTEX							
Benzene[a]	78.1	80.1	95	5.5×10^{-3}	1780	63-79.4	135
Ethylbenzene[b]	106	136.3	9.5	8.7×10^{-3}	160-208	165-254	1349-2200
Toluene[c]	92.1	110.6	22	6.7×10^{-3}	448	295	617
Xylenes[d] (*o*-,*m*-,*p*-)	106.2	137-144	6.7-10	$5.2\text{-}7.6 \times 10^{-3}$	134-213	48-260	1202-1585
Potential Surrogates							
Alkanes:							
Heptane[e]	100.2	98.4	~40	2.06	2.4	2400-8100	45,709
Hexane[e]	86.2	69	100< x <400	1.81	9.5	1250-4100	7,943-12,882
Octane[e]	114.2	125.7	~10	3.21	7×10^{-4}	5500-15,600	10,000-151,356
Cycloalkanes:							
Cyclohexane[e]	84.2	80.7	100	0.19	54.8	480	No data
Naphthalene[f]	128.2	218	8.7×10^{-2}	4.6×10^{-4}	31.7	933	1950

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Chemical	Molecular Weight	Boiling Point (°C)	Vapor Pressure (mm Hg)	Henry's Law Constant (atm-m^3/mole)	Water Solubility (mg/L)	Organic Carbon Partition Coefficient (K_{oc})	Octanol Water Partition Coefficient (K_{ow})
PAHs:							
Anthracene[g]	178.2	340-342	1.7×10^{-5}	8.6×10^{-5}	No Data	1.4×10^{4}	2.8×10^{4}
Benzo(*a*)pyrene[g]	252.3	310-312	5.6×10^{-9}	4.9×10^{-7}	3.8×10^{-9}	5.5×10^{6}	1.55×10^{6}
Chrysene[g]	228.3	448	6.3×10^{-9}	1.0×10^{-6}	1.5×10^{-3}	2.0×10^{5}	4.1×10^{5}
Fluoranthene[g]	202.3	375	5.0×10^{-6}	6.5×10^{-6}	No Data	3.8×10^{4}	7.9×10^{4}
Fluorene[g]	166.2	295	7.1×10^{-4}	6.4×10^{-5}	1.7-2.0	7.3×10^{3}	1.5×10^{4}
Pyrene[g]	202.3	393-404	2.5×10^{-6}	5.1×10^{-6}	0.13-0.17	3.8×10^{4}	8.0×10^{4}

(a) Toxicological Profile for Benzene. Agency for Toxic Substances and Disease Registry (ATSDR). 1991.
(b) Toxicological Profile for Ethylbenzene. ATSDR. 1990b.
(c) Toxicological Profile for Toluene. ATSDR. 1992.
(d) Toxicological Profile for Total Xylenes. ATSDR. 1989a.
(e) CRC Handbook of Chemistry and Physics. 67th ed. 1986-87.
(f) Toxicological Profile for Naphthalene, 2-Methylnaphthalene. ATSDR. 1989c.
(g) Toxicological Profile for Polyaromatic Hydrocarbons. ATSDR. 1989d.

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iii. **Naphthalenes**

Naphthalene is moderately volatile and has a fairly low water solubility, a relatively high K_{ow}, and a moderate affinity for organic carbon (Table 5). These characteristics do not indicate a great tendency to migrate into subsurface soil or groundwater. Biodegradation has been observed in soil and water, although the nature and extent of these processes are site specific (ATSDR, 1989c).

iv. **PAHs**

The PAHs typically include those organic compounds with three or more fused aromatic rings in their structures. The vast majority of the high molecular weight PAHs are not associated with JP-4 fuel. However, those PAHs that are associated with JP-4 fuel represent some of the fuel's heavier compounds.

PAHs are a broad class of compounds with respect to their molecular weights and properties. In general, lower-molecular-weight PAHs (e.g., fluorene, pyrene) are more water soluble and would exhibit great soil mobility than higher-molecular-weight PAHs (Table 5). However, as a chemical group, these compounds are not considered particularly volatile or mobile, and tend to remain associated with soils, rather than leaching into groundwater. The higher-molecular-weight PAHs have much less potential for migration into groundwater given their low water solubility and low K_{oc}s (Table 5). While the primary fate of these compounds in soils is biodegradation (ATSDR, 1989d), the actual extent of biodegradation and subsequent reduction of soil levels cannot realistically be established as a constant because site-specific microorganisms as well as soil and spill conditions are the driving factors in the process.

The relative partitioning of thepotential TPH alternatives across primary environmental media is illustrated in Figure 1.

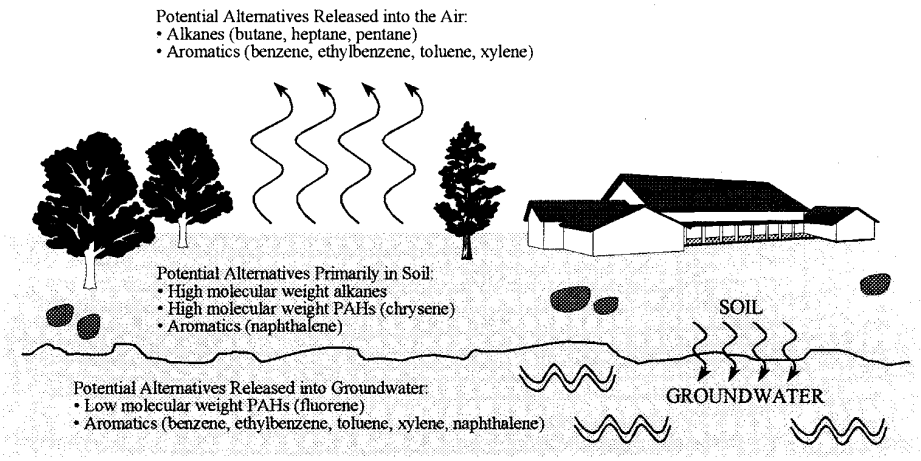

FIGURE 1. Fate and transport of potential TPH alternatives.

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d. ***Temporal Alterations in Distributions of TPH Alternatives***

For the more volatile fuel constituents such as BTEX, naphthalenes, and low-molecular-weight alkanes, the portions of these JP-4 components not volatilized after the initial spill event(s) will enter the surficial and near-surficial soils. Surficial volatilization will continue until such time as the smaller, more hydrophilic constituents (i.e., BTEX, naphthalene, and fluorene) migrate with percolating water, partitioning through subsurface soil and potentially impacting groundwater.

Temporal variations in soil concentrations of relatively nonvolatile fuel constituents, such as higher molecular weight PAHs, long-chain, or branched alkanes, will be much less pronounced. These constituents remain preferentially associated with soil at the site of a spill for significantly longer periods of time than the BTX components. Although the primary fate of PAHs in soils appears to be biodegradation (ATSDR, 1989d), the actual nature and extent of biodegradation will vary widely with such site-specific factors as the size of the spill, the soil type, and the microbes present. It is anticipated that the hydrophobic and bulky alkanes would exhibit similar characteristics in the soil matrix. Lower-molecular-weight PAHs such as fluorene have been shown to exhibit faster migration rates and greater migration distances than their high molecular weight counterparts (ATSDR, 1989d), and would be more likely to reach the water table. The anticipated progression of alterations in the media-specific distributions of potential TPH alternatives, as a function of increasing age of the spill (*weathering*), is qualitatively depicted in Table 6.

e. ***Effects of Fate and Transport on Human Exposure Routes***

Information on temporal variations in the partitioning of JP-4 constituents in site media can be used to predict the relative abundance of JP-4 fuel constituents in select media. This information, when combined with constituent toxicity information, can determine which compounds would effectively be the *risk drivers* at the site. While anticipated risk drivers can be identified based on consideration of exposure routes, physicochemical properties, and toxicity, the extent to which temporal alterations influence the final risk drivers for a spill site is ultimately site specific. Site-specific properties such as the magnitude of precipitation, permeability of the soil, type of soil (fraction of organic carbon present), geological strata, distance to groundwater, and the physical and dynamic nature of the underlying groundwater aquifer(s) will exert great influence on the subsequent fate and transport of any contaminant over time.

i. Soil-to-Groundwater Fate and Transport

Any factor causing temporal alteration in soil or air concentrations can influence which fuel constituent will become the risk driver for a route of exposure, which

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TABLE 6
Anticipated Temporal Variations in Relative Proportions of BTEX and PAHs in Soil and Groundwater

Relative Age of Spill	BTEX [1]	PAHs [1]
Recent, fresh surficial spill	Surface Soil: High levels Groundwater: None	Surface Soil: High levels Groundwater: None
Old spill	Surface Soil: Low levels Groundwater: Low levels; typically benzene	Surface Soil: High to moderate Groundwater: None to traces of low MWr PAHs; (*e.g.*, flourene)
Very Old Spill	Surface Soil: None to trace Groundwater: Low levels; BTEX	Surface Soil: Moderate levels of high MWr PAHs; (*e.g.*, B(a)P) Groundwater: Trace to low levels of low MWr PAHs

[1] Levels described as high, medium/moderate, or low are with respect to the concentrations in virgin fuel

may include ingestion of surface soil or inhalation of vapors. However, the emerging trend toward regulating soil contaminant levels based on groundwater protection may supersede exposures via soil ingestion or vapor inhalation for those compounds that present greater soil mobility (e.g., BTEX, naphthalene, and low-molecular-weight PAHs such as fluorene). For relatively nonmobile TPH alternatives, or those lacking established groundwater protection standards, risks from exposures via soil ingestion or inhalation may still predominate at the site.

Example. In a hypothetical future residential setting, a child/adult living on the site of a fuel spill will breathe air, ingest soil, and ingest potable groundwater. For the case of an older spill site, the surface soil is not likely to contain volatiles, given their propensity to initially volatilize and then migrate into soil over time. For the same reasons, inhalation of volatile compounds will probably not be a primary route of exposure at the older spill site. Ingestion of semivolatile, less mobile fuel constituents (i.e., high-molecular-weight alkanes or bulkier PAHs) in surface soil is more likely to occur, given their greater association with soil. The potential risks from ingesting site groundwater may drive the risk for the more mobile fuel compounds (BTEX). Even at a recent spill site, where migration of compounds to groundwater may not yet have occurred, the typical future land use scenario involving groundwater ingestion will still entail addressing risks from this exposure route, albeit in a predictive manner.

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ii. Summary of Fate and Transport Properties of TPH Alternatives

Higher-molecular-weight PAHs and alkanes, and possibly some naphthalene would appear to remain associated with soil at the site of a spill for significantly longer periods of time than BTEX, while BTEX, naphthalene, and low-molecular-weight PAHs would be anticipated to migrate further, thereby exhibiting a greater potential for groundwater contamination.

2. Toxicity Assessment

In addition to fate and transport properties, information that must be considered for the identification of the most appropriate TPH alternative includes the nature and magnitude of any toxic effects. To this end, toxicity information, established USEPA toxicity values, and any health-based regulatory standards for groundwater and soil were sought for TPH, as well as potential TPH alternatives.

a. Availability of Compound-Specific Toxicity Information

The toxic effects associated with chronic exposures (long term or lifetime) to potential TPH alternatives will be considered for these analyses, as these effects are most representative of exposures associated with land use at fuel sites, and are more conservative (i.e., more protective) of human health.

i. BTEX

The chronic toxicities of the BTEX compounds are driven by the toxic properties of benzene, particularly due to its identification as the sole carcinogen. Benzene is a known carcinogen in animals and humans, both orally and via inhalation. Increased risk of leukemia in occupationally exposed persons (Ott *et al*., 1978, 1981; Rinsky *et al*., 1987; Wong *et al*,. 1983) and in animal studies (Cronkite *et al*., 1984, 1986, 1989; Maltoni *et al*., 1982) supports this conclusion. In addition, benzene has been shown to be harmful to the immune and hematopoietic systems (Snyder *et al*., 1980; Rozen and Snyder, 1985; ATSDR, 1991). Ethylbenzene, toluene, and xylenes share similar types of acute noncarcinogenic toxic effects, primarily manifested as depression of the central nervous system (CNS) and respiratory impairment, with reported effects on the liver, kidneys, and hematopoietic system (ATSDR, 1989b; 1992; 1989c). Some evidence of teratogenicity (adverse effects on fetuses) has been reported for xylenes (ATSDR, 1989a) and ethylbenzene (Andrew *et al*., 1981; ATSDR, 1989b), although conclusive interpretations of these studies are limited.

ii. Alkanes

Alkanes such as hexane, heptane, octane, and cyclohexane exhibit related toxicity following acute exposure, such as CNS depression at fairly high levels. *n*-Hexane

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chronic toxicity includes peripheral nerve damage in workers exposed by inhalation (Iida and Yamamoto, 1973; ACGIH, 1990a) and animals (Spencer, 1980; ACGIH, 1990b). Minimal negative evidence for heptane chronic toxicity was found (API, 1980; Crespi *et al*., 1979). No information was found on octane toxicity in humans or animals. Chronic to subchronic cyclohexane exposures in animals indicate minimal to no observations of neural and other tissue toxicity (ACGIH, 1990b; Patty, 1981-82; Frontali *et al*., 1981), although it has been suggested that cyclohexane may function as a weak tumor promotor (Gupta and Mehrotra, 1990). Additional information on these compounds is limited, as they have not been associated with particularly toxic endpoints.

iii. **Naphthalenes**

Naphthalene carcinogenicity in animals has been studied by the National Toxicology Program (NTP, 1991) and Adkins *et al*. (1986), with equivocal outcomes on carcinogenicity, although it has caused hemolytic anemia following both chronic and acute exposures. Both the liver and the hematopoietic system have been indicated as sites of naphthalene toxicity (ATSDR, 1989c).

iv. **PAHs**

The predominant toxicity associated with PAHs (primarily select high molecular weight PAHs) is carcinogenicity. However, the PAHs that are classed by the USEPA as probable human carcinogens (e.g., benzo(*a*)pyrene, benzo(*a*)anthracene, benzo(*b*)fluoranthene, benzo(*k*)fluoranthene, chrysene, and dibenz(*a,h*)anthracene)* have not been detected in appreciable amounts in jet fuels, with the exception of chrysene (typically present at less than 4 ppb; USEPA, 1980). The carcinogenic effects have been best defined for the PAH benzo(*a*)pyrene, a potent skin and lung carcinogen in animals. In addition, it has been demonstrated that benzo(*a*)pyrene (B(*a*)P) is a cause of adverse reproductive effects and is teratogenic (ATSDR, 1989d). Noncarcinogenic PAHs that have been detected in jet fuels include phenanthrene, anthracene, fluoranthene, pyrene, benzo(*e*)pyrene, and fluorene, which exhibit variable to unknown degrees of toxicity.

b. ***Availability of Toxicity Values***

Most of the potential TPH alternatives have toxicity values that have been established and peer reviewed by the USEPA (USEPA, 1992, 1993a). TPH alternatives with established USEPA toxicity values are shown in Table 7 (BTEX compounds) and Table 8 (non-BTEX compounds).

* The order of potencies for seven PAHs has been estimated as follows (USEPA 1993b); dibenz(*a,h*)anthracene > benzo(*a*)pyrene > benzo(*b*)fluorathene > benzo(*a*)anthracene > indeno(1,2,3-*cd*)pyrene > benzo(*k*)fluoranthene > chrysene.

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TABLE 7
Toxicity Values For BTEX Compounds

Chemical	Chronic Oral R_fD (mg/kg-day)	Inhalation Reference Concentration (mg/m^3)	Oral Slope Factor $(mg/kg/day)^{-1}$	Inhalation Unit Risk $(\mu g/m^3)^{-1}$
Carcinogens:				
Benzene	Not Available	Not Available	2.9×10^{-2}	8.3×10^{-6}
Noncarcinogens:				
Toluene	2×10^{-1}	4×10^{-1}	Not Applicable	Not Applicable
Ethylbenzene	1×10^{-1}	1×10^{0}	Not Applicable	Not Applicable
Xylenes [*o*-,*m*-,*p*-]	2×10^{0}	Not Available	Not Applicable	Not Applicable

A tentative approach for deriving carcinogenic toxicity values for high molecular weight PAHs classed as probable human carcinogens has been proposed by the USEPA ("relative potency estimates"; USEPA, 1993b), although it is currently undergoing technical and policy reviews. This method provides a means for deriving relative cancer slope factors (SFs) for six other high-molecular-weight carcinogenic PAHs (benzo(*a*)anthracene, benzo(*b*)fluoranthene, benzo(*k*)fluoranthene, chrysene, dibenz(*a,h*)anthracene, and indeno(1,2,3-*cd*)pyrene). The basic approach compares the magnitude of the carcinogenic properties of six PAH carcinogens to that of B(*a*)P and normalizes them to B(*a*)P. A PAH-specific adjustment factor (an *order of magnitude* factor) is then applied to either known soil concentrations of these PAHs or to the B(*a*)P SF, to essentially express PAH-specific carcinogenicity in what equates to B(*a*)P equivalents.

However, with the exception of chrysene, these PAHs are not constituents of jet fuels (USEPA, 1980), nor is the PAH in jet fuel most likely to migrate from soil to groundwater (fluorene), carcinogenic. The order of magnitude adjustment factor for chrysene, the sole carcinogenic PAH present in trace amounts in jet fuels, is 0.01 (USEPA, 1993b). When this adjustment factor is applied to B(*a*)P oral SF of 7.3 (mg/kg/d) (USEPA, 1993a), an oral SF of 0.073 (mg/kg/d) can be ascribed to chrysene. This toxicity value is shown in Table 8.

c. Summary of Toxicity and Established Toxicity Values of TPH Alternatives

A comparison of the magnitude of the toxicity values for the carcinogenic JP-4 constituents (oral SFs for benzene and chrysene, Tables 7 and 8) indicates that the

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TABLE 8
Toxicity Values For Additional Potential TPH Substitutes

Chemical	Chronic Oral R_fD (mg/kg-day)	Inhalation Reference Concentration (mg/m^3)	Oral Slope Factor $(mg/kg/day)^{-1}$	Inhalation Unit Risk $(\mu g/m^3)^{-1}$
Polycyclicaromatic Hydrocarbons:				
Anthracene	3×10^{-1}	---	NotApplicable[a]	Not Applicable
Benzo(*e*)pyrene	---	---	NotApplicable[b]	Not Applicable
Chrysene	---	---	0.073[c]	Not Available
Fluoranthene	4×10^{-2}	---	Not Applicable[a]	Not Applicable
Fluorene	4×10^{-2}	---	Not Applicable[a]	Not Applicable
Phenanthrene	---	---	Not Applicable[a]	Not Applicable
Pyrene	3×10^{-2}	---	Not Applicable[a]	Not Applicable
Alkanes: Hexane, Octane, or Cyclohexane	None Available	None Available	Not Applicable	Not Applicable
Naphthalene	4×10^{-2}[d]	Not Available	Not Applicable	Not Applicable

(a) USEPA 1993a. Integrated Risk Information System (IRIS), NLM on-line database was consulted.

(b) Benzo(a)pyrene has an oral slope factor of 7.3 $(mg/kg/day)^{-1}$, but benzo(e)pyrene is not currently considered a carcinogen.

(c) USEPA 1993b. Chrysene oral slope factor derived via "relative potency factor" approach. See text for detailed explanation.

(d) Naphthalene toxicity values are currently undergoing extensive review by the USEPA R_fD Work Group. These values are from the Health Effects Assessment Tables (HEAST) for 1991 (USEPA 1991c). Values are subject to potential alterations in the future.

marginally larger SF is associated with chrysene (0.073 (mg/kg/d) for chrysene; 0.029 (mg/kg/d) for benzene). However, at this time benzene is the only TPH alternative with an oral SF established by the USEPA's Carcinogen Risk Assessment Verification Endeavor (CRAVE). In addition, because the concentration of chrysene in JP-4 fuel tends to be much lower than that of benzene, benzene is more likely to exhibit a greater potential for groundwater contamination than chrysene. Comparisons of the noncarcinogenic toxicity values for TPH alternatives (Tables 7 and 8) indicate that the lowest chronic oral R*f*Ds, and hence the greatest potential for producing adverse health effects under similar exposure conditions, are for naphthalene and several of the PAHs.

3. Availability of Regulatory Standards for Relevant Media

Based on current state and federal trends in regulating BTEX and TPH concentrations in soil, the potential migration of contaminants to groundwater is of primary

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concern for both present and future land use. The approach to determining the soil concentration that corresponds to an acceptable groundwater concentration typically involves identification of a health-based groundwater standard (federal or state), and subsequent modeling of a soil concentration that will not result in a groundwater concentration that exceeds the standard. To varying extents, and with different degrees of scientific rigor, existing or emerging models are being used to derive soil concentrations that maintain groundwater concentrations within federal or state standards.

In some cases, site-specific contingencies are built into the "allowable" soil levels to accommodate site-specific conditions, such as potability of groundwater, distances to well heads, soil type, and soil permeability.* Policies for establishing soil cleanup concentrations that allow for the use of site-specific parameters have greater flexibility than those that attempt to establish a generic soil cleanup concentration applicable to all sites.

In determining soil remediation goals protective of human health, risks associated with both ingestion of soil and ingestion of underlying groundwater under current land use must be determined. The potential for future contamination of any underlying groundwater that may serve as a drinking water source should also be considered, as an active, preventive measure. Groundwater standards for drinking water sources are governed by the federally established SDWA, and exist as enforceable standards termed MCLs. Chemical-specific MCLs are established to be protective of adverse human health effects over a lifetime of drinking-water exposure. As such, the stringency of a health-based MCL is driven by the stringency of the existing oral toxicities. Cleanup efforts for soils would have to ensure that future groundwater concentrations not exceed MCLs for any TPH alternatives. MCLs for potential TPH alternatives are listed in Table 9.

a. ***Summary of Regulatory Standards Information***

The MCL for benzene is more stringent (lower) than the MCLs for ethylbenzene, toluene, and xylenes by 140-, 200-, and 2000-fold factors, respectively. There are no MCLs for alkanes or the PAHs associated with JP-4. There is no MCL for chrysene. The compound with the lowest MCL, and hence the most stringent groundwater criterion, is benzene.

IV. DETERMINATION OF BENZENE AS MOST APPROPRIATE TPH ALTERNATIVE

Selection of the appropriate TPH alternative is based on consideration that influence the magnitude of health risk-based soil cleanup concentrations, in

* For example, Alaska, Idaho, and Washington have developed matrices that allow for the adjustment of soil TPH/BTEX cleanup levels based on site-specific features, including depth to subsurface water, annual precipitation, volume of contaminated soil, and soil or rock type. California's LUFT (Leaking Underground Fuel Tank) manual accommodates annual average precipitation and depth to groundwater in formulating its soil cleanup levels.

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TABLE 9
Maximum Contaminant Levels (MCLs) for BTEX and Potential TPH Alternatives

Chemical	MCL (ppm)[a]
Alkanes (hexane, cyclohexane, octane)	Not Listed
Benzene	0.005
Ethylbenzene	0.7
Naphthalene	Not Listed
PAHs: Benzo(*a*)pyrene[b] Other PAHs (chrysene, fluorene)	 0.0002 None
Toluene	1.0
Xylene	10.0

(a) MCLs are taken from the Final and Proposed Drinking Water Standards (40 CFR 141), July 1992.

(b) Benzo(a)pyrene is not present in jet fuels. It is listed here because it is the only PAH with an MCL.

addition to the previous fate, transport, toxicity, and regulatory standards information.

A. Health Risk-Based Soil Cleanup Concentrations

1. The Human Health Risk Assessment Process

The USEPA approach to human health risk assessment for chemicals essentially follows the approach first articulated by the U.S. National Academy of Sciences (NRC, 1983). The four elements of risk assessment include:

1. Hazard identification establishes the relationship between exposure to a chemical and a specific adverse health effect, and identifies chemicals of concern for all given media.
2. Dose-response assessment describes the quantitative relationship between the amount of a chemical to which individuals come into contact, and the degree and severity of known toxic injury or disease. For noncancer effects, it generates a compound-specific toxicity value, the reference dose (R_fD). For carcinogenic effects, it assigns a cancer weight-of-evidence classification that describes the likelihood that the agent is a human carcinogen, and generates a toxicity value termed the SF.

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3. Exposure assessment describes the quantity and duration of a human population's exposure, expressed as compound-specific intakes, for relevant current and future land use.
4. Risk characterization integrates data, toxicity values, and exposure intakes to quantitatively estimate noncarcinogenic and carcinogenic risk.

Standard equations and exposure parameters exist to ascertain the intake or lifetime average daily dose (LADD) from ingesting a compound in soil (USEPA, 1989). The LADD can then be used to calculate risk (USEPA, 1989):

$$\text{Cancer risk}_{\text{ingestion}} = \text{LADD} \times \text{Oral SF} \quad (1)$$

$$\text{Noncarcinogenic Hazard Quotation}_{\text{ingestion}} \ (\text{HQ}_i) = \text{LADD}/\text{R}_f\text{D} \quad (2)$$

According to the National Oil and Hazardous Substances Contingency Plan (NCP) (40 CFR Part 300), carcinogenic risk greater than 1×10^{-6} is generally regarded to be unacceptable, although this level of risk was described only as a "point of departure" with respect to risk management. In the context of hazardous waste cleanup, site-specific cancer risk between 1×10^{-4} and 1×10^{-6} may be deemed acceptable by the appropriate regulatory authority, depending on site-specific conditions and variables. Risks in excess of 1×10^{-4} are usually not considered anything other than unacceptable. Noncarcinogenic effects are generally considered to be unacceptable when the hazard quotient (HQ) exceeds a value of one (1.0).

a. ***Preliminary Remediation Goals***

An outgrowth of the risk assessment process has been the formulation of methodologies for determining the chemical concentrations corresponding to the upper limits for acceptable carcinogenic or noncarcinogenic "risks" in various media of concern. The USEPA has established a set of guidelines for this risk-based approach to formulating what they term Preliminary Remediation Goals, of PRGs (USEPA, 1991a). Essentially, the risk assessment-based equations for risk and HQ are used to estimate a chemical concentration corresponding to an "acceptable" risk level for a select medium of concern (e.g., soil or groundwater).

PRGs are designed to assist in the analysis and selection of remedial alternatives. They should be in compliance with any applicable or relevant and appropriate requirements (ARARs) and result in acceptable health risks for the given medium at the site. Chemical-specific PRGs are the concentrations of the chemical for a given medium and land use combination. Therefore, two general sources of PRGs are (1) concentrations based on ARARs and (2) concentrations based on health risk assessment. ARARs that must be met include those for the primary

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medium (e.g., soil) as well as other media that could be impacted (e.g., groundwater). Risk-based calculations that set medium-specific concentration limits, using carcinogenic and/or noncarcinogenic toxicity values in conjunction with exposure assumptions, must satisfy the NCP requirements for protection of human health (40 CFR Part 300).

The typical approach advocated by the USEPA in establishing PRGs is to identify PRGs at the site-scoping stage, modify them during and after the remedial investigation (RI) using site-specific information, and ultimately select site remediation levels in the record of decision (ROD). In the context of this report, this might initially involve identification of soil ARARs for potential TPH alternatives and development of PRGs for alternatives lacking ARARs. In general, chemical-specific soil ARARs may not be available, although this report has identified state-specific soil cleanup concentrations for BTEX compounds with varying degrees of "enforceability," ranging from screening or action levels, to guidelines, goals, and actual standards.

PRGs are based on definition of the *future* land use of the site and, in the absence of definitive evidence for an alternate land use scenario (e.g., industrial, agricultural), residential land use, the most conservative is typically assumed. In accordance with USEPA, the land use for the site determines the route(s) of exposure that must be included in the PRG approach. Future industrial land use must include the routes of soil ingestion, coupled with inhalation of soil vapor and soil particulates for an adult worker onsite. Future residential land use requires that PRGs be formulated for the soil ingestion route of exposure, where an individual has been living onsite from birth through 30 years of age. In this manner, human health risk calculations will encompass exposures for both a child and an adult — effectively the most conservative estimates of risk (i.e., they will result in the lowest soil cleanup concentration, as exposure includes that of the most sensitive human receptor).

The approach to formulating a PRG for a single chemical in a single medium (e.g., soil) is the derivation of the soil concentration that will yield either an "acceptable" carcinogenic risk level of 1×10^{-6} or an "acceptable" noncarcinogenic hazard quotient (HQ) of one (1.0). When the potential exists for risks to be generated from exposure to the same chemical in multiple media, an approach similar in rationale, yet slightly more complicated in application, is advocated. Risks associated with concurrent exposure to multiple media (i.e., soil and air), and typically more than one route of exposure (i.e., ingestion and inhalation), are considered in an additive manner. For example, if an adult ingests surficial soil from a given area on a site, while simultaneously inhaling volatile compounds emitted from the soil, the acceptable total carcinogenic risk level for a chemical via *both* exposure pathways would still be 1×10^{-6}, or a noncarcinogenic hazard index of 1.0. The calculation of the corresponding acceptable soil concentration must now incorporate the exposure information for both routes of intake.

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2. Soil PRGs for Potential Jet Fuel Indicators

a. Soil Cleanup Concentrations Based on Soil Ingestion

Using the PRG health risk-based approach, soil cleanup concentrations can be formulated for all chemicals with established toxicity values, for both noncarcinogenic and carcinogenic effects. The equations and assumptions used to calculate the noncarcinogenic PRG for soil based on soil ingestion are shown in Figure 2.

$$THI = \frac{C \times 10^{-6}\ kg/mg \times EF \times IF_{soil/adj}}{R_fD_o \times AT \times 365\ days/year}$$

$$C\ (mg/kg) = \frac{THI \times AT \times 365\ days/year}{1/R_fD_o \times 10^{-6}\ kg/mg \times EF \times IF_{soil/adj}}$$

where:

Parameter	Definition	Default Value
C	Chemical concentration (mg/kg)	None
THI	Target Hazard Index	1.0
R_fD_o	Oral chronic R_fD (mg/kg/day)	Chemical-specific
AT	Averaging time (years)	30 years (equal to exposure duration, incorporated in $IF_{soil/adj}$)
EF	Exposure frequency (day/yr)	350
$IF_{soil/adj}$	Age-adjusted ingestion factor (mg-yr/kg-day)	114

Reduced equation:

$$Risk\text{-}based\ PRG\ (mg/kg\ soil) = 2.7 \times 10^5\ (R_fD_o)$$

FIGURE 2. Residential PRG. Soil ingestion, noncarcinogenic equation.

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$$TR = \frac{SF_o \times C \times 10^{-6}\ kg/mg \times EF \times IF_{soil/adj}}{AT \times 365\ days/year}$$

$$C\ (mg/kg) = \frac{TR \times AT \times 365\ days/year}{SF_o \times 10^{-6}\ kg/mg \times EF \times IF_{soil/adj}}$$

where:

Parameter	Definition	Default Value
C	Chemical concentration (mg/kg)	None
TR	Target excess lifetime cancer risk	10^{-6}
SF_o	Oral slope factor $(mg/kg/day)^{-1}$	Chemical-specific
AT	Averaging time (years)	70
EF	Exposure frequency (day/yr)	350
$IF_{soil/adj}$	Age-adjusted ingestion factor (mg-yr/kg-day)	114

Reduced equation:

$$Risk\text{-}based\ PRG = \frac{0.64}{SF_o}$$

FIGURE 3. Residential PRG. Soil ingestion, carcinogenic equation.

Similarly, equations and assumptions for estimating the carcinogenic PRG for soil based on soil ingestion are shown in Figure 3. Soil PRGs are presented for potential TPH alternatives with established toxicity values, for both carcinogenic and non-carcinogenic toxic endpoints, in Table 10. For carcinogenic and noncarcinogenic effects, the most conservative soil cleanup concentration is considered to drive the risk. The TPH alternatives with the conservative soil PRG estimates are chrysene and benzene, with PRGs of 8.8 and 22 ppm, respectively, based on their carcinogenicity.

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TABLE 10
Soil Concentrations of Potential TPH Alternatives Associated With Maximum "Acceptable" Noncarcinogenic or Carcinogenic Human Health Effects From Soil Ingestion

Carcinogens:		
Chemical	Oral SF $(mg/kg/day)^{-1}$	Soil Concentration (ppm)
Benzene	2.9×10^{-2}	22
Chrysene (PAH)	0.073	8.8
Noncarcinogens:		
Chemical	Oral R_fD (mg/kg/day)	Soil Concentration (ppm)
Anthracene	3×10^{-1}	81,000
Ethylbenzene	1×10^{-1}	27,000
Fluoranthene	4×10^{-2}	10,800
Fluorene	4×10^{-2}	10,800
Naphthalene	4×10^{-2}	10,800
Pyrene	3×10^{-2}	8,100
Toluene	2×10^{-1}	54,000
Xylene	2×10^{0}	540,000

b. ***Soil Cleanup Concentrations for Soil Ingestion and Inhalation Exposure***

When compounds of concern include volatiles, the inhalation pathway can be included along with soil ingestion in the estimation of the soil PRG. USEPA does not specifically mandate this approach for future residential land use, although for industrial land use both pathways are considered for the onsite adult worker. It is not anticipated that risks associated with adult occupational exposure, even with the additional inhalation pathways, will exceed ingestion risks calculated for the child/adult receptor under residential land use. The inclusion of exposure via inhalation of volatiles or airborne particulates requires knowledge of site-specific information on the nature and extent of the soil volatiles contamination (e.g., area of the spill or distribution of volatile samples, depth to encounter of volatiles, air temperature, and regional wind speed, among others). For demonstrative purposes only, modified equations for potential use in estimating noncarcinogenic and carcinogenic soil industrial PRGs, based on ingestion and inhalation exposure routes, are shown in Figures 4 and 5, respectively.

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$$THI = \frac{C \times 10^{-6}\ kg/mg \times EF \times ED \times IR_{soil}}{R_fD_o \times BW \times AT \times 365\ days/year} + \frac{C \times EF \times ED \times IR_{air} \times (1/VF) \times (1/PEF)}{R_fD_i \times BW \times AT \times 365\ days/year}$$

$$C\ (mg/kg) = \frac{THI \times BW \times AT \times 365\ days/year}{ED \times EF \times [((1/R_fD_o) \times 10^{-6}\ kg/mg \times IR_{soil}) + ((1/R_fD_i) \times IR_{air} \times (1/VF + 1/PEF))]}$$

where:

Parameter	Definition	Default Value
C	Chemical concentration (mg/kg)	None
THI	Target Hazard Index	1.0
R_fD_o	Oral Chronic R_fD (mg/kg/day)	Chemical-specific
R_fD_i	Inhalation chronic R_fD (mg/kg/day)	Chemical-specific
BW	Adult body weight (kg)	70
AT	Averaging time (year)	25 (equal to ED)
EF	Exposure frequency (day/yr)	250
ED	Exposure duration (year)	25
IR_{soil}	Soil ingestion rate (mg/day)	50
IR_{air}	Inhalation rate (m^3/day)	20
VF	**Soil-to-air volatilization factor**	**Site, chemical-specific**
PEF	**Particulate emission factor (m^3/kg)**	**Site-specific**

Reduced Equation:

$$Risk\text{-}based\ PRG = \frac{102}{(5 \times 10^{-5}/R_fD_o) + ((1/R_fD_i) \times (20/VF)) + (1/PEF)}$$

FIGURE 4. Commercial/industrial PRG. Ingestion and inhalation, noncarcinogenic equation.

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$$TR = \frac{(SF_o \times C \times 10^{-6}\ kg/mg \times EF \times ED \times IR_{soil})}{BW \times AT \times 365\ days/year} + \frac{SF_i \times C \times EF \times ED \times IR_{air} \times (1/VF + 1/PEF))}{BW \times AT \times 365\ days/year}$$

$$C\ (mg/kg) = \frac{TR \times BW \times AT \times 365\ days/year}{EF \times ED \times [(SF_o \times 10^{-6}\ kg/mg \times IR_{soil}) + (SF_i \times IR_{air} \times (1/VF + 1/PEF))]}$$

where:

Parameter	Definition	Default Value
C	Chemical concentration (mg/kg)	None
TR	Target excess lifetime cancer risk	10^{-6}
SF_o	Oral slope factor $(mg/kg/day)^{-1}$	Chemical-specific
SF_i	Inhalation slope factor $(mg/kg/day)^{-1}$	Chemical-specific
BW	Adult body weight (kg)	70
AT	Averaging time (year)	70
EF	Exposure frequency (day/yr)	250
ED	Exposure duration (year)	25
IR_{soil}	Soil ingestion rate (mg/day)	50
IR_{air}	Inhalation rate (m^3/day)	20
VF	**Soil-to-air volatilization factor**	**Site, chemical-specific**
PEF	**Particulate emission factor (m^3/kg)**	**Site-specific**

Reduced Equation:

$$Risk\text{-}based\ PRG = \frac{2.9 \times 10^{-4}}{((5 \times 10^{-5}) \times SF_o) + (SF_i \times ((20/VF) + (1/PEF)))}$$

FIGURE 5. Commercial/industrial PRG. Ingestion and inhalation, carcinogenic equation.

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Site-specific parameters are indicated by bold, italicized text, to highlight the crucial role of site-specific input when considering the inhalation exposure route. The relationships between the PRGs and the site-specific parameters for the soil-to-air volatilization factor (VF) as well as the particulate emission factor (PEF) are similar (the greater the volatilization and the emission from soil, the lower the soil PRG). In the absence of site-specific information, no quantification of soil cleanup criteria is presented.

c. ***Soil Cleanup Concentrations for Inhalation Exposure Only***

Because of site specificity and the need for modeling of volatilization, partial derivation of a soil PRG based solely on the inhalation exposure route is demonstrated via illustration. Benzene is the only volatile compound that has an inhalation toxicity concentration. The unit cancer risk for benzene inhalation is 8.3×10^{-6} ($\mu g/m^3$) (corresponding to the lifetime risk associated with the continuous inhalation of a 1 $\mu g/m^3$ dose of benzene). A simple proportionality equation allows the determination of an air concentration corresponding to an acceptable benzene risk level of 1 × 10-6 (because 1 $\mu g/m^3$ yields a risk of 8.3×10^{-6}, what benzene concentration yields a risk of 1×10^{-6}?) equal to 0.12 $\mu g/m^3$ (0.037 ppb, using the benzene-specific conversion factor of 1 mg/m^3 = 0.31 ppm [ATSDR, 1991]). This same value was calculated by the USEPA (1990) in *Leaking USTs and Health*. However, estimating the soil concentration corresponding to this "acceptable" air concentration could be modeled *only* for a site-specific condition and exposure scenario, using site-specific input information.

d. ***Assumptions and Limitations of Soil PRGs Estimated for Potential TPH Alternatives***

Soil PRGs for potential TPH alternatives were estimated solely for comparative purposes and determination of which TPH alternative was the predominant risk driver. These PRGs correspond to an assumed future residential land use, and do not include the use of any nonstandardized exposure assumptions (i.e., all USEPA default values for exposure parameters were used; hence, the PRG estimates are not site specific and are fairly conservative). In the absence of USEPA-established CERCLA soil cleanup concentrations (ARARs) for BTEX (or TPH), and state-specific approaches and cleanup standards, the soil ingestion-based PRG may be a relevant consideration, but not necessarily the *final* consideration in setting a remediation standard in the ROD. Analysis of the predominant trend of the states toward establishing soil BTEX cleanup concentrations based on groundwater protection indicated great variability in stages of development and enforcement of this approach. Hence, use of more traditional health protective approaches (i.e., such as relying on soil ingestion as the primary exposure route, as opposed to deriving an "acceptable" soil concentration from a groundwater standard) may receive variable weight in a risk management decision-making process.

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e. ***Relative Soil Cleanup Concentrations***

The carcinogens chrysene and benzene yield the most conservative (i.e., lowest) soil PRGs (Table 10). Substantially more toxicity information exists for benzene, and the carcinogenic endpoint has been studied extensively for multiple routes of exposure. Definitive carcinogenic toxicity values have been established for benzene (the oral SF and the inhalation unit risk). Chrysene, on the other hand, has substantially less supporting toxicity information. In addition, it has been assigned a relative potency factor as a means of *adjusting* its carcinogenicity relative to that of benzo(*a*)pyrene. To date there is no definitive oral SF for chrysene. From the human health perspective, the overall weight of evidence for benzene carcinogenicity and the existence of recognized cancer SF information makes benzene a better candidate for a TPH alternative than chrysene.

B. **Summary of the Basis for Selection of Benzene as Indicator of Choice**

The physicochemical properties of benzene influencing its potential for groundwater impact, the magnitude of and scientific understanding of its toxicity, and the availability of an established toxicity value point to benzene as the alternative of choice for JP-4. Chrysene, the sole carcinogenic PAH in JP-4 considered as a possible alternative, is not as viable an alternative, given its less definitive cancer toxicity value, the lack of sufficient data regarding noncarcinogenic health effects, the absence of an MCL, and the smaller potential to impact groundwater. Naphthalene is not a viable choice, given the lesser magnitude of the toxicity associated with napthalene, the lack of an established toxicity value, and the lack of an MCL. The paucity of toxicity information for alkanes and the lack of established toxicity values for chronic adverse endpoints limits their consideration. This information, coupled with the demonstration of a benzene-driven soil PRG (the most conservative PRG), supports selection of benzene as the TPH alternative of choice.

V. **IMPLICATIONS OF BENZENE AS THE JP-4 JET FUEL INDICATOR FOR SOIL REMEDIATION**

A. **The Potential for Simultaneous Achievement of Benzene and TPH Soil Cleanup Concentrations — A Comparative Approach**

The degree of health and environmental protection that could be provided by the use of TPH soil cleanup concentrations at petroleum hydrocarbon-contaminated sites was compared to the degree of protection provided by cleanup of benzene to its soil PRG (a residual risk of 10^{-6}). A direct health risk-based comparison was not possible because of the inability to assess health risks for TPH and the lack of

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historical risk-based approaches to establishing TPH cleanup concentrations. The following two hypothetical illustrations demonstrate this point.

1. ***Remediation to a Conservative TPH Soil Cleanup Concentration (Detection Limit)***

Hypothesis 1: Cleaning up site soil to the conservative TPH method detection limit (10 ppm) will simultaneously achieve acceptable benzene risk levels.

To avoid site-specific complexities, several simplifying points and assumptions were used: (1) the estimated soil cleanup concentration for BTEX is driven by benzene, (2) soil ingestion is the principal exposure route, (3) a risk level of 10^{-6} is conservatively estimated to be achieved at a benzene soil concentration of 22 ppm (the benzene soil PRG), (4) the lowest soil cleanup level proposed by a state for TPH is 10 ppm (based on the current method detection level for TPH in soils), and (5) 100% of the TPH concentration is conservatively assumed to be benzene (e.g., the maximally detectable amount, 10 ppm, is solely due to benzene in surface soil). Using these assumptions, the most conservative TPH-based soil cleanup level, 10 ppm, will allow simultaneous achievement of the risk-based benzene soil PRG (22 ppm).

The hypothesis is limited by consideration of only the soil medium and an ingestion pathway. Factoring the groundwater medium (or air) or a groundwater-protective cleanup strategy into the illustration will impact the ability to cleanup to TPH background to allow achievement of benzene cleanup concentrations, in a site-specific manner. The second limitation involves the assumption that all TPH is benzene, a purposely erroneous stipulation used solely for "worst case" illustrative purposes (typically, jet fuel contains less than 18% of total benzenes [benzene and substituted benzenes], and extensive volatilization of these compounds follows any spill).

2. ***Remediation to a Benzene Health Risk-Based Soil Cleanup Concentration (PRG)***

Hypothesis 2: Cleaning up a site to a benzene 10^{-6} risk level (22 ppm) will achieve TPH cleanup to the method detection level (10 ppm).

If BTEX was considered to be 100% benzene and was cleaned up to the 10^{-6} risk level of 22 ppm in soil, the TPH method detection limit (10 ppm) may or may not be achieved. The bulk components of JP-4, the alkanes, may still be present in soil at a concentration greater than 10 ppm. If fuel release occurred substantially in the past, it is more likely that cleanup to a 10^{-6} benzene risk level would be protective of TPH, as fate and transport processes could result in reduction of the initial high TPH (alkane) levels. PAHs, the TPH components in soil (in addition

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to benzene) that possess significant toxicity (e.g., chrysene), are present in relatively small concentrations in JP-4 jet fuel, and are not expected to contribute extensively to TPH.

An alternative to this comparative approach could encompass a simplified cost-benefit analysis (i.e., remediation of 1 yd^3 of soil cleaned to a TPH cleanup level of 10 ppm vs. cleaned to a benzene [BTEX] cleanup level of 22 ppm), and could yield economic considerations. The potential for an acceptable benzene soil cleanup level to result in an acceptable TPH soil level, and vice versa, is best presented at the site-specific level, accounting for site-specific factors such as the type and nature of the fuel release, as well as the time from spill.

B. **The Potential for Alteration of the Benzene Risk-Based Soil Cleanup Concentration (PRG)**

The factors that most influence any risk-based cleanup concentrations (e.g., PRGs) for a chemical of concern are (1) the predetermined "acceptable" level of risk, (2) measures of toxicity, and (3) site-specific exposure parameters. As benzene carcinogenicity is anticipated to drive the site risk estimates, two components specifically examined in greater detail were the basis for the benzene SF and exposure assessment strategies that might be employed at Air Force JP-4 sites.

1. The "Acceptable" Human Health Risk Level

The target risk level for Superfund sites for carcinogenic effects is usually 1×10^{-6} (based on the NCP's point of departure for analysis of remedial alternatives) (USEPA, 1991a). However, the interpretation of this point of departure is based on the following: "For known or suspected carcinogens, acceptable exposure levels are generally concentration levels that represent an excess upper bound lifetime cancer risk to an individual of between 10^{-4} and 10^{-6}" (40 CFR Part 300). Thus, depending on site-specific conditions (e.g., severity of the biological effect, potency of the chemical of concern, size of the potentially exposed population, and degree of potential future exposure based on future land-use projections), 10^{-5} or 10^{-4} may be more appropriate predetermined levels of "acceptable" risk. In addition, state-specific interpretations of acceptable risk may vary as well (i.e., California, where "acceptable" equates to 10^{-5} risk levels), although non-CERCLA sites would be the best candidate sites for state jurisdiction taking precedence.

2. The Benzene Cancer Slope Factor

The USEPA's approach to deriving the cancer SF for benzene (USEPA, 1985b) is based on consideration of data obtained primarily from three epidemiology studies

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of workers exposed to benzene occupationally via inhalation (Ott *et al*., 1978; Rinsky *et al*., 1981; Wong *et al*., 1983). In all studies, the critical endpoint was cancer mortality attributable to leukemias. Information regarding the concentrations of benzene and durations of exposure were used to generate "dose groups" with benzene-related leukemia mortalities associated with each group, which were then used to derive dose-response curves. Finally, different cancer risk models were combined with different exposure parameters to generate cancer unit risks.* A final unit risk estimate of 2.6×10^{-2} ppm was converted by USEPA to an oral SF of 2.9×10^{-2} (mg/kg/d) (the value shown in Table 7), using standard conversion methods** (USEPA, 1989).

a. Potential for Alteration of the Benzene SF

Based on the current USEPA documentation on the derivation of the benzene SF (USEPA, 1985b) and consideration of additional studies that estimate SFs, the potential for appreciably altering the benzene SF is not anticipated to be significant.

Typical uncertainties associated with SF formulation are not applicable to the approach used for benzene. The benzene SF was estimated from human data, necessitating no interspecies extrapolation, and peer review suggests data were obtained from the best available human studies. Variable risk models (relative and absolute risk) and exposure metrics (cumulative and weighted-cumulative exposure) were used, and the traditional, conservative LMS model was not used. The benzene SF was presented as the geometric mean of the maximum likelihood estimates (MLEs), as opposed to the standard approach for estimating the SF as the 95th upper percentile bound.

Additional reports and papers (Paxton *et al.*, 1994a, b; Crump, 1994) have addressed the potential for alteration of the USEPA benzene SF. However, the extent to which these have been reviewed, either by external peer review or the USEPA, has not been directly ascertained. Therefore, for purposes of this paper, no alternate values or distributions are utilized.

3. Alternative Methods for Determining Exposure Estimates

a. Use of Site-Specific Exposure Parameters

Current USEPA exposure assessment methodology suggests a series of standard default exposure routes and assumptions for use with discrete current and future land use scenarios. While the exposure routes themselves may be applicable to a specific site, the majority of the standard exposure assumptions advocated for use

* The risk associated with a unit dose of benzene equal to 1 ppm.

** Conversion assumes 1 ppm benezene = 3.26 mg/m^3, adult body weight = 70 kg and adult inhalation rate = 20 m^1/d.

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in estimating chemical intakes are not site specific, nor are they necessarily the most current, relevant numerical values. Historically, the use of alternate standard assumptions or the development of site-specific assumptions has been met with varying degrees of acceptance by regulatory agencies, although the existing guidelines for use of these assumptions (USEPA, 1989, 1991b) and the guidelines regarding the formulation of site-specific PRGs (USEPA, 1991a) advocate site-specific information wherever possible. Site-specific information and exposure routes will vary with the location, magnitude, and nature of the spill or leak, as well as with the local human populations, regional topology and hydrogeology, and land use.

The potential for exposure of humans who come in contact with the site of a former JP-4 spill or leak can be influenced by factors such as (1) the identification of the current and future land uses at the site (e.g., current land use that is active, inactive, industrial, residential, or agricultural; future land use that is similar to current, or involves conversion to industrial, residential, or agricultural), (2) the identification of the human receptor of greatest concern under these land uses (e.g., a worker in an industrial setting, a child in a residential setting, or a farmer in an agricultural setting), (3) the physical nature of the site (e.g., heavily vegetated, bare topsoil, pavement, geographically limited access, fencing, depth to a potable aquifer; geological stratification), (4) the size/volume of the spill or leak, and (5) the age of the spill or leak. Site-specific considerations and the use of site-specific exposure parameters, whenever feasible, are crucial to the process of developing soil cleanup criteria that accurately reflect site risks.

b. ***The Monte Carlo Approach***

Most exposure estimates are a multiplicative combination of average, conservative, and worst case exposure assumptions that yield a point estimate for the intake of a chemical. There are three major disadvantages to this approach: (1) there is no way of knowing the actual degree of uncertainty and conservatism in an assessment (i.e., the exposure estimate, and subsequently the risk level, lacks a depiction of its inherent variation), (2) the selection of upper limit values for many exposure variables may result in scenarios that rarely occur (e.g., what is the likelihood of an individual ingesting the maximum soil amount per day, for every day of the maximum number of exposure days, for the maximum number of years the individual could live near site?), and (3) because many exposure variables are at or near their maxima, performing sensitivity analyses is of limited value. A distributional approach to exposure estimates, such as a Monte Carlo simulation* approach, is a viable alternative to point estimation.

Monte Carlo simulation is a procedure for solving problems involving random variation (chance or probability) where time does not play a major role (Law and Kelton, 1982; Hillier and Lieberman, 1986). While it has been widely used by

* There are three classes of methods generally used for simulating exposure under uncertainty: (1) sensitivity analysis, (2) probabilistic error propagation, and (3) fuzzy sets. Monte Carlo simulation is in the class of probabilistic ewrror propagation (Lipton and Shaw, 1992).

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statisticians, systems analysts, and engineers for many years for problems that are not amenable to solution by experimentation (e.g., estimating critical values, the power of a new hypothesis test, and the effect of uncertainty on complex systems), its use in human health risk assessment is relatively recent (e.g., Burmaster *et al*., 1990; ENVIRON, 1991; Burmaster and von Stackelberg, 1991; Hawkins, 1991; RiskFocus, 1990, 1991a, b). Monte Carlo simulation can be used to estimate distributions for exposure assumptions without altering the basic structure of the exposure estimate as first described by the National Research Council (1983).

In both the "traditional" and Monte Carlo approaches to exposure assessment, the analyst first constructs a model for a chemical-specific LADD (*intake*), consisting of relationships between random variables. In the "traditional" approach to risk assessment, point estimates for each of the variables in the intake equation are chosen (e.g., the 95th percentile upper confidence limit on the mean of the groundwater sample concentrations, the 90th percentile of the distribution of adult water consumption), yielding a point estimate of intake for which, because different percentiles are used,* it is not possible to know what *combined* percentile to assign to the overall expression of intake. In a Monte Carlo simulation model, the analyst determines a continuous or discrete distribution for each of the random variables in the model's intake equation, defined in terms of the probability density function (PDF) or the cumulative distribution function (CDF). Input values for each exposure variable are randomly selected from the appropriate distributions and used to derive an intake estimate, a process that is repeated thousands of times to yield a distribution of daily intakes. From this intake distribution, a specific intake can be selected (e.g., the average or mean intake, median intake, or 95th percentile upper confidence limit on the intake) that, in combination with the appropriate toxicity value, can be used to calculate risk.

A workshop cosponsored by USEPA and the University of Virginia attempted to assess the state of the art in selecting input distribution functions (emphasizing their application to environmental risks) and to establish theoretically sound and defensible foundations on which to generate future guidelines for USEPA use in the selection of probability distributions (UVA, 1993). The issue papers and workshop participants concluded that the selection of the input distributions is critical and attempted to propose means to advance the state of the art. There was no consensus on the use of specific distributions, the exception being mutual agreement on the need for use of scientifically defensible, rationally chosen, site-specific distributions.

c. Application of the Monte Carlo Approach to Groundwater Ingestion

A comparison of point estimation and Monte Carlo simulation of LADD and cancer risk is performed for a hypothetical site where groundwater is the medium

* In some cases *no* distribution-based percentiles are used, such as an exposure frequency of 350 d per year based on the assumption that people are away from home 2 weeks per year.

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of concern and offsite residents are the population of concern based on their use of groundwater contaminated with benzene (assumed present at the MCL, 5 ppb) as a drinking water source. Point and distributional intakes are derived using the USEPA model for intake of a compound via ingestion of water (USEPA, 1989; Equation 8)):

$$\text{Intake} = \frac{\text{CW} \times \text{IR} \times \text{EF} \times \text{ED}}{\text{BW} \times \text{AT}} \tag{3}$$

where:

Intake	intake (mg/kg/d)
CW	chemical concentration in water (mg/l)
IR	ingestion rate (l/d)
EF	exposure frequency (d/year)
ED	exposure durations (years)
BW	body weight (kg)
AT	averaging time (d)

Figure 6 presents the input for deriving the standard, point estimate for groundwater intake (LADD), with a benzene concentration of 5 ppb. Figure 7 presents the input distribution variables used in a Monte Carlo estimation of groundwater intake. The point estimate of the LADD, 5.9×10^{-3} mg/kg/d (Figure 6), corresponds to greater than the 100th percentile on the distributional analysis (1.6×10^{-4}, off scale) in Figure 8. If the 95th percentile was of interest, the resulting estimate from the distributional analysis would be 4×10^{-5} mg/kg/d, a much lower (147-fold) exposure estimate than the point estimate. The effect of the distributional analysis on the risk estimate is shown in Figure 9. The cancer risk estimated by use of the point estimate LADD and the benzene oral SF is 1.7×10^{-4} (essentially 2×10^{-4}) (Figure 6), while the 95th percentile for the cancer risk based on the distributional LADD analysis (Figure 9) would predict 1.2×10^{-6} (essentially 1×10^{-6}). This is effectively a 200-fold reduction in risk from the simple point estimate approach.

Lloyd *et al.* (1992) used a Monte Carlo simulation to evaluate the New Jersey Department of Environmental Protection and Energy (NJDEPE) approach for calculating residential surface soil cleanup standards for benzene. The authors considered only a soil ingestion pathway. The NJDEPE point estimate for the benzene cleanup concentration is 3 mg/kg, which is well below the 1st percentile of the overall distribution determined by Lloyd *et al*. This indicates that greater than 99% of all cleanup standards generated by the distribution approach are greater than 3 mg/kg, making the NJDEPE estimate a very conservative value. A similar type of distributional evaluation of the NJDEPE benzene soil cleanup standard was conducted by Gephart *et al*. (1994) using an emerging distributional sampling technique called Latin hypercube. Results indicated that 89.5% of the cleanup values were greater than 3 mg/kg, supporting the Monte Carlo predictions.

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Point estimate:

$$LADD = \frac{0.005\,mg/\ell \times 2.0\,\ell/day \times 350\,days/year \times 30\,years}{70\,kg \times 70\,years \times 365\,days/year} = 5.87 \times 10^{-5}\ mg/kg/day$$

$$Cancer\ risk = 5.87 \times 10^{-5}\,mg/kg/day \times 0.029\,(mg/kg/day)^{-1} = 1.7 \times 10^{-6}$$

FIGURE 6. Calculating LADD and cancer risk using point estimates.

VI. CONCLUSIONS AND FUTURE DIRECTIONS

There is no established USEPA regulatory policy for BTEX or TPH soil cleanup concentrations, to date, although work is ongoing toward establishing guidelines for soil cleanup concentrations based on protection of groundwater. Cleanup typically falls under state jurisdiction, which entails variable state-specific approaches to setting BTEX and/or TPH soil cleanup levels. State-specific soil cleanup concentrations for BTEX are based primarily on protection of human health via protection of groundwater and/or protection of human health for the more traditional soil ingestion route. State-specific soil cleanup concentrations for TPH are based primarily on consideration of one or more BTEX components in specific fuels with extrapolation to corresponding TPH concentrations, as well as approaches with decreasing scientific bases.

Among the potential alternatives for TPH at JP-4 spill sites, benzene appears most appropriate based on its toxicity (carcinogenicity), weight-of-evidence cancer classification (Class A carcinogen), mobility in the environment, potential for migration to groundwater, and presence at numerous JP-4-contaminated sites (using the U.S. Air Force Installation Restoration Program Information Management System [IRPIMS] database, in conjunction with historical information on JP-4 site-specific contamination provided by U.S. Air Force IRP project managers, both benzene and TPH were present at a minimum of 40% of these sites). Based on these parameters, risk-based soil cleanup concentrations based on BTEX tend to be driven by benzene, and risks associated with exposure to benzene in groundwater used as a drinking water source are anticipated to dominate risks from benzene in other media. However, if faced with the need for regulatory compliance with both BTEX and TPH cleanup standards, remediation to a benzene soil cleanup concentration will not necessarily achieve simultaneous TPH soil cleanup.

Benzene cancer risk is determined from the benzene SF and potential for exposure. When the potential for alteration of benzene risk-based cleanup concentrations is explored by examining components of toxicity and exposure that can

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Scenario: Ingestion of benzene in water

$$LADD = \frac{C \times IR \times EF \times ED}{BW \times LS \times CF}$$

where:

LADD	=	Lifetime Average Daily Dose (mg/kg/day)
C	=	Concentration (mg/liter)
IR	=	Ingestion rate (liters/day)
EF	=	Exposure frequency (days/year)
ED	=	Exposure duration (years)
BW	=	Body weight (kg)
LS	=	Life span (years)
CF	=	Conversion factor (365 days/year)

$$Cancer\ risk = LADD \times CPF$$

where:

LADD	=	Lifetime Average Daily Dose (mg/kg/day)
CPF	=	Cancer potency factor $(mg/kg/day)^{-1}$

Input distributions:

C	Point value (5×10^{-3} mg/L; benzene MCL)
IR	Cumulative[1] (Min = 0.4, Max = 2; 19.2 % = 0.4, 39.6 % = 0.96, 60 % = 1.28, 80 % = 1.7, 100 % = 1.96)
EF	Triangular (minimum = 250, most likely = 350, maximum = 365)
ED	Cumulative[1] (Min = 1, Max = 75; 25 % = 4, 50 % = 8, 75 % = 15, 90 % = 26, 95 % = 33, 100 % = 47)
BW	Equal chance of selecting male or female body weight Male (ln lb): Lognormal)[1] ($\mu = 5.13$, $\sigma = 0.17$) Female (ln lb): Lognormal[1] ($\mu = 4.96$, $\sigma = 0.20$)
CPF	Point value ($(0.029\ mg/kg/day)^{-1}$)

[1] Distributions from Exposure Factors Sourcebook, American Industrial Health Council (AIHC, 1994)

FIGURE 7. Estimating a distribution of human daily intakes.

influence risk estimates, two points are apparent: the potential for appreciably altering the benzene SF is not anticipated to be significant and there is no scientific consensus on use of specific distributions of exposure parameters. However, scientifically defensible, rationally chosen, site-specific distributions should be used to estimate exposure.

Based on the conclusions of this study, several alternatives to the use of TPH cleanup standards for JP-4 jet fuel-related soil remediation present themselves, as

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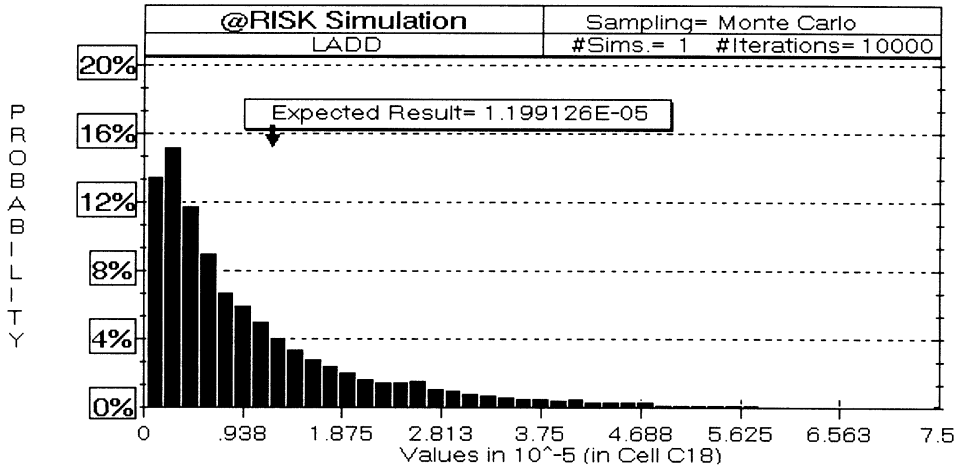

FIGURE 8. Distribution vs. point estimate of a groundwater to drinking water LADD.

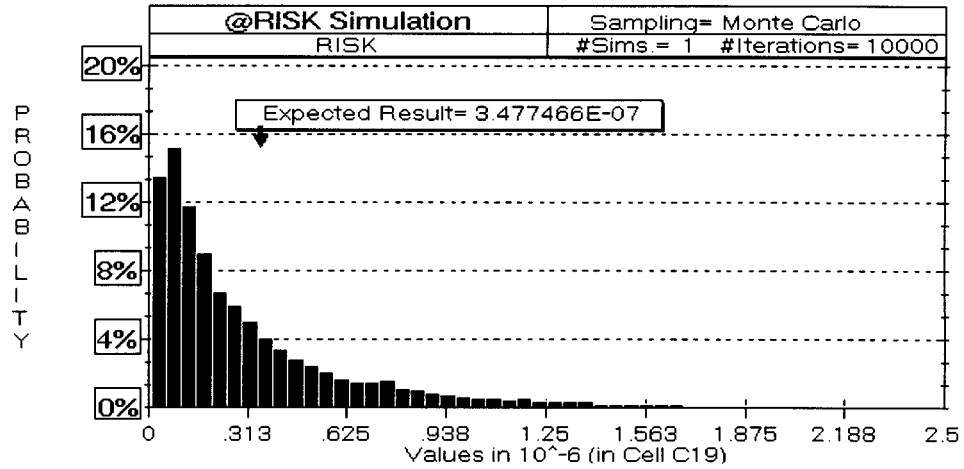

FIGURE 9. Distribution vs. point estimate of a groundwater to drinking water cancer risk.

well as implications for non-JP-4 petroleum products. Whether they relate to JP-4 fuel or to other petroleum products, the issues of their utility and applicability as short-term vs. long-term solutions remain to be considered. Short-term considerations, specifically in the case of JP-4, could include the adaptation of benzene as a TPH alternative. Research and funding efforts could focus on formulating a scientifically sound approach to soil cleanup concentrations for benzene, amenable to site-specific manipulation, based on protection of groundwater. A cost-benefit analysis could be undertaken for soil remediation of benzene and TPH, using

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current, acceptable remediation methods and applying a site-specific approach, to provide an economic basis for comparison of either standard. Considerations for the long term could include focusing research and funding efforts on the characterization of TPH, including chemical characterization, potential toxic effects, fate and transport, and the utility of TPH in the risk assessment process. Whether TPH is considered a methodological entity, discrete petroleum products, chemical subsets of TPH, or as individual compounds, a comprehensive evaluation should enable the pinpointing of specific areas that warrant targeted research efforts aimed at filling data gaps.

Several questions germane to the establishment of cleanup standards for fuels or petroleum products in general can be posed. (1) Do compounds that remain associated with soils at fuel or petroleum product spill sites (the effective non-BTEX components of TPH) warrant their own standards, and should their basis be founded on health, aesthetics, or other considerations? In the face of a dearth of information on health effects for many alkane components of fuels, informed decision-making is hindered. (2) Should there be specific standards for individual petroleum products? Certain state-specific soil cleanup goals already take into consideration the nature of the fuel (i.e., gasoline vs. diesel), based on their variable composition. The results of an evaluation of alternatives to a TPH standard performed for a fuel other than JP-4 would have a different result than that presented here. For fuels with high concentrations of high molecular weight, carcinogenic PAHS, for example, benzene could not be the sole indicator compound. (3) If TPH is retained as a soil cleanup standard, should there be provisional soil cleanup standards specific for the age, and more importantly, the depth of the spill or leak? TPH for surficial soil remediation will not be comprised of the same subset of chemicals as TPH in subsurface soil. Ongoing and future research should provide answers to these and other questions. Currently a national effort is underway, in the form of the TPH Criteria Working Group (TPHCWG), to analyze the present state of the science for TPH and to assess current methods for defining TPH and their implications for remediation.

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