Sources Of Toxicity Values
For Constituents Of Motor Fuels
Relevant To Leaking Underground Storage Tank
Site Characterization and Risk Assessment

U.S. Environmental Protection Agency
Office of Land and Emergency Management
Office of Underground Storage Tanks
Washington, D.C.

December 2019

DISCLAIMER

This document provides technical information to EPA, state, tribal, and local agencies. This document does not impose any requirements or obligations on EPA, states, or local or tribal governments, or the regulated community. Please make decisions regarding a particular situation based on statutory and regulatory authority. Decision-makers retain the discretion to use the information contained in this document as they deem necessary and appropriate.

Contents

Introduction

Purpose, Scope, And Applicability

Federal, state, and international agencies develop chemical toxicity values[1] for a variety of risk assessment purposes. However, the various sources of toxicity values may not be familiar to broad audiences. Thus, the U.S. Environmental Protection Agency's (EPA's) Office of Underground Storage Tanks (OUST) and senior scientists in the Office of Land and Emergency Management (OLEM)[2], collaborated on developing this document and the appendices to provide the Regions, states, and tribes with a consolidated reference of toxicity values. The Appendices provide methodology for developing risk-based screening values for a select group of constituents of motor fuels, that is gasoline and diesel fuel, that may be of concern (especially due to the potential for vapor intrusion) at leaking underground storage tank (UST) sites.

Although EPA developed this document primarily to be used for typical UST sites, users may find it helpful when addressing petroleum contamination at non-UST sites. Some of these sites may include refineries, petrochemical plants, terminals, aboveground storage tank farms, pipelines, and large scale fueling and storage operations at federal facilities, or sites with releases of non-petroleum chemicals including landfills, hazardous waste disposal sites, and sites with comingled plumes of petroleum and chlorinated solvents. Other OLEM program offices – the Office of Superfund Remediation and Technology Innovation (OSRTI), Office of Resource Conservation and Recovery (ORCR), Federal Facilities Restoration and Reuse Office (FFRRO), and Office of Brownfields and Land Reuse (OBLR) – may address these sites.

This document provides information on the different sources of toxicity values, criteria on selecting appropriate toxicity values, other non-EPA led efforts to increase consistency and transparency in selecting toxicity values for hazardous waste and cleanup sites. EPA recognizes that, because of the size and diversity of the regulated community, states are in the best position to implement their own UST programs. The federal UST program does not prescribe human health values for contaminants; implementing authorities should use toxicity values appropriate for the contaminants present, the specific characteristics of exposure, for example residential vs industrial, and the routes of exposure, for example inhalation, ingestion, dermal absorption.

---

[1] A numerical expression of a substance's exposure-response relationship that is used in risk assessments (see *Risk Assessment Guidance for Superfund, Volume I: Human Health Evaluation Manual (Part A) Interim Final* (EPA/540/1-89/002 December 1989), Chapter 7, *Definitions for Chapter 7*, p.7-3. *https://www.epa.gov/sites/production/files/2015-09/documents/rags_a.pdf*)

[2] OLEM was formerly known as the Office of Solid Waste and Emergency Response (OSWER).

Constituents of Motor Fuels

Motor fuels typically consist of a complex and variable mixture of petroleum hydrocarbons and are classified as chemical substances of unknown or variable composition, complex reaction products or biological materials (UVCB) (OECD, 2016).[3] The variability of the substances in terms of chemical identity, properties and percent makes them difficult to assess for hazard, exposure and risk. Table 1 lists a number of constituents of motor fuels, but this is not an exhaustive list of chemicals because motor fuels are comprised of hundreds of individual compounds. Petroleum hydrocarbons (PHCs) present in petroleum fuels generally belong to one of two major groups: aromatics and aliphatics. The aromatic PHCs are characterized as having one or more benzene rings. Benzene, toluene, ethylbenzene, and the three isomers of xylene are collectively referred to as BTEX; each of these has only a single benzene ring. Naphthalene is a polycyclic aromatic hydrocarbon (PAH) that is comprised of two benzene rings. The aliphatics are non-aromatic PHCs consisting of straight-chains, branched chains, or nonaromatic rings. Examples of aliphatic hydrocarbons are the groups the alkanes, the alkenes, and the alkynes.

Although BTEX represent the group of PHCs that receive the most attention at typical leaking UST sites, they are not the only compounds that may pose a risk to human health. Petroleum fuels may also contain a variety of non-PHC volatile organic chemicals (VOCs) as additives to enhance performance. For example, fuel oxygenates have typically been ethers – such as diisopropyl ether (DIPE), and methyl-tertiary-butyl ether (MTBE) – or alcohols – such as ethanol and tertiary-butyl alcohol (TBA). At typically older UST sites where leaded gasoline from leaks or overfills was released into the environment, in addition to the organic lead compounds tetraethyl lead (TEL) and tetramethyl lead (TML), the lead scavengers ethylene dibromide (EDB), and 1,2-dichloroethane (1,2-DCA), may also be present.[4] Other PHCs, for example naphthalene, may also pose a risk to human health.

Overview Of Toxicity Values

There are different types of toxicity values, and depending on the type of values, and the units, they are used differently. Toxicity values generally represent an exposure rate that identifies the amount of a substance that one may be exposed to per unit of time (for example milligrams per kilogram per body weight per day (mg/kg bw-day). Carcinogens are generally represented by the increase in risk per unit increase in exposure, such as increased risk per mg/kg bw-day or microgram per cubic meter ($\mu g/m^3$). To estimate risk, these toxicity values are used in equations that combine the toxicity value with exposure factors, for example, the amount ingested, inhaled or absorbed; the receptor's body weight; and the frequency and duration of the exposure.

---

[3] For more information about UVCBs see: EPA (2015c) accessible at *https://www.epa.gov/sites/production/files/2015-05/documents/uvcb.pdf*, Clark, et al. (2013), and Swick, et al. (2013).

[4] Leaded gasoline for on-road automotive fuel was phased-out in 1996; however, it is still used for certain off-road applications such as automobile racing and in aviation fuel (Avgas).

To complicate matters, there are a variety of adjustments to the data that may be made. Some toxicity values are based on laboratory animal studies, and the doses or concentrations have been adjusted to account for the differences between lab animals and humans; for example,

Table 1. Selected Constituents Of Motor Fuels.

Chemical Name [synonyms]	CASRN
Benzene [Benzol, Phenyl Hydride]*	71-43-2
n-Butanol [1-Butanol, Butyl alcohol, 1-Hydroxybutane, n-Propyl carbinol]*	71-36-3
Ethylene dibromide (EDB) [1,2-Dibromoethane, Ethylene bromide, Glycol dibromide]*	106-93-4
Ethylene dichloride (EDC) [1,2-Dichloroethane (1,2-DCA), Ethylene chloride, Glycol dichloride]*	107-06-2
Diisopropyl Ether (DIPE) [Isopropyl ether, Diisopropyl oxide, 2-Isopropoxy propane]*	108-20-3
Ethanol [Alcohol, Cologne spirit, Ethyl alcohol, EtOH, Grain alcohol]*	64-17-5
Ethyl Tert-Butyl Ether (ETBE) [2-Ethoxy-2-methylpropane, Ethyl 1,1-dimethylethyl ether]*	637-92-3
Ethylbenzene [Ethylbenzol, Phenylethane]*	100-41-4
Isobutyl Alcohol (IBA) [Isobutanol, Isopropylcarbinol, 2-Methyl-1-propanol]*	78-83-1
Isooctane [2,2,4-trimethylpentane, Isobutyltrimethylmethane]*	540-84-1
Methanol [Carbinol, Methyl Alcohol, Wood Alcohol]*	67-56-1
Methylcyclopentadienyl manganese tricarbonyl (MMT) [CI-2, Combustion Improver-2, Manganese tricarbonylmethylcyclopentadienyl, 2-Methylcyclopentadienyl manganese tricarbonyl]*	12108-13-3
Methyl tert-Butyl Ether (MTBE) [tert-Butyl methyl ether, Methyl-1,1-dimethylethyl ether, 2-Methoxy-2-methyl propane]*	1634-04-4
Naphthalene [Naphthalin, Tar camphor, White tar]*	91-20-3
Tertiary Amyl Ethyl Ether (TAEE) [2-Ethoxy-2-methylbutane; Ethyl tert-pentyl ether; Ethyl tert-amyl ether; 2-Ethyl-2-ethoxypropane]#	919-94-8

Chemical Name [synonyms]	CASRN

Tertiary Amyl Methyl Ether (TAME)
  [tert-Pentyl methyl ether; 1,1-Dimethyl propylmethyl ether; Methyl-tert-
  pentyl ether]*
	994-05-8

Tertiary Butyl Alcohol (TBA)
  [tert-Butyl alcohol; 2-Methyl-2-propanol;Trimethyl carbinol; 2-
  Methylpropan-2-ol; 1,1-Dimethylethanol]*
	75-65-0

Tetra Ethyl Lead (TEL) [Lead tetraethyl; Tetraethylplumbane]*	78-00-2
Tetra Methyl Lead (TML) [Tetramethylplumbane]*	75-74-1
Toluene [Methyl benzene, Methyl benzol, Phenyl methane, Toluol]*	108-88-3
1,2,3-Trimethylbenzene [Hemellitol, Hemimellitene]*	526-73-8
1,2,4-Trimethylbenzene [Pseudocumene]*	95-63-6
1,3,5-Trimethylbenzene [Mesitylene, Symmetrical trimethylbenzene, sym-Trimethylbenzene]*	108-67-8
Xylenes (mixture of 3 isomers below) [dimethylbenzene; Methyl toluene; Xylol]@	1330-20-7
Meta-Xylene [m-xylene; 1,3-Dimethylbenzene; m-Xylol]*	108-38-3
Ortho-Xylene [o-xylene; 1,2-Dimethylbenzene; o-Xylol]*	95-47-6
Para-Xylene [p-xylene; 1,4-Dimethylbenzene; p-Xylol]*	106-42-3
Synonyms sources: *NIOSH Pocket Guide to Chemical Hazards (https://www.cdc.gov/niosh/npg/default.html) #NIST Chemistry WebBook (http://webbook.nist.gov/chemistry/) @New Jersey Department of Health – Hazardous Substance Fact Sheet (http://nj.gov/health/eoh/rtkweb/documents/fs/2014.pdf)	

they are adjusted to reflect human equivalent doses, sometimes abbreviated as HED. In other instances, they are not adjusted. Some toxicity values are adjusted for general public exposures, for example 24 hours per day, 7 days per week for 70 years, while others may be adjusted to reflect worker exposures, for example 8 hours per day, 5 days per week, 50 weeks per year for 30 years. Finally, some toxicity values incorporate uncertainty factors to account for what is not known about the toxicity, while others do not. The point is not to suggest that some values are necessarily better than others, rather, it is important to understand the basis

for the derivation of the toxicity values, as these reflect certain assumptions regarding the exposure scenario and receptors, and therefore you may need to account for differences between the toxicity values and your scenario of interest.

There are also different levels of vetting of toxicity values. Some toxicity values are based on rigorous and transparent analytical processes, with extensive peer and public review, for example EPA IRIS assessments. Other toxicity values are derived from less rigorous procedures, but still may be useful for screening purposes or to bound uncertainties due to data gaps, for example toxicity values pulled from the literature or derived from analogue data or read-across techniques.

There are multiple sources of, and approaches to selecting, toxicity values for use in risk characterization. This document provides a brief overview (with links to related information) of the sources and approaches listed below:

- Toxicity values from government sources, such as EPA, Canada, the European Union (EU), and various state agencies.
- Toxicity values from published, peer-reviewed literature.
- Unpublished toxicity values derived from toxicological studies.
- Use of analogue data and category approaches.
- Qualitative approaches based on structural alerts.

Appendices A through D provide methodology on calculating risk-based screening levels. These Appendices are intended to offer options for selecting sources for toxicity information and do not dictate the use of calculated values, or the equations themselves, by any particular UST program. Appendix A provides equations for calculating target screening levels for contaminants in indoor air. Appendices B, C, and D provide methodologies for calculating screening values for groundwater, soil gas, and soil, respectively, by back-calculating from a target indoor air concentration derived by using the equations in Appendix A. This approach produces site-specific screening levels that can be compared to actual, measured concentrations in groundwater, soil gas, and soil. As these media samples are typically collected during site characterization, additional sampling –for example indoor air sampling – may not be necessary if measured concentrations at the site are below the respective calculated screening levels. Appendix E lists all of the sources of information cited in this document in alphabetical order with hyperlinks.

Regulatory And Screening Level Risk-Based Concentrations

Some programs use toxicity values to derive concentrations that incorporate exposure assumptions, which can then be compared to measurements or estimates of contaminants in different environmental media. These values may be regulatory, such as a maximum contaminant level (MCL) for drinking water, in terms of milligrams per liter (mg/L), or screening level, such as the risk screening levels (RSL) derived for use in the Superfund Program. If you have an MCL or RSL, you may need only to compare the measured or predicted concentration

in the media to the derived risk-based concentration to determine if it exceeds the risk-based level.

The toxicity values and media-specific concentrations can both be useful in assessing risk, but it is important to know what you are dealing with, for example rate or concentration, and pay particular attention to the units as these direct how to calculate risk.

The OLEM Toxicity Value Hierarchy

The Office of Land and Emergency Management (formerly EPA's Office of Solid Waste and Emergency Response or OSWER), which houses the federal UST program, issued a 2003 memorandum that recommends hierarchy of toxicity values for use by the Superfund program; *Human Health Toxicity Values In Superfund Risk Assessments* (OSWER Directive 9285.7-53). The 2003 memorandum outlined a three-tiered hierarchy of toxicity values:

- Tier 1 – EPA's Integrated Risk Information System (IRIS)
- Tier 2 – EPA's Provisional Peer-Reviewed Toxicity Values (PPRTVs)
- Tier 3 – Other Toxicity Values

These recommendations described below were developed for EPA's Superfund program, not the UST program, but are considered appropriate to use for selecting toxicity values when addressing contamination at leaking UST sites.

Tier 1: Integrated Risk Information System Toxicity Values

EPA's Integrated Risk Information System (IRIS) toxicity values are generally the preferred source of human health toxicity values; they represent the highest quality science based human health assessments regarding the toxicity of chemicals. The IRIS database contains compound-specific hazard identification and dose-response assessments and, for a given compound, may include one or more toxicity values including reference dose (*RfD*), reference concentration (*RfC*), drinking water unit risk value, cancer slope factor, and inhalation unit risk (*IUR*) value. They are generally based on laboratory animal data and may include adjustments to derive human equivalent doses or concentrations. These assessments undergo internal peer review, interagency review, and public comment, as well as an external panel peer review that is open to the public. Unfortunately, not all chemicals have IRIS assessments, nor do all IRIS assessments have a full suite of toxicity values, that is cancer and non-cancer for dermal, inhalation, and oral routes of exposure, and IRIS only contains chronic exposure values.

Tier 2: Provisional Peer Reviewed Toxicity Values

Provisional peer reviewed toxicity values (PPRTVs) are the second tier of OLEM human health toxicity values in the recommended hierarchy for the Superfund and Resource Conservation and Recovery Act (RCRA) hazardous waste programs. PPRTVs are developed by the Superfund

Health Risk Technical Support Center (STSC)[5] for chemicals that do not have IRIS values or are for less than chronic durations of exposure[6]. The STSC derives the values following a thorough literature review using generally the same methods, sources of data, and guidance the IRIS program uses, but the chemicals developed into PPRTVs typically have smaller databases of information. As with the IRIS toxicity values, they may include reference doses, reference concentrations, cancer slope factors, or inhalation unit risk values. They are generally based on laboratory animal data and may include adjustments to derive human equivalent doses or concentrations. PPRTVs are, like IRIS values, internally and externally peer reviewed. However, unlike IRIS values, PPRTVs are developed specifically for the Superfund program and are intended to be provisional; when an IRIS value becomes available, any existing PPRTV is removed from the database. In fall 2009, EPA began to include appendix screening values to the assessments where the data did not support development of a PPRTV, but they were sufficient to allow derivation of quantitative estimates with greater levels of uncertainty. EPA has less confidence in provisional screening toxicity values than PPRTVs and they Tier 3 values.

Tier 3: Other Toxicity Values

Tier 3 includes additional EPA and non-EPA sources of toxicity information. These may include toxicity values developed by other federal – such as Agency for Toxicity and Disease Registry, Occupational Safety and Health Administration – or state agencies – such as California Environmental Protection Agency, Hawai'i Department of Health, Massachusetts Department of Environmental Protection, New Jersey Department of Environmental Protection, and Washington Department of Ecology – or they may come from other countries, such as the European Union, Canada, and Australia.

Because several relevant Tier 3 values may be available for a given chemical, it may be necessary to determine a preferred value. It is important to recognize that there are similarities and differences in the way organizations develop toxicity values. When evaluating potential toxicity values, give priority to sources that provide information based on similar methods and procedures as those use for Tier 1 and Tier 2, such as methods, sources, transparency, peer review, and contain values that are peer reviewed and publicly available. It is also important to be mindful of the basis for the derivation of the toxicity value, as discussed above, such as

---

[5] The STSC is managed by the U.S. EPA's National Center for Environmental Assessment (NCEA) in Cincinnati, Ohio. The STSC provides technical support to EPA program and regional offices in the area of human health risk assessment. Examples include the development of Provisional Peer-Reviewed Toxicity Value (PPRTV) assessments, scientific consultations, and support for interpreting U.S. EPA publications and other guidance, and risk assessment methods research on chemical pollutants. For further information, contact 513-569-7300.

[6] IRIS usually only provides chronic toxicity values, but PPRTV's are also derived for subchronic exposure durations.

occupational, general population or consumer; acute, subchronic, chronic, to make sure it is applicable and sufficiently protective for the scenario of interest.[7]

Two notable efforts attempt to improve the consistency and transparency of processes used for selecting toxicity values:

- In 2007, The Environmental Council of the States (ECOS) released an issue paper *Identification and Selection of Toxicity Vales/Criteria for CERCLA and Hazardous Waste Site Risk Assessments in the Absence of IRIS Values*. This paper provides guidance and a suggested framework, in the form of seven recommendations, for identifying and selecting toxicity values when IRIS values are not available. The ECOS paper stresses that risk assessors should continue to identify the most scientifically defensible toxicity value and that the selecting individuals have a robust understanding of the available sources of toxicity data and their strengths and weaknesses so that the most appropriate toxicity value is selected.
- In 2013, OSWER released the *Tier 3 Toxicity Value White Paper*, which provides recommendations on processes to improve the transparency and consistency for identifying, evaluating, selecting, documenting, and communicating Tier 3 toxicity values. The white paper does not provide a ranking of Tier 3 sources. Instead, it recommends that priority be given to toxicity values:
    - derived using hazard identification and dose-response assessments that are consistent with EPA methodologies,
    - from sources that are transparent about the methods and processes used to develop values,
    - are publicly available, and
    - that have undergone peer review.

Be cautious using toxicity values that do not meet these criteria.

Potential sources of Tier 3 toxicity values include but are not limited to:

Agency For Toxic Substances And Disease Registry (ATSDR). ATSDR calculates minimal risk levels (MRLs), which are estimates of daily human exposure to a hazardous substance that is likely to be without appreciable risk of adverse non-cancer health effects over a specified duration of exposure. These substance-specific estimates, which are intended to serve as screening levels, are used by ATSDR health assessors and other responders to identify contaminants and potential health effects that may be of concern at hazardous waste sites.

---

[7] The Health Effects Assessment Summary Tables (HEAST) is one example of an outdated database. It contains older information on chemicals of interest to Superfund and the Resource Conservation and Recovery Act (RCRA). HEAST values are no longer being generated or reviewed. Unlike IRIS or PPRTV values, not all HEAST values went through formal peer review or an EPA review process, and interim values are also included in the tables. EPA does not recommend using them.

EPA Program Offices. Other program offices in EPA may derive toxicity values or employ toxicity values derived by others to develop regulatory criteria or screening values. Assessors may have to mine the documentation to identify relevant toxicity values. EPA program offices include:

- Office of Water, which provides Human Health Criteria that include the derivation of toxicity values: https://www.epa.gov/wqc/national-recommended-water-quality-criteria-human-health-criteria-table.
- Office of Air and Radiation, which provides Dose-Response Assessments for Hazardous Air Pollutants: https://www.epa.gov/fera/dose-response-assessment-assessing-health-risks-associated-exposure-hazardous-air-pollutants
- Office of Chemical Safety and Pollution Prevention, which addresses chemicals under the Toxic Substances Control Act (TSCA): https://www.epa.gov/chemicals-under-tsca.

State Agencies. Several state agencies developed toxicity values for various petroleum hydrocarbons and other chemicals. These state agencies include, but are not limited to:

- California Office Of Environmental Health Hazard Assessment (OEHHA): Toxicity Criteria Database.
- Hawai'i Department of Health: Environmental Hazard Evaluation (EHE) and Environmental Action Levels (EALs)
- Massachusetts Department of Environmental Protection: 2016 Standards & Guidelines for Contaminants in Massachusetts Drinking Water
- New Jersey Department of Environmental Protection: Remediation Standards
- Washington Department of Ecology: Reference Doses for Petroleum Mixtures

International Sources. Several international agencies and organizations have developed toxicity values for various petroleum hydrocarbons and other chemicals. Organizations throughout the EU may, in some cases, use different equations or assumptions in risk assessment reports, but the reports are likely to be peer-reviewed, and it may be useful to mine for toxicity values that can then be used as points of departure in EPA's equations. A helpful reference for EU risk approaches is the European Chemicals Agency's (ECHA) *Guidance on Information Requirements and Chemical Safety Assessment*. Additional international sources include:

- International Programme on Chemical Safety (IPCS). IPCS in cooperation with the Canadian Centre for Occupational Health and Safety (CCOHS) developed INCHEM, which "consolidates current, internationally peer-reviewed chemical safety-related publications and database records from international bodies, for public access." INCHEM contains "information on chemicals commonly used throughout the world, which may also occur as contaminants in the environment and food. It consolidates information from a number of intergovernmental organizations whose goal it is to assist in the sound management of chemicals."
- European Chemicals Agency. In addition to providing a searchable database of Information on Chemicals, "ECHA is the driving force among regulatory authorities in implementing the European Union's ground-breaking chemicals legislation for the

benefit of human health and the environment as well as for innovation and competitiveness. ECHA helps companies to comply with the legislation, advances the safe use of chemicals, provides information on chemicals and addresses chemicals of concern."[8] ECHA's website also provides information about the EU's approach to the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH). REACH became effective on June 1, 2007.

- European Commission's Joint Research Centre (JRC), Publications Repository. The JRC Publications Repository is an online service giving access to data about research publications such as articles, working papers, preprints, technical reports, conference papers and data sets in various digital formats. Where available, links are provided to the full-text of the publication. Content is organized around *Communities and Collections* which correspond to administrative entities. Each collection may contain an unlimited number of items.

- The National Industrial Chemicals Notification and Assessment Scheme (NICNAS). Implemented by the Australian Government Department of Health, NICNAS "is intended to help protect the Australian people and the environment by assessing the risks of industrial chemicals and providing information to promote their safe use. Their focus is the industrial use of chemicals. This covers a broad range of chemicals used in inks, plastics, adhesives, paints, glues, solvents, cosmetics, soaps and many other products."

Sources Of Environmental Concentrations Or Levels For Assessing Risks

National Drinking Water Regulations. EPA's Office of Water develops primary and secondary National Drinking Water Standards. Primary standards are legally enforceable maximum contaminant levels that apply to public water systems, taking into account health risks, cost and technology. Secondary standards are non-enforceable guidelines regulating contaminants in drinking water that may cause cosmetic effects, for example skin or tooth discoloration, or aesthetic effects, for example taste, odor, or color. EPA recommends secondary standards to water systems but does not require systems to comply. However, states may choose to adopt them as enforceable standards. EPA's Office of Water also develops health advisories, which provide information on contaminants that can cause human health effects and are known or anticipated to occur in drinking water.

Regional Screening Levels (RSL) Tables. EPA provides a compilation of screening level concentrations in the regional screening level (RSL) tables. The RSL tables provide comparison values, for example concentrations, for residential and commercial or industrial exposures to soil, air, and tapwater as drinking water. The concentrations are derived from toxicity values, for example reference dose, reference concentration, cancer slope factor, and inhalation unit risk, selected from the highest tier available and specific scenario or receptor exposure factors, for example child resident or industrial worker. Many of chemicals in the table have one or more missing toxicity values. EPA's RSL workgroup updates the RSL tables approximately every

---

[8] Data included in this database have not been verified by ECHA, rather it reflects the interpretation of the submitter. In addition, the full study is generally not available, making it difficult to assess the quality of the data.

six months, but the workgroup does not necessarily review values from all potential sources. Additionally, they do not derive toxicity values when none are available.

The [RSL web site](#) is the source of screening levels for all EPA regions. On the RSL website you will find tables of risk-based screening levels, calculated using the latest toxicity values, default exposure assumptions, and physical and chemical properties, as well as a calculator where you can change default parameters to reflect site-specific risks.

In addition to serving as a consolidated source of toxicity information from the highest tier available, RSL tables provide screening levels (SLs) derived using chemical specific toxicity values and default exposure factors according to risk assessment guidance from EPA's Superfund program[9]. The RSL website is a source of SLs for all EPA regions, and unified use of these SLs at Superfund sites promotes national consistency. For EPA's Superfund program, individual regions may still develop non-consensus screening values or choose to use Tier 3 values not included in the RSL table.

Occupational Safety and Health Administration (OSHA). OSHA provides permissible exposure limits [(PELs)](#) to protect workers[10] against the health effects of exposure to hazardous chemicals in air. PELs are regulatory limits on the amount or concentration of a substance in the air. They may also contain a skin designation that alerts workers to potential irritation and sensitization concerns. OSHA PELs are based on an 8-hour time weighted average (TWA) exposure. PELs are addressed in specific standards for the general industry, shipyard employment, and the construction industry. However, note that many PELs are outdated. In fact, the official OSHA website cautions: "OSHA recognizes that many of its permissible exposure limits (PELs) are outdated and inadequate for ensuring protection of worker health (https://www.osha.gov/dsg/annotated-pels/)."

Additional Sources Of Information And Tools For Risk Assessment

U.S. Geological Survey (USGS) Health-Based Screening Levels (HBSLs). The USGS National Water-Quality Program has recently updated information in its searchable online database of [HBSLs](#) for sources of drinking water. All HBSL values in the database have been updated to reflect EPA's most recent methods and exposure assumptions for establishing drinking-water guidelines.

"HBSLs are non-enforceable benchmark concentrations of contaminants in water. These screening levels supplement federal drinking-water standards and guidelines, which are not available for many of the hundreds of contaminants analyzed in sources of drinking water.

---

[9] The *Risk Assessment Guidance for Superfund (RAGS)* document is comprised of a number of separate sections that are accessible at *https://www.epa.gov/risk/risk-assessment-guidance-superfund-rags-part*.

[10] OSHA PELs apply only to occupational exposures. PELs are NOT appropriate to evaluate general population risks. It may be possible to access original documentation and identify the point of departure to calculate a toxicity value that is appropriate for the general population, and sensitive subpopulations.

Using HBSLs can provide a human-health context when evaluating the quality of sources of drinking water and help prioritize monitoring efforts."

The USGS database contains more than 800 contaminants and allows users to easily find information on drinking-water benchmarks and guidelines, such as current EPA drinking-water benchmarks MCLs and Human Health Benchmarks for Pesticides (HHBPs) and other water quality benchmarks that may be helpful, as it includes screening levels for sediment, fish and shellfish: https://www.usgs.gov/mission-areas/water-resources/science/water-quality-benchmarks-contaminants?qt-science_center_objects=0#qt-science_center_objects. The web site also includes guidance on the use of benchmarks.

The Risk Assessment Information System (RAIS). The Risk Assessment Information System (RAIS) began in 1996 under the Department of Energy's (DOE's) Oak Ridge Operations Office to provide a clearing house for risk assessment information used to evaluate and remediate legacy contamination from the Manhattan Project.[11] The RAIS was designed to provide all risk assessment processes in a transparent forum for the public, subcontractors, and State and Federal regulators. Guidance documents, tutorials, databases, historical information, toxicity values, screening levels and risk models have been integrated into the RAIS. There are also links to a suite of EPA risk assessment guidance documents, models, and databases. Where available, the RAIS provides comprehensive data on chemical toxicity, and physical and biological parameter values useful in conducing human exposure or ecological risk assessments, or both. Chemical toxicity values are drawn from sources using the same 3 tier hierarchy described previously.

Vapor Intrusion Screening Level Calculator. EPA provides a source of exposure values for indoor air concentrations of volatile chemicals in the Vapor Intrusion Screening Levels (VISL) Calculator.[12] VISLs for human health protection are generally recommended, medium-specific, risk-based screening-level concentrations intended for use in identifying areas or buildings that may warrant further investigation and mitigation as appropriate.

The VISLs include target indoor air screening levels for long-term, that is chronic exposures that consider the potential for cancer and non-cancer effects of vapor-forming chemicals. The VISLs also include subsurface screening levels for comparison to sampling results for sub-slab soil gas, near-source soil gas, and groundwater. These subsurface screening levels are back-calculated from the target indoor air screening levels for chronic exposures using medium-specific, generic attenuation factors that reflect generally reasonable worst-case conditions (EPA, 2015b,

---

[11] The RAIS server is housed at the DOE's Oak Ridge National Laboratory. DOE's cleanup contractor, URS|CH2M Oak Ridge LLC (UCOR), continues to support the RAIS to maintain the information and to update databases and tools based on new guidance through a contract with the University of Tennessee.

[12] The user's guide for the VISL calculator provides additional information about derivation of the indoor air and subsurface screening levels. In 2018, the VISL calculator became available as an online calculator, replacing previous versions in MS-Excel workbooks. The VISL now uses the same database as the RSLs for toxicity values and physiochemical parameters and will be automatically updated during the semi-annual RSL updates.

Appendix B). VISLs are not automatically response action levels, although EPA recommends that similar calculation algorithms be employed to derive cleanup levels; see EPA, 2015b, Section 7.6 for more information.

The VISL calculator allows users to specify an exposure scenario, target risk for carcinogens and target hazard for non-carcinogens, and the average groundwater temperature at a site. It then calculates screening levels for the target indoor air concentration, sub slab and exterior soil gas concentrations, and ground water concentration.

An individual subsurface sampling result that exceeds the respective, chronic screening level does not establish that vapor intrusion will pose an unacceptable human health risk to building occupants. Conversely, these generic, single-chemical VISLs do not account for the cumulative effect of all vapor-forming chemicals that may be present. Thus, if multiple chemicals that have a common, non-cancer toxic effect are present, a significant health threat may exist at a specific building or site even if none of the individual substances exceeds its VISL.

It is important to note that while the VISL calculator provides generic vapor intrusion attenuation factors, it does not account for biodegradation of biodegradable organic contaminants such as petroleum hydrocarbons and other motor fuel constituents. As a result, subsurface screening levels determined by the VISL calculator are likely higher than necessary for aerobically-biodegradable VOCs. For additional guidance on determining screening levels for petroleum hydrocarbons and other fuel constituents present in the subsurface as the result of a release from a regulated UST, see EPA's *Technical Guide For Addressing Petroleum Vapor Intrusion At Leaking Underground Storage Tank Sites* (EPA 510-R-15-001, 2015)*.

Databases. These sources can be used to identify potential toxicity values, or points of departure to calculate toxicity values, in the absence of authoritative toxicity values. The calculation of toxicity values based on points of departure such as NOAELs, LOAELs requires more expertise to select key studies, taking into consideration factors such as data quality and applicability, select the appropriate point of departure, perform extrapolations to derive human equivalent dose, and apply uncertainty factors. Assessors interested in taking this approach should refer to EPA guidance relevant to human health risk assessment: *https://www.epa.gov/risk/risk-assessment-guidelines*.

- EPA CompTox Chemistry Dashboard: "Responding to the need for *high-quality, structure-curated, open data* to meet the various needs of the environmental sciences and computational toxicology communities, EPA developed the CompTox Chemistry Dashboard. CompTox integrates diverse types of relevant domain data through a cheminformatics layer, built upon a database of curated substances linked to chemical structures. These data include physicochemical, environmental fate and transport, exposure, usage, in vivo toxicity, and in vitro bioassay data, surfaced through an integration hub with link-outs to additional EPA data and public domain online resources. Batch searching allows for direct chemical identifier (ID) mapping and downloading of multiple data streams in several different formats. This facilitates fast

access to available structure, property, toxicity, and bioassay data for collections of chemicals (hundreds to thousands at a time). Advanced search capabilities are available to support, for example, non-targeted analysis and identification of chemicals using mass spectrometry. The contents of the chemistry database, presently containing more than 800,000 substances, are available as public domain data for download. The chemistry content underpinning the Dashboard has been aggregated over the past 15 years by both manual and auto-curation techniques within EPA's DSSTox project. DSSTox chemical content is subject to strict quality controls to enforce consistency among chemical substance-structure identifiers, as well as list curation review to ensure accurate linkages of DSSTox substances to chemical lists and associated data. The Dashboard provides support for a broad array of research and regulatory programs across the worldwide community of toxicologists and environmental scientists."

Toxicity values, if available are listed under *Hazard* and provided in tabular form which includes the type of toxicity value, for example NOAEL, LOAEL); the risk assessment class, for example chronic, subchronic, acute; the value; study type; exposure route; species; and source. The table can be sorted and downloaded. The assessor must select the appropriate value or values from the table.

- [Hazardous Substances Data Bank (HSDB)](). "HSDB is a toxicology database that focuses on the toxicology of potentially hazardous chemicals. It provides information on human exposure, industrial hygiene, emergency handling procedures, environmental fate, regulatory requirements, nanomaterials, and related areas." HSDB provides summary information on hazard, that may include toxicity values, and available data. The assessor must select the appropriate value or values that are summarized within the *Human Health Effects* or *Animal Toxicity Studies* sections, or both. The information in HSDB has been assessed by a Scientific Review Panel. HSDB is one of the group of databases comprising TOXNET® (TOXicology Data NETwork).

  TOXNET® covers chemicals and drugs, diseases and the environment, environmental health, occupational safety and health, poisoning, risk assessment and regulations, and toxicology. It is managed by the [Toxicology and Environmental Health Information Program]() in the [Division of Specialized Information Services]() of the [National Library of Medicine]().

  "TOXNET® provides information on:
  - Specific chemicals, mixtures, and products
  - Chemical nomenclature
  - Chemicals that may be associated with a disease, condition or symptom
  - Chemicals associated with consumer products, occupations, hobbies, and more
  - Special toxic effects of chemicals in humans and/or animals
  - Citations from the scientific literature"

- **Health & Environmental Research Online (HERO) Database.** The [HERO]() database includes more than 600,000 scientific references and data from the peer-reviewed literature used by EPA to develop its regulations and includes the IRIS database, PPRTVs,

and integrated science assessments[13]. These assessments supported by HERO characterize the nature and magnitude of health risks to humans and the ecosystem from pollutants and chemicals in the environment. HERO is an evergreen database, this means new studies are continuously added so scientists can keep abreast of current research. Imported references are systematically sorted, classified and made available for search and citation.

Analogue and Category Approaches. For chemicals without toxicity values, it may be possible to use an analogue approach where a comparison is made between the target chemical and structurally similar chemicals that have similar physical chemical properties and functional groups. An analogue with relevant toxicological data can then be used to assess risks associated with the target chemical via read-across. EPA developed several tools to identify analogues of chemicals of interest, including the Analog Identification Methodology (AIM), and the Chemistry Dashboard (CompTox).

The category approach is an extension of the analogue approach, whereby a category is defined based on:
- molecular structure a new chemical must have to be included in the category,
- boundary conditions such as molecular weight, equivalent weight, the log of the octanol/water partition coefficient (log P), or water solubility, that would determine inclusion in (or exclusion from) a category, and
- standard hazard and fate tests to address concerns for the category (EPA, 2010).

The intergovernmental Organisation for Economic Cooperation and Development (OECD) identified an advantage of a chemical category assessment approach as the identification of consistent patterns of characteristics and health effects within a category serves to increase the confidence and reliability of the results for all of the individual chemicals that fit within the category definition, compared to evaluation of data using the single analogue approach (OECD, 2014). The OECD Existing Chemicals Database contains a number of examples where groups of chemicals were assessed using category approaches, published as screening information datasets (SIDS). EPA and OECD collaborated on developing many of these category documents under the High Production Volume Chemicals Program. Chemicals were assessed and grouped, and the results were published as SIDS.[14] OECD also produced guidance on the characterization of hydrocarbon solvents for assessment purposes (OECD, 2016). The guidance includes suggestions that might be helpful for identifying chemical characteristics relevant to analogue and category approaches.

Category and analogue approaches have been applied in the EPA PPRTV program. Lizarraga et al. (2019) presents a case study illustrating how the read-across approach was applied to derive

---

[13] Integrated Science assessments provide input into establishing National Ambient Air Quality Standards (NAAQS).
[14]or example, see the SIDS document for the C7-C9 Aliphatic Hydrocarbon Solvents Category, available at: *https://hpvchemicals.oecd.org/ui/handler.axd?id=afd8ccb9-af39-43ca-b49c-5034972e75dc*.

toxicity values for p,p'-dichlorodiphenyldichloroethene (p,p'-DDE). Candidate chemicals were identified based on chemical structure. Physicochemical properties, toxicokinetics, in vitro bioactivity and laboratory animal studies on analogues were collected and assessed, using a weight of evidence approach to select the best analogue to use to derive toxicity values for p,p'-DDE (Lizarraga et al., 2019).

   Predictive Approaches. In the absence of toxicological data, it may be possible to glean information on potential toxicological hazards based on chemical structure. Chemical structure can provide information about putative biological activity and potential hazard. Some structural alerts, such as for genotoxicity and sensitization, are quite well characterized. Computer models, such as the OECD QSAR Toolbox and the online tool OCHEM, provide information about the scientific basis for a structural alert. A qualitative assessment of risk based on the presence of structural alerts can be used to highlight the potential presence of hazards. Structural alerts are commonly used in the early phases of drug development to screen out molecules that are likely to be problematic (Shushko et al, 2012). In chemical risk assessment, they can be used to inform risk management decisions, such as the need for personal protective equipment, but generally do not provide sufficient information to quantify risk, or risk reduction from mitigation actions. EPA has incorporated structural alerts and predictive models into chemical assessments for regulatory purposes under the Toxic Substances Control Act (TSCA).[15]

References Cited

Clark, *et al.*, 2013. A GHS-consistent approach to health hazard classification of petroleum
   substances, a class of UVCB substances. *Reg Tox Pharm* 67:409-420.

EPA. 2010. TSCA new chemicals program, chemical categories report.
   http://www.epa.gov/oppt/newchems/pubs/npcchemicalcategories.pdf

EPA. 2015a. *Technical Guide for Addressing Petroleum Vapor Intrusion at Leaking Underground
   Storage Tank Sites* (EPA 510-R-15-001). Office of Underground Storage Tanks.
   *https://www.epa.gov/sites/production/files/2015-06/documents/pvi-guide-final-6-10-
   15.pdf*

EPA. 2015b. *OSWER Technical Guide for Assessing and Mitigating the Vapor Intrusion Pathway
   From Subsurface Sources To Indoor Air* (OSWER Publication 9200.2-154). Office of Solid
   Waste and Emergency Response.
   http://www.epa.gov/oswer/vaporintrusion/

---

[15] For more information, see "*Using Predictive Methods to Assess Hazard under TSCA*" at
https://www.epa.gov/tsca-screening-tools/using-predictive-methods-assess-hazard-under-tsca#models.

EPA. 2015c. Toxic Substances Control Act Inventory Representation for Chemical Substances of Unknown or Variable compositions, Complex reaction products and Biological Materials: UVCB Substances.
https://www.epa.gov/sites/production/files/2015-05/documents/uvcb.pdf

EPA. 2018a. *Vapor Intrusion Screening Level (VISL) Calculator: User's Guide*. Office of Solid Waste and Emergency Response.
https://www.epa.gov/vaporintrusion/visl-users-guide

EPA. 2018b. *Vapor Intrusion Screening Level (VISL) Calculator*. Office of Solid Waste and Emergency Response.
https://epa-visl.ornl.gov/cgi-bin/visl_search

Lizarraga L.E., Dean J.L., Kaiser P., Wesselkamper S.C., Lambert J.C., Zhao Q.J. 2019. A case study on the application of an expert-driven read-across approach in support of a quantitative risk assessment of p,p'-dichlorodiphenyldichloroethane. *Regulatory Toxicology and Pharmacology* 103:301-313.

OECD. 2014. *Guidance on Grouping of Chemicals, Second Edition. No. 194*. Organisation for Economic Cooperation and Development ENV/JM/MONO(2014)4.
http://www.oecd.org/publications/guidance-on-grouping-of-chemicals-second-edition-9789264274679-en.htm

OECD. 2016. *Guidance for Characterising Hydrocarbon Solvents for Assessment Purposes Series on Testing and Assessment No. 230*. Organisation for Economic Cooperation and Development ENV/JM/MONO(2015)52.
http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=env/jm/mono(2015)52&doclanguage=en

Swick, *et al.*, 2013. Gasoline risk management: A compendium of regulations, standards and industry practices. *Reg Tox Pharm* 70: S80-S92.

Appendix A
Calculation Of Risk-Based Target Concentrations For Selected Motor Fuel Constituents In Indoor Air

EPA's guidance document, *Risk Assessment Guidance for Superfund (RAGS)*[16] is the source of the equations in this Appendix. EPA's risk assessment practices have evolved over time and some sections are dated. For example, Part F provides supplemental guidance for inhalation risk assessment and was revised in 2009; it replaces older methodology that used inhalation slope factors (SF_i) with newer methodology that instead uses inhalation unit risk (IUR) values.

Target indoor air concentrations are calculated using the equations presented below. $C_{ia,c}$ is the target indoor air concentration for carcinogens (Equation A-1) and $C_{ia,nc}$ is the target indoor air concentration for non-carcinogens (Equation A-2). Each of the toxicity values is weighted by the appropriate exposure factors to determine the target indoor air screening concentrations. The smaller value of $C_{ia,c}$ or $C_{ia,nc}$ is used as the target indoor air screening value.

$$C_{ia,c} = \frac{TCR \cdot ATc \cdot 365\ (days/year) \cdot 24 (hours/day)}{EF \cdot ED \cdot ET \cdot IUR}$$ Equation A-1

For carcinogens, the inhalation unit risk (IUR) is the appropriate toxicity value. Weighting factors are: TCR, which is the target cancer risk (generally equal to 1.0E-06); ATc, which is the averaging time for cancer risk; and EF, ED, and ET, which are exposure parameters (exposure frequency, exposure duration, and exposure time).

$$C_{ia,nc} = \frac{THQ \cdot RfC \cdot ATnc \cdot 365 \cdot 24 \cdot 1000 (ug/mg)}{EF \cdot ED \cdot ET}$$ Equation A-2

For non-carcinogens, the reference concentration (RfC) is the appropriate toxicity value. Weighting factors are: THQ, which is the Target Hazard Quotient (generally equal to 1); $ATnc$, which is the averaging time non-cancer risk; and EF, ED, and ET, which are exposure parameters (exposure frequency, exposure duration, and exposure time).

Example calculations using Equations A-1 and A-2 are presented in Table A-1 for selected motor fuel constituents in indoor air under a residential exposure scenario. Generally, the lowest of the cancer and non-cancer values is chosen as the appropriate screening level. Note that cancer screening levels ($C_{ia,c}$) are consistently lower than non-cancer screening levels ($C_{ia,nc}$), thus the cancer screening levels would generally be used to assess risk to receptors for a given chemical.

---

[16] EPA's *RAGS* guidance is accessible at *https://www.epa.gov/risk/risk-assessment-guidance-superfund-rags-part.*

Table A-1. Example Target Residential Indoor Air Concentrations For Selected Motor Fuel Constituents

Chemical	IUR (µg/m³)⁻¹	RfC (mg/m³)	C_{ia} (µg/m³)	
			Cancer (TCR=1.0E-06)	Non-cancer (THQ=1.0)
Benzene	7.8E-06	3.0E-02	3.6E-01	31.3
Toluene	NA	5.0E+00	*	5214
Ethylbenzene	2.5E-06***	1.0E+00	1.1E+00	1043
Xylenes (all 3 isomers)	NA	1.0E-01	*	104
Naphthalene	3.4E-05***	3.0E-03	8.3E-02	3.1
1,2-Dibromoethane (EDB)	6.0E-04	9.0E-03	4.7E-03	9.4
1,2-Dichloroethane (1,2-DCA)	2.6E-05	7.0E-03**	1.1E-01	7.3
Diisopropyl ether (DIPE)	NA	7.0E-01**	*	730
Methyl Tertiary-Butyl Ether (MTBE)	2.6E-07***	3.0E+00	1.1E+01	3.1

All values for *IUR* and *RfC* are from IRIS (Tier 1) unless otherwise noted:
* = cannot calculate due to lack of *IUR*
** = PPRTV (Tier 2)
*** = Other (Tier 3)
NA = value not available in any of the 3 tiers
Values (and units) of other variables used in these example residential calculations (equations in Table A-1) are:

Variable	Cancer (c)	Non-Cancer (nc)
ATc or *ATnc* (years)	70	26
ED (years)	26	26
EF (days/year)	350	350
ET (hours/day)	24	24

The exposure factors above are consistent with those in *Human Health Evaluation Manual, Supplemental Guidance: Update of Standard Default Exposure Factors* OSWER Directive 9200.1-120 (*https://www.epa.gov/sites/production/files/2015-11/documents/oswer_directive_9200.1-120_exposurefactors_corrected2.pdf*)

After a target indoor air screening level (C_{ia}) has been established, the next step is to determine vapor source concentrations in the field and assess whether these are high enough to potentially pose a threat of vapor intrusion. Site characterization activities typically involve sampling soil, soil gas, and/or groundwater. Analytical data from these samples enables site-specific screening levels to be calculated using the target indoor air screening level as a starting point and back-calculating. Appendices B through D provide example calculations for determining screening levels for volatile contaminants in groundwater, soil gas, and soil, respectively. If the highest measured concentration is lower than the calculated screening level for the same medium, then there should be no potential for vapor intrusion and additional sampling – for instance, indoor air sampling – would not be necessary. If the highest measured concentration is higher than the calculated screening level, there is a potential for vapor intrusion and additional sampling should be conducted. Refer to EPA's petroleum vapor intrusion guidance (EPA, 2015a) if the contaminants are from a regulated UST, or EPA's more general vapor intrusion guidance (EPA, 2015b) if the source is something else.

Note: it is important to realize that an individual subsurface sampling result that exceeds the screening level does not necessarily establish that vapor intrusion will pose an unacceptable human health risk to building occupants. Conversely, these generic, single-chemical screening levels do not account for the cumulative effect of all vapor-forming chemicals that may be present. Thus, if multiple chemicals that have a common, non-cancer toxic effect are present, a significant health threat may exist at a specific building or site even if none of the individual substances exceeds its vapor intrusion screening level (see discussion of non-cancer hazard index in EPA (2015b) Section 7.4.1).

Appendix B
Calculation Of Risk-Based Screening Concentrations For Selected Motor Fuel Constituents In Groundwater

After target indoor air screening levels (C_{ia}) have been established, for example by using the equations and procedures described in Appendix A, the next step is to determine vapor source concentrations and assess whether these are high enough to potentially pose a threat of vapor intrusion. The equations below allow for calculation of groundwater screening levels based on target indoor air screening levels derived from the equations in Appendix A. The groundwater screening level can then be compared to actual field measurements of groundwater concentrations. If the highest measured groundwater concentration is lower than the calculated screening level for groundwater, then there should be no potential for vapor intrusion and additional sampling – for instance, indoor air sampling – would not be necessary. If the highest measured groundwater concentration is higher than the calculated screening level, there is a potential for vapor intrusion and additional sampling should be conducted. Refer to EPA's petroleum vapor intrusion guidance (EPA, 2015a) if the contaminants are from a regulated UST, or EPA's more general vapor intrusion guidance (EPA, 2015b) if the source is something else.

$$C_{gw} = \frac{C_{ia}}{\alpha_{gw} \cdot 1000 \cdot HLC} \qquad \text{Equation B-1}$$

C_{gw} is the screening concentration in groundwater (µg/L). C_{ia} is the target indoor air screening level concentration (µg/m^3). α_{gw} is the groundwater vapor intrusion attenuation factor (unitless). HLC is the unitless Henry's Law constant. 1,000 is the number of liters (L) per m^3 (to convert from units of µg/m^3 to µg/L).

$$C_{ia} = C_{gw} \cdot \alpha_{gw} \cdot 1000 \cdot HLC \qquad \text{Equation B-2}$$

C_{ia} is the target indoor air screening level concentration (µg/m^3) and represents an upper bound for indoor air screening concentration. C_{gw} is the screening concentration in groundwater (µg/L). α_{gw} is the groundwater vapor intrusion attenuation factor (unitless). 1,000 is the number of liters (L) per m^3 (to convert from units of µg/m^3 to µg/L). HLC is the unitless Henry's Law constant.

Appendix C
Calculation Of Risk-Based Screening Concentrations For Selected
Motor Fuel Constituents In Soil Gas

After target indoor air screening levels (C_{ia}) have been established, the next step is to determine vapor source concentrations and assess whether these are high enough to potentially pose a threat of vapor intrusion. The equations below, C-1 and C-2, allow for calculation of soil gas screening levels based on target indoor air screening levels derived from the equations in Appendix A. These soil gas screening levels can then be compared to actual field measurements of soil gas concentrations. If the highest measured soil gas concentration is lower than the calculated screening level for soil gas, then there should be no potential for vapor intrusion and additional sampling – for instance, indoor air sampling – would not be necessary. If the highest measured soil gas concentration is higher than the calculated screening level, there is a potential for vapor intrusion and additional sampling should be conducted. Refer to EPA's petroleum vapor intrusion guidance (EPA, 2015a) if the contaminants are from a regulated UST, or EPA's more general vapor intrusion guidance (EPA, 2015b) if the source is something else.

$$C_{sg} = \frac{C_{ia}}{\alpha_{sg}}$$
<div align="right">Equation C-1</div>

C_{sg} is the screening concentration in soil gas (μg/m^3). NOTE: C_{esg}, as from Appendix D, may be substituted for C_{sg}. C_{ia} is the target indoor air screening level concentration (μg/m^3). α_{sg} is the soil gas vapor intrusion attenuation factor (unitless).

$$C_{ia} = C_{sg} \cdot \alpha_{sg}$$
<div align="right">Equation C-2</div>

C_{ia} is the target indoor air screening level concentration (μg/m^3) and represents an upper bound on indoor air screening concentration. C_{sg} is the screening concentration in soil gas (μg/m^3). Note: C_{esg}, as from Appendix D, may be substituted for C_{sg}. α_{sg} is the soil gas vapor intrusion attenuation factor (unitless).

Appendix D
Calculation Of Risk-Based Screening Concentrations For Selected
Motor Fuel Constituents In Soil

A risk-based screening level can be determined for motor fuel constituents in soil samples by first calculating the estimated soil gas concentration (C_{esg}) from the concentration in a representative soil sample and then using this value following the procedure in Appendix C to assess whether the soil concentration is high enough to potentially pose a threat of vapor intrusion. If the highest measured soil concentration is lower than the calculated screening level, then there should be no potential for vapor intrusion and additional sampling – for instance, indoor air sampling – would not be necessary. If the highest measured soil concentration is higher than the calculated screening level, there is a potential for vapor intrusion and additional sampling should be conducted. Refer to EPA's petroleum vapor intrusion guidance (EPA, 2015a) if the contaminants are from a regulated UST, or EPA's more general vapor intrusion guidance (EPA, 2015b) if the source is something else.

To calculate C_{esg}, the approach is to use the vapor pressure of the pure liquid, Raoult's Law, and the temperature of the subsurface to estimate the partial pressure of the fuel component in the soil gas in equilibrium with an oily phase liquid. The relationship between C_{esg} and P_i is,

$$C_{esg}[\mu g/m^3] = \frac{p_i \bullet MW_i}{82 \bullet K} \qquad\qquad \text{Equation D-1}$$

Where p_i is the equilibrium partial pressure of chemical i in the vapor phase [atm] at the temperature of the subsurface environment, MW_i is the molecular weight of chemical i, and K is the temperature in degrees Kelvin.

The formula assumes the universal gas law

$$PV = nRT \qquad\qquad \text{Equation D-2}$$

where P is pressure, V is volume, n is the number of moles, T is the temperature and R is the Universal Gas Constant with a value of $8.2 \bullet 10^{-5}$ $m^3 \bullet atm \bullet K^{-1} \bullet mole^{-1}$.

Assuming that:
(1) the bulk concentrations of a particular fuel component, such as benzene, determined in a soil sample (mg benzene/kg soil) is dominated by benzene present in LNAPL or residual NAPL,
(2) that an analysis of total petroleum hydrocarbon or TPH (mg TPH/kg soil) is equivalent to the quantity of hydrocarbon fuel in the soil present as LNAL or residual NAPL,
(3) the partial pressure of the fuel component can be described by Raoult's Law (Kirchstetter et al. (1999), their equation 1),

$$p_i = \gamma_i\, x_i p_i^o \qquad\qquad \text{Equation D-3}$$

Where γ_i is the activity coefficient of chemical *i* in the NAPL; x_i is the mole fraction of chemical *i* in the NAPL, and p_i^o is the vapor pressure of the pure chemical *i* at the temperature of the subsurface [atm].

For fuel components other than alcohols, the value of the activity coefficient (γ_i) is usually near 1.0. Table 2 in Harley et al. (2000) provides values of (γ_i) for a range of fuel components. A fuel NAPL in contact with porewater in the subsurface will lose almost all of its ethanol to the porewater. The measured activity coefficients in Table 2 are an upper boundary on the value of (γ_i) in NAPL in the subsurface, while the UNIFAC activity coefficients are a lower boundary. To be conservative, for a spill of E10, use the values of the measured activity coefficients in calculations.

A value for X_i can be estimated as follows;

$$X_i = \frac{C_i/MW_i}{C_{TPH}/100}$$

Equation D-4

where C_i is the concentration of chemical *i* in soil or sediment [mg/kg], MW_i is the molecular weight of chemical *i*, and C_{TPH} is the concentration of TPH in the soil or sediment [mg/kg]. Equation D-4 assumes that the mean molecular weight of gasoline is 100 amu.

The value of p_i^o can be calculated using the Wagner equation as described in Harley et al. (2000) equation 3 and Kirchstetter et al. (1999) equation 2. Note that there is a typographical error in equation 2 of Kirchstetter et al. (1999). Equation 3 in Harley et al. (2000) is correct. The Wagener equation calculates a value of p_i^o [atm] as follows,

$$p_i^o = p_c \bullet p_r^o$$

Equation D-5

where p_c [atm] is the critical pressure of chemical *i* and $p^o{}_r$ *is a correction factor*. The correction factor is calculated as follows:

$$\ln p_r^o = \frac{a\left(1-T/T_c\right)+b(1-T/T_c)^{1.5}+ c(1-T/T_c)^3+ d(1-T/T_c)^6}{T/T_c}$$

Equation D-6

where T_c [degrees K] is the critical temperature of the chemical, and *T* is the subsurface temperature [degrees K], and the coefficients *a, b, c* and *d* are fitting factors. Values for *P$_c$, T$_c$, a, b, c, and d* are available in Appendix 4 in the Supporting Information of Kirchstetter et al. (1999). Table D-1 presents calculated values of p_i^o for several fuel hydrocarbons over the range of temperatures that can be expected in groundwater.

Table D-1. Estimated Vapor Pressures Of Selected Components Of Gasoline At Groundwater Temperatures.

	p_i^o (atm)				
	5 °C	**10 °C**	**15 °C**	**20 °C**	**25 °C**
Benzene	4.6E-02	6.0E-02	7.7E-02	9.9E-02	1.3E-01
Toluene	1.2E-02	1.6E-02	2.2E-02	2.9E-02	3.7E-02
Ethylbenzene	3.6E-03	5.0E-03	6.9E-03	9.4E-03	1.3E-02
o-Xylene	2.4E-03	3.4E-03	4.7E-03	6.5E-03	8.8E-03
m-Xylene	3.1E-03	4.4E-03	6.0E-03	8.2E-03	1.1E-02
p-Xylene	3.3E-03	4.6E-03	6.3E-03	8.6E-03	1.2E-02
naphthalene	4.8E-05	7.6E-05	1.2E-04	1.8E-04	2.7E-04
MTBE	1.4E-01	1.7E-01	2.2E-01	2.7E-01	3.3E-01

Table D-2 corrects p_i^o for activity and converts from [atm] to [µg/m³]. The Estimated Soil Gas Concentration (C$_{esg}$) can then be calculated as follows:

$$C_{esg} = x_i \bullet (\gamma_i \, p_i^o)$$

Equation D-7

where x_i is calculated from the concentrations of chemical $_i$ and TPH in soil or sediment by equation D-4 and the value of $\gamma_i \, p_i^o$ is taken from Table D-2.

Table D-2. Estimated Values Of $\gamma_i \, p^o{}_i$ For Selected Components Of Gasoline At Groundwater Temperatures.

	$\gamma_i \, p_i^o$ (µg/m³)				
	5 °C	**10 °C**	**15 °C**	**20 °C**	**25 °C**
Benzene	4.6E-02	6.0E-02	7.7E-02	9.9E-02	1.3E-01
Toluene	1.2E-02	1.6E-02	2.2E-02	2.9E-02	3.7E-02
Ethylbenzene	3.6E-03	5.0E-03	6.9E-03	9.4E-03	1.3E-02
o-Xylene	2.4E-03	3.4E-03	4.7E-03	6.5E-03	8.8E-03
m-Xylene	3.1E-03	4.4E-03	6.0E-03	8.2E-03	1.1E-02
p-Xylene	3.3E-03	4.6E-03	6.3E-03	8.6E-03	1.2E-02
naphthalene	4.8E-05	7.6E-05	1.2E-04	1.8E-04	2.7E-04
MTBE	1.4E-01	1.7E-01	2.2E-01	2.7E-01	3.3E-01

REFERENCES FOR APPENDIX D

Harley, R.A., S.C. Coulter-Burke, and T.S. Yeung. 2000. Relating Liquid Fuel and Headspace Vapor Composition for California Reformulated Gasoline Samples Containing Ethanol. *Environmental Science & Technology* 34: 4088-4094.

Kirchstetter, T.W., B.C. Singer, R.A. Harley, G.R. Kendall and J.M. Hesson. 1999. Impact of California Reformulated Gasoline on Motor Vehicle Emissions. 2. Volatile Organic Compound Speciation and Reactivity. *Environmental Science & Technology* 33: 329-336.

Appendix E
Links For Sources Of Toxicity Information

Agency for Toxic Substances and Disease Registry (ATSDR) Minimal Risk Levels (MRLs): *http://www.atsdr.cdc.gov/mrls/index.asp*

Analogue Identification Methodology (AIM): *https://www.epa.gov/tsca-screening-tools/analog-identification-methodology-aim-tool*

California Office of Environmental Health Hazard Assessment, Toxicity Criteria Database: *http://oehha.ca.gov/tcdb/index.asp*

CompTox (EPA's chemistry dashboard): *https://comptox.epa.gov/dashboard*

ECOS. Identification and Selection of Toxicity Vales/Criteria for CERCLA and Hazardous Waste Site Risk Assessments in the Absence of IRIS Values: *https://www.ecos.org/wp-content/uploads/2016/05/FINAL-ECOS-PV-Paper-4-23-07.pdf*

EPA. 2003. *Human Health Toxicity Values In Superfund Risk Assessments. (*OSWER Directive 9285.7-53): *https://nepis.epa.gov/Exe/ZyPDF.cgi/91015CKS.PDF?Dockey=91015CKS.PDF*

EPA. 2014. Human Health Evaluation Manual, Supplemental Guidance: Update of Standard Default Exposure Factors (OSWER Directive 9200.1-120): *https://www.epa.gov/sites/production/files/2015-11/documents/oswer_directive_9200.1-120_exposurefactors_corrected2.pdf*

EPA. 2015a. *Technical Guide for Addressing Petroleum Vapor Intrusion at Leaking Underground Storage Tank Sites* (EPA 510-R-15-001): *https://www.epa.gov/sites/production/files/2015-06/documents/pvi-guide-final-6-10-15.pdf*

EPA. 2015b. *OSWER Technical Guide for Assessing and Mitigating the Vapor Intrusion Pathway From Subsurface Sources To Indoor Air* (OSWER Publication 9200.2-154): *http://www.epa.gov/oswer/vaporintrusion/*

EPA. 2018a. *Vapor Intrusion Screening Level (VISL) Calculator: User's Guide*: *https://www.epa.gov/vaporintrusion/visl-users-guide*

EPA. 2018b. *Vapor Intrusion Screening Level (VISL) Calculator*: *https://epa-visl.ornl.gov/cgi-bin/visl_search*

EPA Chemicals Under the Toxic Substances Control Act (TSCA): *https://www.epa.gov/chemicals-under-tsca*

EPA Office of Water, National Drinking Water Standards:
http://water.epa.gov/drink/contaminants/index.cfmv

EPA. *Risk Assessment Guidance for Superfund (RAGS)*: *https://www.epa.gov/risk/risk-assessment-guidance-superfund-rags-part*.

EPA Risk Assessment Portal:
http://www.epa.gov/risk/

European Chemicals Agency (ECHA):
https://echa.europa.eu/information-on-chemicals/registered-substances

European Commission's Joint Research Centre (JRC), Publications Repository:
http://publications.jrc.ec.europa.eu/repository/

Hawai'i Department of Health, Environmental Hazard Evaluation and Environmental Action Levels: *http://eha-web.doh.hawaii.gov/eha-cma/Leaders/HEER/EALs*

Hazardous Substances Data Bank (HSDB): *https://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB*

Health & Environmental Research Online (HERO) Database: *http://hero.epa.gov/*

HEAST Database: *http://epa-heast.ornl.gov/*

ICPS INCHEM: *http://www.inchem.org/*

Integrated Risk Information System (IRIS): *http://www.epa.gov/iris/*

Massachusetts Department of Environmental Protection, 2014 Standards & Guidelines for Contaminants in Massachusetts Drinking Water:
http://www.mass.gov/eea/agencies/massdep/water/drinking/standards/standards-and-guidelines-for-drinking-water-contaminants.html

National Ambient Air Quality Standards (NAAQS) Table:
https://www.epa.gov/criteria-air-pollutants/naaqs-table

National Industrial Chemicals Notification and Assessment Scheme (NICNAS):
https://www.nicnas.gov.au/

New Jersey Department of Environmental Protection, Remediation Standards:
http://www.state.nj.us/dep/srp/guidance/rs/

New Jersey Department of Health – Hazardous Substance Fact Sheet:
http://nj.gov/health/eoh/rtkweb/documents/fs/2014.pdf

NIH NLM Hazardous Substances Data Bank: *https://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB*

NIOSH Pocket Guide to Chemical Hazards: *https://www.cdc.gov/niosh/npg/default.html*

NIST Chemistry WebBook: *http://webbook.nist.gov/chemistry/*

Occupational Safety and Health Administration (OSHA), Permissible Exposure Limits (PELs): *https://www.osha.gov/dsg/annotated-pels/index.html*

OCHEM:
https://ochem.eu/home/show.do

OECD Cooperative Chemicals Assessment Programme (CoCAP): *http://www.oecd.org/env/ehs/risk-assessment/cocap-cooperative-chemicals-assessment-programme.htm*

OECD Existing Chemicals Database: *https://hpvchemicals.oecd.org/ui/Default.aspx*

OECD QSAR Toolbox:
http://www.oecd.org/chemicalsafety/risk-assessment/oecd-qsar-toolbox.htm

Provisional Peer-Reviewed Toxicity Values (PPRTV): *http://hhpprtv.ornl.gov/index.html*

Regional Screening Level Tables: *https://www.epa.gov/risk/regional-screening-levels-rsls*

Registration, Evaluation, Authorisation, and Restriction of Chemicals (REACH) database: *https://echa.europa.eu/regulations/reach/understanding-reach*

Risk Assessment Information System (RAIS): *https://rais.ornl.gov/*

Tier 3 Toxicity Value White Paper: *https://www.epa.gov/sites/production/files/2015-11/documents/tier3-toxicityvalue-whitepaper.pdf*

TOXNET (TOXicology Data NETwork): *https://toxnet.nlm.nih.gov/*

U.S. Geological Survey (USGS) Health-Based Screening Levels (HBSLs): *https://usgs.us17.list-manage.com/track/click?u=25dfe86acf8f5c5a5fc3519af&id=022ed733e9&e=b3f136dedb*

Using Predictive Methods to Assess Hazard under TSCA: *https://www.epa.gov/tsca-screening-tools/using-predictive-methods-assess-hazard-under-tsca#models*

Washington Department of Ecology, Reference Doses for Petroleum Mixtures:
https://fortress.wa.gov/ecy/clarc/FocusSheets/petroToxParameters.pdf