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SUBJECT: Risk-Based Concentration Table, July - December 1995

FROM: Roy L. Smith, Ph.D.
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TO: RBC Table mailing list

Attached is the EPA Region III risk-based concentration (RBC) table, which we distribute semi-annually to all interested parties.

IMPORTANT MESSAGE

EPA Region III has established a homepage on the World Wide Web which you can find at http://earth1.epa.gov:80/ or http://www.epa.gov/. Our homepage will soon include the RBC table in downloadable form. We strongly encourage all RBC table users having Internet access to obtain the table electronically rather than on paper. In this way, users can obtain the most current issue immediately in a form that can be used directly as input for risk assessment calculations. This distribution method will also save large amounts of paper and cost substantially less.

For those lacking Internet access, it's once again time to re-register to receive a paper copy of the RBC table. We need to hear from you periodically to ensure that you still have an interest and that we have your correct address. Please fax your registration request to Vanessa Sizer at 215-597-9890, including your name, address, and phone number. Please don't phone to re-register; we need hard copy to document your continued interest. If we don't hear from you by March 30, 1996, we'll assume you no longer need a paper copy. Thanks for your cooperation.

CONTENTS, USES, AND LIMITATIONS OF THE RBC TABLE

The table contains reference doses and carcinogenic potency slopes (obtained from IRIS through September 1, 1995, HEAST through May 1995, the EPA-NCEA Superfund Health Risk Technical Support Center, and other EPA sources) for nearly 600 chemicals. These toxicity constants have been combined with "standard" exposure scenarios to calculate RBCs--chemical concentrations corresponding to fixed levels of risk (*i.e.*, a hazard quotient of 1, or lifetime cancer risk of 10^{-6}, whichever occurs at a lower concentration) in water, air, fish tissue, and soil.

The RBC table also includes soil screening levels (SSLs) for protection of groundwater

and air. Most SSLs were obtained directly from EPA/OSWER's proposed SSL guidance document, to which we have added some additional SSLs based on the same methodology. Sources of SSLs are noted in the table. SSLs incorporate the same exposure assumptions as RBCs, plus additional assumptions needed for inter-media extrapolation. SSLs are therefore distinct from RBCs, and should be used only in the framework proposed in the OSWER document (available from NTIS as document numbers 9355.4-1, PB95-965530, or EPA540/R-94/105).

The Region III toxicologists use RBCs to screen sites not yet on the NPL, respond rapidly to citizen inquiries, and spot-check formal baseline risk assessments. The background materials provide the complete basis for all the calculations, with the intent of showing users exactly how the RBCs were developed. Simply put, RBCs are risk assessments run in reverse. For a single contaminant in a single medium, under standard default exposure assumptions, the RBC corresponds to the target risk or hazard quotient.

RBCs also have several important limitations. Specifically excluded from consideration are (1) transfers from soil to air and groundwater, and (2) cumulative risk from multiple contaminants or media. Also, the toxicity information in the table has been assembled by hand, and (despite extensive checking and years of use) may contain errors. It's advisable to cross-check before relying on any RfDs or CPSs in the table. If you find any errors, please send me a note.

Many users want to know if the risk-based concentrations can be used as valid no-action levels or cleanup levels, especially for soils. The answer is a bit complex. First, it is important to realize that the RBC table does not constitute regulation or guidance, and should not be viewed as a substitute for a site-specific risk assessment. For sites where:

1. A single medium is contaminated;

2. A single contaminant contributes nearly all of the health risk;

3. Volatilization or leaching of that contaminant from soil is expected not to be significant;

4. The exposure scenarios used in the RBC table are appropriate for the site;

5. The fixed risk levels used in the RBC table are appropriate for the site; and

6. Risk to ecological receptors is expected not to be significant;

the risk-based concentrations would probably be protective as no-action levels or cleanup goals. However, to the extent that a site deviates from this description, as most do, the RBCs would not necessarily be appropriate.

To summarize, the table should generally not be used to (1) set cleanup or no-action levels at CERCLA sites or RCRA Corrective Action sites, (2) substitute for EPA guidance for preparing baseline risk assessments, or (3) determine if a waste is hazardous under RCRA.

ANSWERS TO FREQUENTLY ASKED QUESTIONS

To help you better understand the RBC table, here are answers to our most often-asked questions:

1. How can the age-adjusted inhalation factor (11.66) be less than either the inhalation rate for a child (12) or for an adult (20)?

Age-adjusted factors are not intake rates, but rather partial calculations which have different units than intake rates do. The fact that these partial calculations have values similar to intake rates is really coincidental, an artifact of the similar magnitude of years of exposure and time-averaged body weight.

2. Why does arsenic appear in the RBC table separately as a carcinogen and a non-carcinogen, while other contaminants do not?

Arsenic is double-entered to ensure that the risk assessor realizes that non-carcinogenic concerns are significant for arsenic. Otherwise, one might be tempted to accept a 1e-4 risk (37 ppm in residential soil), when the oral reference dose would be exceeded at 23 ppm.

Also, EPA has a little-known risk management policy for arsenic (dating from 1988) that suggests that arsenic-related cancer risks of up to 1e-3 can be accepted because the cancers are squamous cell carcinomas with a low mortality rate. Thus, noncarcinogenic RBCs represent an important limitation on acceptable arsenic concentrations.

3. Many contaminants have no inhaled reference dose or carcinogenic potency slope in IRIS, yet these numbers appear in the RBC table with IRIS given as the source. Where did the numbers come from?

Most inhaled reference doses and potency slopes in the RBC table are converted from reference concentrations and unit risk values which do appear in IRIS. These conversions assume 70-kg persons inhaling 20 m^3/d. For example, the inhalation unit risk for arsenic (4.3e-3 risk per $\mu g/m^3$) is divided by 20 m^3/d and multiplied by 70 kg times 1000 μg/mg, yielding a CPSi of 15.1 risk per mg/kg/d.

4. Why does the RBC table base soil RBCs for cadmium and manganese on reference doses that apply only to drinking water?

The RBC table's use of the drinking water RfDs for cadmium and manganese reflects (1) the limited space available in the already-crowded table, and (2) the intended use of the table as a screening tool rather than a source of cleanup levels (thereby making false positives acceptable). For a formal risk assessment, Region III would use the food RfDs for soil ingestion.

At this time, only two substances (as far as we know) have distinct oral RfDs for water and food--cadmium and manganese. Adding the two food RfDs to the table would require an entire column, which would be about 99.9% blank. The table has become so crowded that it would be difficult to accommodate another column. Also, we given this problem a relatively low

priority because the table's primary purpose is to identify environmental problems needing further study. RBCs were never intended for uncritical use as cleanup levels, merely to identify potential problems which need a closer look.

5. What is the source of the child inhalation rate of 12 m3/d?

The calculation comes from basic physiology. It's a scaling of the mass-specific 20 m3/d rate for adults from a body mass of 70 kg to 15 kg, using the 2/3 power of mass, as follows:

Let: IRcm = mass-specific child inhalation rate (m3/kg/d)
IRc = child inhalation rate (m3/d)

20 m3/d ÷ 70kg = 0.286 m3/kg/d (mass-specific adult inhalation rate)

$0.286 \text{ m3/kg/d} \times (70^{.67}) = (\text{IRcm}) \times (15^{.67})$

$\text{IRcm} = (0.286) \times (70^{.67}) \div (15^{.67}) = 0.286 \times 2.807 = 0.803 \text{ m3/kg/d}$

IRc = IRcm x 15kg = 0.803 m3/kg/d x 15kg = 12.04 m3/d

A short (but algebraically equivalent) way to do the conversion:

$20 \times (15 \div 70)^{.333} = 11.97$ (different from, but actually more correct than, 12.04 because of rounding error in the long form).

6. Can the oral RfDs in the RBC table be applied to dermal exposure?

Not directly. EPA's Office of Research and Development is working on dermal RfDs for some substances, but has not yet produced any final values. When dermal RfDs do appear, they will undoubtedly be based on absorbed dose rather than administered dose. Oral RfDs are (usually) based on administered dose and therefore tacitly include a GI absorption factor. Thus, any use of oral RfDs in dermal risk calculations would have to involve removing this absorption factor.

*7. The exposure variables table in the RBC background document lists the averaging time for non-carcinogens as "ED*365". What does that mean?*

ED is exposure duration, in years. Multiplying ED by 365 simply converts the duration to days. In fact, the ED term is included in both the numerator and denominator of the RBC algorithms for non-cancer risk, canceling it altogether. We expressed the algorithm this way to allow users to realize this. The total exposure is really corrected only by EF (days exposed per year) divided by 365. (Note that this explanation applies to noncarcinogenic risk only; for carcinogens, exposure is pro-rated over the number of days in a 70-year life span.)

8. Why is inorganic lead not included in the RBC table?

The reason lead is missing from the RBC table is simple, and fundamental: EPA has no

reference dose or potency slope for inorganic lead, so it wasn't possible to calculate risk-based concentrations. EPA considers lead a special case because:

(1) Lead is ubiquitous in all media, so human exposure comes from multiple sources. Comparing single-medium exposures with a reference dose would be misleading.

(2) If EPA did develop a reference dose for lead by the same methods other reference doses, we would probably find that most people already exceed it. Since EPA already knows this and is moving aggressively to lower lead releases nationally, such findings at individual sites would be irrelevant and unduly alarming.

(3) EPA decided to take a new approach to separate important lead exposures from trivial ones. EPA developed a computer model (the IEUBK model) which predicts children's blood lead concentrations using lead levels in various media as inputs. The idea is to evaluate a child's entire environment, and reduce lead exposures in the most cost-effective way.

On the practical side, there are several EPA policies which effectively substitute for RBCs. The EPA Office of Solid Waste has released a detailed directive on risk assessment and cleanup of residential soil lead. The directive recommends that soil lead levels less than 400 ppm be considered safe for residential use. Above that level, the document suggests collecting certain types of data and modeling children's blood lead with the IEUBK model. For the purposes of the RBC table, the de facto residential soil number would be 400 mg/kg. For water, we suggest 15 ppb (from the national EPA Action Level), and for air, the National Ambient Air Quality Standard.

9. Where did the potency slopes for carcinogenic PAHs come from?

The source of the potency slopes for PAHs is "Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons", Final Draft, EPA Environmental Criteria and Assessment Office, Cincinnati, OH. It's available from NTIS as document number ECAO-CIN-842 (March, 1993). The slopes are expressed in terms of order-of-magnitude equivalence factors relating the compounds to benzo[a]pyrene; we have converted these TEQs to potency slopes to fit the format of the table.

10. May I please have a copy of the January 1991 RBC table?

We're sorry, but no. The RBC table doesn't represent regulation or guidance, so past issues should have no legal importance. Each time we update the table we destroy all obsolete copies, electronic and paper. We do this to ensure that only one set of RBCs, that based on current information, exists at any time.

11. I've noticed that some soil RBCs are 1 million parts per million. Since some of these substances are liquids, that's obviously ridiculous. What is that basis for these calculations?

A soil RBC of 1 million parts per million means that no amount of the contaminant in soil will cause a receptor to exceed the oral reference dose by incidental ingestion of soil. In

fact, some contaminants would have RBCs of more than 1 million ppm, but the algorithms cap concentrations at 100%. The reason we retain these admittedly impossible numbers is to let users see that the contaminant is not a threat via soil ingestion.

However, it's important to realize that the RBC calculations do not consider the potential of soil contaminants to leach to groundwater or escape to air by volatilization or dust entrainment. To consider these inter-media transfers, it's necessary to either monitor air and groundwater, or to use a model. Measured or modeled air and groundwater concentrations should then be compared to the RBCs for air and tap water.

We have begun to incorporate inter-media transfers into the RBC table in the form of soil screening levels (SSLs). However, EPA Headquarters has proposed only about a hundred SSLs so far, so the list is still rather short.

12. Please elaborate on the meaning of the 'W' source code in the table.

The "W" code means that a reference dose or potency slope for a contaminant is currently not present on either IRIS or HEAST, but that it once was present on either IRIS or HEAST and was removed. Such withdrawal usually indicates that consensus on the number no longer exists among EPA scientists, but not that EPA believes the contaminant to be unimportant. Older versions of the RBC table had separate codes for IRIS and HEAST withdrawals, but we changed to a single code for both because, after all, it hardly matters.

We retain withdrawn numbers in the table because we still need to deal with these contaminants during the sometimes very long delays before replacement numbers are ready. We take the position that for the purpose of screening an obsolete RBC is better than none at all. The 'W' code should serve as a clear warning that before making any serious decision involving that contaminant you will need to develop an interim value based on current scientific understanding.

If you are assessing risks at a site where a major contaminant is coded "W", consider working with your Regional EPA risk assessor to develop a current toxicity constant. If the site is being studied under CERCLA, the EPA-NCEA Regional Technical Support group may be able to assist.

13. Can I get copies of supporting documents for interim toxicity constants which are coded "E" in the RBC table?

Unfortunately, Region 3 does not have a complete set of supporting documents. The EPA-NCEA Superfund Health Risk Technical Support Center prepares these interim toxicity constants in response to site-specific requests from Regional risk assessors, and sends the documentation only to the requestor. The RBC tables contain only the interim values (those with "E" codes) that we've either requested ourselves or otherwise obtained copies of. There may be many more interim values of which we are unaware. Also, we don't receive automatic updates when NCEA revisits a contaminant, so it's likely that some interim values in the RBC table are obsolete.

It has been NCEA's policy to deny requests for documentation of interim toxicity constants. Although Region 3 has sometimes provided this documentation on request, for the above-stated reasons we have no assurance that the documentation, or even the interim numbers, are current. We've decided to discontinue distributing information that may be misleading. If one of the "E"-coded contaminants is a major risk contributor at your site, we strongly suggest that you work with EPA to develop an up-to-date reference dose or slope factor.

CHANGES IN THIS ISSUE OF THE RBC TABLE

New or revised EPA toxicity constants are now marked with "**" before the contaminant name. This is to help users quickly pick out substances with new RBCs. Formerly these contaminants were printed in underlined boldface type that copied badly. A new basis code, "M" for MCL, has been added to the upper right corner of each page. This code denotes soil screening levels for groundwater protection that are based on EPA Maximum Contaminant Levels.

If you want to raise issues or get answers to questions about the RBC table, please call the Technical Support Help Line at 215-597-1116. The line has a voice mail system to take your calls if we're not available. We'll return your call as soon as we can. Please limit calls to RBC issues; if you have a question about applying RBCs to a site, please call the EPA Regional office handling the project. Thanks for your help and cooperation, and we hope the RBC table continues to be a useful resource.

Attachment

EPA Region III Risk-Based Concentration Table

Background Information

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October 4, 1995

Development of Risk-Based Concentrations

General

Separate carcinogenic and non-carcinogenic risk-based concentrations were calculated for each compound for each pathway. The concentration in the table is the lower of the two, rounded to two significant figures. The following terms and values were used in the calculations:

Exposure variables	**Value**	**Symbol**
General:		
Carcinogenic potency slope oral (risk per mg/kg/d):	*	CPSo
Carcinogenic potency slope inhaled (risk per mg/kg/d):	*	CPSi
Reference dose oral (mg/kg/d):	*	RfDo
Reference dose inhaled (mg/kg/d):	*	RfDi
Target cancer risk:	1e-06	TR
Target hazard quotient:	1	THQ
Body weight, adult (kg):	70	BWa
Body weight, age 1-6 (kg):	15	BWc
Averaging time carcinogens (d):	25550	ATc
Averaging time non-carcinogens (d):	ED*365	ATn
Inhalation, adult (m3/d):	20	IRAa
Inhalation, child (m3/d):	12	IRAc
Inhalation factor, age-adjusted (m3-y/kg-d):	11.66	IFAadj
Tap water ingestion, adult (L/d):	2	IRWa
Tap water ingestion, age 1-6 (L/d):	1	IRWc
Tap water ingestion factor, age-adjusted (L-y/kg-d):	1.09	IFWadj
Fish ingestion (g/d):	54	IRF
Soil ingestion, adult (mg/d):	100	IRSa
Soil ingestion, age 1-6 (mg/d):	200	IRSc
Soil ingestion factor, age adjusted (mg-y/kg-d):	114.29	IFSadj
Residential:		
Exposure frequency (d/y):	350	EFr
Exposure duration, total (y):	30	EDtot
Exposure duration, age 1-6 (y):	6	EDc
Volatilization factor (L/m3):	0.5	K

Exposure variables	Value	Symbol
Occupational:		
Exposure frequency (d/y):	250	EFo
Exposure duration (y):	25	EDo
Fraction of contaminated soil ingested (unitless)	0.5	FC

*: Contaminant-specific toxicological constants. The priority among sources of toxicological constants was as follows: (1) IRIS, (2) HEAST, (3) HEAST alternative method, (4) EPA-NCEA Superfund Health Risk Technical Support Center, (5) withdrawn from IRIS or HEAST, and (6) other EPA documents. Each source was used only if numbers from higher-priority sources were unavailable. The EPA Superfund Health Risk Technical Support Center, part of the EPA National Center for Environmental Assessment in Cincinnati, develops provisional RfDs and CPSs on request for contaminants not in IRIS or HEAST. These provisional values are labeled "E = EPA-NCEA provisional" in the table. It is possible they may be obsolete. If one of the "E" constants is important to a Superfund risk assessment, consider requesting, through a Regional risk assessor, a new provisional value.

Age-adjusted factors

Because contact rates with tap water, ambient air, and residential soil are different for children and adults, carcinogenic risks during the first 30 years of life were calculated using age-adjusted factors. These factors approximated the integrated exposure from birth until age 30 by combining contact rates, body weights, and exposure durations for two age groups - small children and adults. The age-adjusted factor for soil was obtained from RAGS IB; the others were developed by analogy.

Air inhalation

$$IFAadj \ \frac{m^3 \cdot y}{kg \cdot d} = \frac{EDc \cdot IRAc}{BWc} + \frac{(EDtot - EDc) \cdot IRAa}{BWa}$$

Tap water ingestion

$$IFWadj \ \frac{L \cdot y}{kg \cdot d} = \frac{EDc \cdot IRWc}{BWc} + \frac{(EDtot - EDc) \cdot IRWa}{BWa}$$

Soil ingestion

$$IFSadj \ \frac{mg \cdot y}{kg \cdot d} = \frac{EDc \cdot IRSc}{BWc} + \frac{(EDtot - EDc) \cdot IRSa}{BWa}$$

Residential water

Volatilization terms were calculated only for compounds with a mark in the "VOC" column. Compounds having a Henry's Law constant greater than 10^{-5} were considered volatile. The list may be incomplete, but is unlikely to include false positives. The equations and the volatilization factor (K, above) were obtained from RAGS IB. Oral potency slopes and reference doses were used for both oral and inhaled exposures for volatile compounds lacking inhalation values. Inhaled potency slopes were substituted for unavailable oral potency slopes only for volatile compounds; inhaled RfDs were substituted for unavailable

oral RfDs for both volatile and non-volatile compounds. RBCs for carcinogens were based on combined childhood and adult exposure; for non-carcinogens RBCs were based on adult exposure.

Carcinogens

$$RBC\ \frac{\mu g}{L} = \frac{TR \cdot ATc \cdot 1000\ \frac{\mu g}{mg}}{EFr \cdot ([\,K \cdot IFAadj \cdot CPSi\,] + [\,IFWadj \cdot CPSo\,])}$$

Non-carcinogens

$$RBC\ \frac{\mu g}{L} = \frac{THQ \cdot BWa \cdot ATn \cdot 1000\ \frac{\mu g}{mg}}{EFr \cdot EDtot \cdot \left(\frac{K \cdot IRAa}{RfDi} + \frac{IRWa}{RfDo}\right)}$$

Ambient air

Oral potency slopes and references were used where inhalation values were not available. RBCs for carcinogens were based on combined childhood and adult exposure; for non-carcinogens RBCs were based on adult exposure.

Carcinogens

$$RBC\ \frac{\mu g}{m^3} = \frac{TR \cdot ATc \cdot 1000\ \frac{\mu g}{mg}}{EFr \cdot IFAadj \cdot CPSi}$$

Non-carcinogens

$$RBC\ \frac{\mu g}{m^3} = \frac{THQ \cdot RfDi \cdot BWa \cdot ATn \cdot 1000\ \frac{\mu g}{mg}}{EFr \cdot EDtot \cdot IRAa}$$

Edible fish

All RBCs were based on adult exposure.

Carcinogens

$$RBC\ \frac{mg}{kg} = \frac{TR \cdot BWa \cdot ATc}{EFr \cdot EDtot \cdot \frac{IRF}{1000\ \frac{g}{kg}} \cdot CPSo}$$

Non-carcinogens

$$RBC\ \frac{mg}{kg} = \frac{THQ \cdot RfDo \cdot BWa \cdot ATn}{EFr \cdot EDtot \cdot \frac{IRF}{1000\ \frac{g}{kg}}}$$

Commercial/industrial soil ingestion

RBCs were based on adult occupational exposure, including an assumption that only 50% of total soil ingestion is work-related.

Carcinogens

$$RBC\ \frac{mg}{kg} = \frac{TR \cdot BWa \cdot ATc}{EFo \cdot EDo \cdot \frac{IRSa}{10^6\ \frac{mg}{kg}} \cdot FC \cdot CPSo}$$

Non-carcinogens

$$RBC\ \frac{mg}{kg} = \frac{THQ \cdot RfDo \cdot BWa \cdot ATn}{EFo \cdot EDo \cdot \frac{IRSa}{10^6\ \frac{mg}{kg}} \cdot FC}$$

Residential soil ingestion

RBCs for carcinogens were based on combined childhood and adult exposure; RBCs for non-carcinogens were based on childhood exposure only.

Carcinogens

$$RBC\ \frac{mg}{kg} = \frac{TR \cdot ATc}{EFr \cdot \frac{IFSadj}{10^6\ \frac{mg}{kg}} \cdot CPSo}$$

Non-carcinogens

$$RBC\ \frac{mg}{kg} = \frac{THQ \cdot RfDo \cdot BWc \cdot ATn}{EFr \cdot EDc \cdot \frac{IRSc}{10^6\ \frac{mg}{kg}}}$$

Development of Soil Screening Levels

General

In December 1994 the EPA Office of Solid Waste and Emergency Response proposed Soil Screening Guidance (Document 9355.4-1, PB95-963530, EPA540/R-94/101, available through NTIS at 703-487-4650). This draft document provides (1) a framework in which soil screening levels are to be used, (2) a detailed methodology for calculating soil screening levels, and (3) soil screening levels for 107 substances.

Consistent with this new guidance, the risk-based concentration table now includes two columns of generic soil screening levels (SSLs). OSWER's 107 proposed soil screening levels have been added verbatim. In addition, the proposed SSL methodology has been used to calculate soil screening levels for more substances, which are also included in the

new table. The table clearly distinguishes the OSWER SSLs from the "unofficial" ones.

These SSLs provide reasonable maximum estimates of transfers of contaminants from soil to other media. One column contains soil concentrations protective of groundwater quality; the other contains soil concentrations protective of air quality. "Protective" is defined in the same terms as the risk-based concentrations for tap water and air -- that residential contact scenarios will yield a fixed upper bound risk of 10^{-6} or a fixed hazard quotient of 1 (whichever occurs at the lower concentration).

OSWER's SSLs should be used only within the framework proposed in the guidance document. The additional SSLs included in the RBC table are intended for the same uses (although they obviously carry less weight than the formally proposed numbers).

The SSLs are based on the following assumptions:

Input variables	**Value**	**Symbol***
Surface soil moisture content (g/g)	0.1	W_s
Vadose zone soil moisture content (kg/kg)	0.2	W_v
Surface soil bulk density (g/cm^3)	1.5	ρ_{bs}
Vadose zone soil bulk density (kg/L)	1.5	ρ_{bv}
Surface soil particle density (g/cm^3)	2.65	ρ_{ss}
Vadose zone soil particle density (g/cm^3)	2.65	ρ_{sv}
Total surface soil porosity (L pore /L soil)	0.43	N_s
Total vadose zone soil porosity (L pore/L soil)	0.43	N_v
Air-filled surface soil porosity (L air/L soil)	0.28	θ_{as}
Water-filled surface soil porosity (L water/L soil)	0.15	θ_{ws}
Air-filled vadose zone soil porosity (L air/L soil)	0.13	θ_{av}
Water-filled vadose zone soil porosity (L water/L soil)	0.30	θ_{wv}
Organic carbon fraction of surface soil (g/g)	0.006	FOC_s
Organic carbon fraction of vadose zone soil (g/g)	0.002	FOC_v
Dispersion factor for 0.5 acres (g/m^{2}s per kg/m^3)	35.1	Q/C
Particulate emission factor (m^3/kg)	6.79e+08	PEF
Exposure interval (s)	9.50e+08	T
Dilution-attenuation factor (unitless)	10	DAF

*: Symbols were adjusted, variables were rearranged, and derived and chemical-specific variables were omitted for simplicity and clarity. Presentation of the input variables in a single table using the same terms as in the OSWER SSL document would have been confusing. The terms used here are generally similar to OSWER's, and can easily be compared with the SSL guidance document.

With two exceptions described in the following section, SSL calculations were based on the same algorithms presented in the OSWER draft SSL guidance document. For details of the calculations (and for general background information on SSLs), I strongly recommend

consulting that document. The "unofficial" SSLs were developed under the following conditions:

Soil Screening Levels for Inhalation

Inhaled reference doses and potency slopes were used if available. If inhalation values were not available, oral RfDs and potency slopes were substituted. SSLs were calculated only for substances for which aqueous solubility, Koc, Henry's Law constant, and diffusivity in air were available. SSLs were calculated only for substances for which a volatilization factor could be calculated. This was done because OSWER's large proposed particulate emission factor rendered it pointless to estimate SSLs for particulate emissions alone. The final calculated SSL shown in the RBC table is the smaller of the risk-based SSL and the soil saturation concentration. All calculated SSLs were rounded to 2 significant figures.

The OSWER risk algorithms for inhalation were revised in order to be consistent with the rest of the RBC table. Only calculated SSLs were affected by this; SSLs proposed by OSWER are presented verbatim. Calculated SSLs for inhalation of carcinogens were based on an integrated lifetime exposure rather than adult exposure. SSLs for inhalation of noncarcinogens were based on adult exposure for 350 days per year rather than 365 days per year. The following algorithms were used to calculate inhalation SSLs:

Carcinogens

$$SSL\ \frac{mg}{kg} = \frac{TR \cdot ATc}{EFr \cdot IFAadj \cdot \left(\frac{1}{VF} + \frac{1}{PEF}\right) \cdot CPSi}$$

Non-carcinogens

$$SSL\ \frac{mg}{kg} = \frac{THQ \cdot BWa \cdot ATn \cdot RfDi}{EFr \cdot EDtot \cdot IRAa \cdot \left(\frac{1}{VF} + \frac{1}{PEF}\right)}$$

Soil Screening Levels for Groundwater Use

All algorithms were as proposed by OSWER. MCLs were used as target groundwater concentrations if available. If MCLs were unavailable the risk-based concentration in the "tap water" column of the RBC table was used as the target groundwater concentration. All SSLs for groundwater are based on a dilution-attenuation factor (DAF) of 10. Since these SSLs scale linearly with DAF, the SSLs for DAF=1 would be ten times lower. They were omitted to conserve space. All groundwater SSLs were rounded to 2 significant figures and capped at unity.

Sources: I=IRIS H=HEAST A=HEAST alternate W=Withdrawn from IRIS or HEAST E=EPA-NCEA Regional Support provisional value O=Other EPA documents.

Basis: C=carcinogenic effects N=noncarcinogenic effects E=EPA draft Soil Screening Level S=soil saturation concentration M=EPA MCL.

Contaminant	CAS	RfDo mg/kg/d	RfDi mg/kg/d	CPSo kg·d/mg	CPSi kg·d/mg	VOC	Risk-Based Concentrations: Tap Water µg/L	Ambient Air µg/m3	Fish mg/kg	Soil Ingestion: Industrial mg/kg	Soil Ingestion: Residential mg/kg	Soil Screening Levels- Transfers from Soil to: Air mg/kg	Groundwater mg/kg
Acephate	30560191	4.00E-03 I		8.70E-03 I			7.7 C	0.72 C	0.36 C	660 C	73 C		
Acetaldehyde	75070		2.57E-03 I		7.70E-03 I		94 N	0.81 C					
Acetochlor	34256821	2.00E-02 I					730 N	73 N	27 N	41000 N	1600 N		
Acetone	67641	1.00E-01 I					3700 N	370 N	140 N	200000 N	7800 N	62000 E	8 E
Acetone cyanohydrin	75865	7.00E-02 H	4.00E-02 A				2600 N	150 N	95 N	140000 N	5500 N		
Acetonitrile	75078	6.00E-03 I	1.43E-02 A				220 N	52 N	8.1 N	12000 N	470 N		
Acetophenone	98862	1.00E-01 I	5.71E-06 W			X	0.042 N	0.021 N	140 N	200000 N	7800 N		
Acifluorfen	62476599	1.30E-02 I					470 N	47 N	18 N	27000 N	1000 N		
Acrolein	107028	2.00E-02 H	5.71E-06 I				730 N	0.021 N	27 N	41000 N	1600 N		
Acrylamide	79061	2.00E-04 I		4.50E+00 I	4.55E+00 I		0.015 C	0.0014 C	0.0007 C	1.3 C	0.14 C		
Acrylic acid	79107	5.00E-01 I	2.86E-04 I				18000 N	1 N	680 N	1E+06 N	39000 N		
Acrylonitrile	107131	1.00E-03 H	5.71E-04 I	5.40E-01 I	2.38E-01 I		0.12 C	0.026 C	0.0058 C	11 C	1.2 C		
Alachlor	15972608	1.00E-02 I		8.00E-02 H			0.84 C	0.078 C	0.039 C	72 C	8 C		
Alar	1596845	1.50E-01 I					5500 N	550 N	200 N	310000 N	12000 N		
Aldicarb	116063	1.00E-03 I					37 N	3.7 N	1.4 N	2000 N	78 N	570 S	0.036 M
Aldicarb sulfone	1646884	1.00E-03 I					37 N	3.7 N	1.4 N	2000 N	78 N		
Aldrin	309002	3.00E-05 I		1.70E+01 I	1.71E+01 I		0.004 C	0.00037 C	0.00019 C	0.34 C	0.038 C	0.5 E	0.005 E
Ally	74223646	2.50E-01 I					9100 N	910 N	340 N	510000 N	20000 N		
Allyl alcohol	107186	5.00E-03 I					180 N	18 N	6.8 N	10000 N	390 N		
Allyl chloride	107051	5.00E-02 W	2.86E-04 I				1800 N	1 N	68 N	100000 N	3900 N		
Aluminum	7429905	1.00E+00 E					37000 N	3700 N	1400 N	1E+06 N	78000 N		
Aluminum phosphide	20859738	4.00E-04 I					15 N	1.5 N	0.54 N	820 N	31 N		
Amdro	67485294	3.00E-04 I					11 N	1.1 N	0.41 N	610 N	23 N		
Ametryn	834128	9.00E-03 I					330 N	33 N	12 N	18000 N	700 N		
m-Aminophenol	591275	7.00E-02 H					2600 N	260 N	95 N	140000 N	5500 N		
4-Aminopyridine	504245	2.00E-05 H					0.73 N	0.073 N	0.027 N	41 N	1.6 N		
Amitraz	33089611	2.50E-03 I					91 N	9.1 N	3.4 N	5100 N	200 N		
Ammonia	7664417		2.86E-02 I				1000 N	100 N					
Ammonium sulfamate	7773060	2.00E-01 I					7300 N	730 N	270 N	410000 N	16000 N		
Aniline	62533		2.86E-04 I	5.70E-03 I			10 N	1 N	0.55 C	1000 C	110 C	45 N	0.03 I
Antimony and compounds	7440360	4.00E-04 I					15 N	1.5 N	0.54 N	820 N	31 N		
Antimony pentoxide	1314609	5.00E-04 H					18 N	1.8 N	0.68 N	1000 N	39 N		
Antimony potassium tartrate	304610	9.00E-04 H					33 N	3.3 N	1.2 N	1800 N	70 N		
Antimony tetroxide	1332316	4.00E-04 H					15 N	1.5 N	0.54 N	820 N	31 N		
Antimony trioxide	1309644	4.00E-04 H					15 N	1.5 N	0.54 N	820 N	31 N		
Apollo	74115245	1.30E-02 I					470 N	47 N	18 N	27000 N	1000 N		
Aramite	140578	5.00E-02 H		2.50E-02 I	2.49E-02 I		2.7 C	0.25 C	0.13 C	230 C	26 C		
Arsenic	7440382	3.00E-04 I					11 N	1.1 N	0.41 N	610 N	23 N	380 E	15 E
**Arsenic (as carcinogen)	7440382			1.50E+00 I	1.51E+01 I		0.045 C	0.00041 C	0.0021 C	3.8 C	0.43 C	380 E	15 E

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Arsine	7784421		1.43E-05 I				0.52 N	0.052 N					
Assure	76578148	9.00E-03 I					330 N	33 N	12 N	18000 N	700 N		
Asulam	3337711	5.00E-02 I					1800 N	180 N	68 N	100000 N	3900 N		
Atrazine	1912249	3.50E-02 I		2.22E-01 H			0.3 C	0.028 C	0.014 C	26 C	2.9 C		
Avermectin B1	65195553	4.00E-04 I					15 N	1.5 N	0.54 N	820 N	31 N		
Azobenzene	103333			1.10E-01 I	1.08E-01 I		0.61 C	0.058 C	0.029 C	52 C	5.8 C		
Barium and compounds	7440393	7.00E-02 I	1.43E-04 A				2600 N	0.52 N	95 N	140000 N	5500 N	350000 E	32 E
Baygon	114261	4.00E-03 I					150 N	15 N	5.4 N	8200 N	310 N		
Bayleton	43121433	3.00E-02 I					1100 N	110 N	41 N	61000 N	2300 N		
Baythroid	68359375	2.50E-02 I					910 N	91 N	34 N	51000 N	2000 N		
Benefin	1861401	3.00E-01 I					11000 N	1100 N	410 N	610000 N	23000 N		
Benomyl	17804352	5.00E-02 I					1800 N	180 N	68 N	100000 N	3900 N		
Bentazon	25057890	2.50E-03 I					91 N	9.1 N	3.4 N	5100 N	200 N		
Benzaldehyde	100527	1.00E-01 I				☒	610 N	370 N	140 N	200000 N	7800 N		
Benzene	71432		1.71E-03 E	2.90E-02 I	2.90E-02 I	☒	0.36 C	0.22 C	0.11 C	200 C	22 C	0.5 E	0.02 E
Benzenethiol	108985	1.00E-05 H					0.37 N	0.037 N	0.014 N	20 N	0.78 N		
Benzidine	92875	3.00E-03 I		2.30E+02 I	2.35E+02 I		0.00029 C	0.00003 C	0.00001 C	0.025 C	0.0028 C	1.3 C	1.100E-06 C
Benzoic acid	65850	4.00E+00 I					150000 N	15000 N	5400 N	1E+06 N	310000 N	320 S	280 E
Benzotrichloride	98077			1.30E+01 I			0.0052 C	0.00048 C	0.00024 C	0.44 C	0.049 C	0.012 C	0.000073 C
Benzyl alcohol	100516	3.00E-01 H					11000 N	1100 N	410 N	610000 N	23000 N		
Benzyl chloride	100447			1.70E-01 I		☒	0.062 C	0.037 C	0.019 C	34 C	3.8 C	0.5 C	0.0003
Beryllium and compounds	7440417	5.00E-03 I		4.30E+00 I	8.40E+00 I		0.016 C	0.00075 C	0.00073 C	1.3 C	0.15 C	690 E	180 E
Bidrin	141662	1.00E-04 I					3.7 N	0.37 N	0.14 N	200 N	7.8 N		
Biphenthrin (Talstar)	82657043	1.50E-02 I					550 N	55 N	20 N	31000 N	1200 N		
1,1-Biphenyl	92524	5.00E-02 I					1800 N	180 N	68 N	100000 N	3900 N	9000 S	110 N
Bis(2-chloroethyl)ether	111444			1.10E+00 I	1.16E+00 I	☒	0.0092 C	0.0054 C	0.0029 C	5.2 C	0.58 C	0.3 E	0.0003 E
Bis(2-chloroisopropyl)ether	39638329	4.00E-02 I		7.00E-02 H	3.50E-02 H	☒	0.26 C	0.18 C	0.045 C	82 C	9.1 C		
Bis(chloromethyl)ether	542881			2.20E+02 I	2.17E+02 I	☒	0.00005 C	0.00003 C	0.00001 C	0.026 C	0.0029 C	0.00004 C	1.000E-07 C
Bis(2-chloro-1-methylethyl)ether				7.00E-02 W	7.00E-02 W		0.96 C	0.089 C	0.045 C	82 C	9.1 C		
Bis(2-ethylhexyl)phthalate (DEHP)	117817	2.00E-02 I		1.40E-02 I			4.8 C	0.45 C	0.23 C	410 C	46 C	210 E	11 E
Bisphenol A	80057	5.00E-02 I					1800 N	180 N	68 N	100000 N	3900 N		
Boron (and borates)	7440428	9.00E-02 I	5.71E-03 H				3300 N	21 N	120 N	180000 N	7000 N		
Boron trifluoride	7637072		2.00E-04 H				7.3 N	0.73 N					
Bromodichloromethane	75274	2.00E-02 I		6.20E-02 I		☒	0.17 C	0.1 C	0.051 C	92 C	10 C	1800 E	0.3 E
Bromoethene	593602				1.10E-01 H	☒	0.096 C	0.057 C					
Bromoform (tribromomethane)	75252	2.00E-02 I		7.90E-03 I	3.85E-03 I	☒	2.4 C	1.6 C	0.4 C	720 C	81 C	46 E	0.5 E
Bromomethane	74839	1.40E-03 I	1.43E-03 I			☒	8.7 N	5.2 N	1.9 N	2900 N	110 N	2 E	0.1 E
4-Bromophenyl phenyl ether	101553	5.80E-02 O					2100 N	210 N	78 N	120000 N	4500 N		
Bromophos	2104963	5.00E-03 H					180 N	18 N	6.8 N	10000 N	390 N		

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Bromoxynil	1689845	2.00E-02 I					730 N	73 N	27 N	41000 N	1600 N		
Bromoxynil octanoate	1689992	2.00E-02 I					730 N	73 N	27 N	41000 N	1600 N		
1,3-Butadiene	106990				9.80E-01 I	☒	0.011 C	0.0064 C				0.0013 C	0.000072 C
1-Butanol	71363	1.00E-01 I					3700 N	370 N	140 N	200000 N	7800 N	9700 E	8 E
Butyl benzyl phthalate	85687	2.00E-01 I					7300 N	730 N	270 N	410000 N	16000 N	530 E	68 E
Butylate	2008415	5.00E-02 I					1800 N	180 N	68 N	100000 N	3900 N		
sec-Butylbenzene	135988	1.00E-02 E				☒	61 N	37 N	14 N	20000 N	780 N	80 S	0.27 M
tert-Butylbenzene	104518	1.00E-02 E				☒	61 N	37 N	14 N	20000 N	780 N		0.27 M
Butylphthalyl butylglycolate	85701	1.00E+00 I					37000 N	3700 N	1400 N	1E+06 N	78000 N		
Cacodylic acid	75605	3.00E-03 H					110 N	11 N	4.1 N	6100 N	230 N		
**Cadmium and compounds	7440439	5.00E-04 I	5.71E-05 E		6.30E+00 I		18 N	0.00099 C	0.68 N	1000 N	39 N	920 E	6 E
Caprolactam	105602	5.00E-01 I					18000 N	1800 N	680 N	1E+06 N	39000 N		
Captafol	2425061	2.00E-03 I		8.60E-03 H			7.8 C	0.73 C	0.37 C	670 C	74 C		
Captan	133062	1.30E-01 I		3.50E-03 H			19 C	1.8 C	0.9 C	1600 C	180 C		
Carbaryl	63252	1.00E-01 I					3700 N	370 N	140 N	200000 N	7800 N	0.34 S	23 N
Carbofuran	1563662	5.00E-03 I					180 N	18 N	6.8 N	10000 N	390 N		
**Carbon disulfide	75150	1.00E-01 I	2.00E-01 I			☒	1000 N	730 N	140 N	200000 N	7800 N	11 E	14 E
Carbon tetrachloride	56235	7.00E-04 I	5.71E-04 E	1.30E-01 I	5.25E-02 I	☒	0.16 C	0.12 C	0.024 C	44 C	4.9 C	0.2 E	0.03 E
Carbosulfan	55285148	1.00E-02 I					370 N	37 N	14 N	20000 N	780 N		
Carboxin	5234684	1.00E-01 I					3700 N	370 N	140 N	200000 N	7800 N		
Chloral	75876	2.00E-03 I					73 N	7.3 N	2.7 N	4100 N	160 N		
Chloramben	133904	1.50E-02 I					550 N	55 N	20 N	31000 N	1200 N		
Chloranil	118752			4.03E-01 H			0.17 C	0.016 C	0.0078 C	14 C	1.6 C		
Chlordane	57749	6.00E-05 I		1.30E+00 I	1.29E+00 I		0.052 C	0.0049 C	0.0024 C	4.4 C	0.49 C	10 E	2 E
Chlorimuron-ethyl	90982324	2.00E-02 I					730 N	73 N	27 N	41000 N	1600 N		
Chlorine	7782505	1.00E-01 I					3700 N	370 N	140 N	200000 N	7800 N		
Chlorine dioxide	10049044		5.71E-05 I				2.1 N	0.21 N					
Chloroacetaldehyde	107200	6.90E-03 O					250 N	25 N	9.3 N	14000 N	540 N		
Chloroacetic acid	79118	2.00E-03 H					73 N	7.3 N	2.7 N	4100 N	160 N		
2-Chloroacetophenone	532274		8.57E-06 I				0.31 N	0.031 N					
4-Chloroaniline	106478	4.00E-03 I					150 N	15 N	5.4 N	8200 N	310 N	1200 S	0....
Chlorobenzene	108907	2.00E-02 I	5.71E-03 A			☒	39 N	21 N	27 N	41000 N	1600 N	94 E	0.6 E
Chlorobenzilate	510156	2.00E-02 I		2.70E-01 H	2.70E-01 H		0.25 C	0.023 C	0.012 C	21 C	2.4 C		
p-Chlorobenzoic acid	74113	2.00E-01 H					7300 N	730 N	270 N	410000 N	16000 N		
4-Chlorobenzotrifluoride	98566	2.00E-02 H					730 N	73 N	27 N	41000 N	1600 N	86 N	7.5 N
2-Chloro-1,3-butadiene	126998	2.00E-02 A	2.00E-03 H			☒	14 N	7.3 N	27 N	41000 N	1600 N		
1-Chlorobutane	109693	4.00E-01 H				☒	2400 N	1500 N	540 N	820000 N	31000 N		
Chlorodibromomethane	124481	2.00E-02 I		8.40E-02 I		☒	0.13 C	0.075 C	0.038 C	68 C	7.6 C	1900 E	0.2 E
**1-Chloro-1,1-difluoroethane	75683	I	1.43E+01			☒	87000 N	52000 N					

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Chlorodifluoromethane	75456		1.43e+01 I			☒	87000 N	52000 N					
Chloroethane	75003	4.00E-01 E	2.86E+00 I			☒	8600 N	10000 N	540 N	820000 N	31000 N	2600 S	33 N
2-Chloroethyl vinyl ether	110758	2.50E-02 O				☒	150 N	91 N	34 N	51000 N	2000 N		
Chloroform	67663	1.00E-02 I		6.10E-03 I	8.05E-02 I	☒	0.15 C	0.078 C	0.52 C	940 C	100 C	0.2 E	0.
Chloromethane	74873			1.30E-02 H	6.30E-03 H	☒	1.4 C	0.99 C	0.24 C	440 C	49 C	0.063 C	0.0066 C
4-Chloro-2,2-methylaniline hydrochloride	3165933			4.60E-01 H			0.15 C	0.014 C	0.0069 C	12 C	1.4 C		
4-Chloro-2-methylaniline	95692			5.80E-01 H			0.12 C	0.011 C	0.0054 C	9.9 C	1.1 C		
beta-Chloronaphthalene	91587	8.00E-02 I					2900 N	290 N	110 N	160000 N	6300 N	2.8 S	140 N
o-Chloronitrobenzene	88733			2.50E-02 H		☒	0.42 C	0.25 C	0.13 C	230 C	26 C		
p-Chloronitrobenzene	100005			1.80E-02 H		☒	0.59 C	0.35 C	0.18 C	320 C	35 C		
2-Chlorophenol	95578	5.00E-03 I					180 N	18 N	6.8 N	10000 N	390 N	53000 E	2 E
2-Chloropropane	75296		2.86E-02 H			☒	170 N	100 N				22 N	0.64 N
Chlorothalonil	1897456	1.50E-02 I		1.10E-02 H			6.1 C	0.57 C	0.29 C	520 C	58 C		
o-Chlorotoluene	95498	2.00E-02 I				☒	120 N	73 N	27 N	41000 N	1600 N	1200 N	5.6 N
Chlorpropham	101213	2.00E-01 I					7300 N	730 N	270 N	410000 N	16000 N		
Chlorpyrifos	2921882	3.00E-03 I					110 N	11 N	4.1 N	6100 N	230 N		
Chlorpyrifos-methyl	5598130	1.00E-02 H					370 N	37 N	14 N	20000 N	780 N		
Chlorsulfuron	64902723	5.00E-02 I					1800 N	180 N	68 N	100000 N	3900 N		
Chlorthiophos	60238564	8.00E-04 H					29 N	2.9 N	1.1 N	1600 N	63 N		
Chromium III and compounds	16065831	1.00E+00 I	5.71E-07 W				37000 N	0.0021 N	1400 N	1E+06 N	78000 N		
Chromium VI and compounds	18540299	5.00E-03 I			4.20E+01 I		180 N	0.00015 C	6.8 N	10000 N	390 N	140 E	1
Coal tar	8001589				2.20E+00 W			0.0028 C					
Cobalt	7440484	6.00E-02 E					2200 N	220 N	81 N	120000 N	4700 N		
Coke Oven Emissions	8007452				2.17E+00 I			0.0029 C					
**Copper and compounds	7440508	4.00E-02 E					1500 N	150 N	54 N	82000 N	3100 N		
Crotonaldehyde	123739	1.00E-02 W		1.90E+00 H	1.90E+00 W		0.035 C	0.0033 C	0.0017 C	3 C	0.34 C		
Cumene	98828	4.00E-02 I	2.57E-03 H				1500 N	9.4 N	54 N	82000 N	3100 N	81 N	65 N
Cyanides:													
Barium cyanide	542621	1.00E-01 W					3700 N	370 N	140 N	200000 N	7800 N		
Calcium cyanide	592018	4.00E-02 I					1500 N	150 N	54 N	82000 N	3100 N		
Copper cyanide	544923	5.00E-03 I					180 N	18 N	6.8 N	10000 N	390 N		
Cyanazine	21725462	2.00E-03 H		8.40E-01 H			0.08 C	0.0075 C	0.0038 C	6.8 C	0.76 C		
Cyanogen	460195	4.00E-02 I					1500 N	150 N	54 N	82000 N	3100 N		
Cyanogen bromide	506683	9.00E-02 I					3300 N	330 N	120 N	180000 N	7000 N		
Cyanogen chloride	506774	5.00E-02 I					1800 N	180 N	68 N	100000 N	3900 N		
Free cyanide	57125	2.00E-02 I					730 N	73 N	27 N	41000 N	1600 N		
Hydrogen cyanide	74908	2.00E-02 I	8.57E-04 I				730 N	3.1 N	27 N	41000 N	1600 N		
Potassium cyanide	151508	5.00E-02 I					1800 N	180 N	68 N	100000 N	3900 N		
Potassium silver cyanide	506616	2.00E-01 I					7300 N	730 N	270 N	410000 N	16000 N		

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Silver cyanide	506649	1.00E-01 I					3700 N	370 N	140 N	200000 N	7800 N		
Sodium cyanide	143339	4.00E-02 I					1500 N	150 N	54 N	82000 N	3100 N		
**Thiocyanate		2.00E-02 E					730 N	73 N	27 N	41000 N	1600 N		
Zinc cyanide	557211	5.00E-02 I					1800 N	180 N	68 N	100000 N	3900 N		
Cyclohexanone	108941	5.00E+00 I				☒	30000 N	18000 N	6800 N	1E+06 N	390000 N		
Cyclohexlamine	108918	2.00E-01 I					7300 N	730 N	270 N	410000 N	16000 N		
Cyhalothrin/Karate	68085858	5.00E-03 I					180 N	18 N	6.8 N	10000 N	390 N		
Cypermethrin	52315078	1.00E-02 I					370 N	37 N	14 N	20000 N	780 N		
Cyromazine	66215278	7.50E-03 I					270 N	27 N	10 N	15000 N	590 N		
Dacthal	1861321	1.00E-02 I					370 N	37 N	14 N	20000 N	780 N		
Dalapon	75990	3.00E-02 I					1100 N	110 N	41 N	61000 N	2300 N		
Danitol	39515418	2.50E-02 I					910 N	91 N	34 N	51000 N	2000 N		
DDD	72548			2.40E-01 I			0.28 C	0.026 C	0.013 C	24 C	2.7 C	37 S	0.
DDE	72559			3.40E-01 I			0.2 C	0.018 C	0.0093 C	17 C	1.9 C	10 S	0.5 E
DDT	50293	5.00E-04 I		3.40E-01 I	3.40E-01 I		0.2 C	0.018 C	0.0093 C	17 C	1.9 C	80 E	1 E
Decabromodiphenyl ether	1163195	1.00E-02 I				☒	61 N	37 N	14 N	20000 N	780 N		
Demeton	8065483	4.00E-05 I					1.5 N	0.15 N	0.054 N	82 N	3.1 N		
Diallate	2303164			6.10E-02 H		☒	0.17 C	0.1 C	0.052 C	94 C	10 C		
Diazinon	333415	9.00E-04 H					33 N	3.3 N	1.2 N	1800 N	70 N	5400 S	2.8 N
Dibenzofuran	132649	4.00E-03 E					150 N	15 N	5.4 N	8200 N	310 N	120 S	120 N
1,4-Dibromobenzene	106376	1.00E-02 I				☒	61 N	37 N	14 N	20000 N	780 N		
1,2-Dibromo-3-chloropropane	96128		5.71E-05 I	1.40E+00 H	2.42E-03 H	☒	0.048 C	0.21 N	0.0023 C	4.1 C	0.46 C	1.9 N	0.00061 M
1,2-Dibromoethane	106934		5.71E-05 H	8.50E+01 I	7.70E-01 I	☒	0.00075 C	0.0081 C	0.00004 C	0.067 C	0.0075 C	0.0058 C	0.00018 M
Dibutyl phthalate	84742	1.00E-01 I					3700 N	370 N	140 N	200000 N	7800 N	100 E	120 E
Dicamba	1918009	3.00E-02 I					1100 N	110 N	41 N	61000 N	2300 N		
1,2-Dichlorobenzene	95501	9.00E-02 I	4.00E-02 A			☒	270 N	150 N	120 N	180000 N	7000 N	300 E	6 E
1,3-Dichlorobenzene	541731	8.90E-02 O				☒	540 N	320 N	120 N	180000 N	7000 N		
1,4-Dichlorobenzene	106467		2.29E-01 I	2.40E-02 H		☒	0.44 C	0.26 C	0.13 C	240 C	27 C	7700 E	1 E
3,3'-Dichlorobenzidine	91941			4.50E-01 I			0.15 C	0.014 C	0.007 C	13 C	1.4 C	52 S	0.01 E
1,4-Dichloro-2-butene	764410				9.30E+00 H	☒	0.0011 C	0.00067 C					
Dichlorodifluoromethane	75718	2.00E-01 I	5.71E-02 A			☒	390 N	210 N	270 N	410000 N	16000 N	37 N	7..
1,1-Dichloroethane	75343	1.00E-01 H	1.43E-01 A			☒	810 N	520 N	140 N	200000 N	7800 N	980 E	11 E
1,2-Dichloroethane (EDC)	107062		2.86E-03 E	9.10E-02 I	9.10E-02 I	☒	0.12 C	0.069 C	0.035 C	63 C	7 C	0.3 E	0.01 E
1,1-Dichloroethylene	75354	9.00E-03 I		6.00E-01 I	1.75E-01 I	☒	0.044 C	0.036 C	0.0053 C	9.5 C	1.1 C	0.04 E	0.03 E
1,2-Dichloroethylene (cis)	156592	1.00E-02 H				☒	61 N	37 N	14 N	20000 N	780 N	1500 E	0.2 E
1,2-Dichloroethylene (trans)	156605	2.00E-02 I				☒	120 N	73 N	27 N	41000 N	1600 N	3600 E	0.3 E
1,2-Dichloroethylene (mixture)	540590	9.00E-03 H				☒	55 N	33 N	12 N	18000 N	700 N		
2,4-Dichlorophenol	120832	3.00E-03 I					110 N	11 N	4.1 N	6100 N	230 N	4800 S	0.5 E
2,4-Dichlorophenoxyacetic Acid (2,4-D)	94757	1.00E-02 I				☒	61 N	37 N	14 N	20000 N	780 N	7000 S	1.7 M

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4-(2,4-Dichlorophenoxy)butyric Acid	94826	8.00E-03 I					290 N	29 N	11 N	16000 N	630 N		
1,2-Dichloropropane	78875		1.14E-03 I	6.80E-02 H		☒	0.16 C	0.092 C	0.046 C	84 C	9.4 C	11 E	0.02 E
2,3-Dichloropropanol	616239	3.00E-03 I					110 N	11 N	4.1 N	6100 N	230 N		
1,3-Dichloropropene	542756	3.00E-04 I	5.71E-03 I	1.75E-01 H	1.30E-01 H	☒	0.077 C	0.048 C	0.018 C	33 C	3.7 C	0.1 E	0.001
Dichlorvos	62737	5.00e-04 I	1.43E-04 I	2.90E-01 I			0.23 C	0.022 C	0.011 C	20 C	2.2 C	3.5 C	0.00072 C
Dicofol	115322			4.40E-01 W			0.15 C	0.014 C	0.0072 C	13 C	1.5 C		
Dicyclopentadiene	77736	3.00E-02 H	5.71E-05 A			☒	0.42 N	0.21 N	41 N	61000 N	2300 N		
Dieldrin	60571	5.00E-05 I		1.60E+01 I	1.61E+01 I		0.0042 C	0.00039 C	0.0002 C	0.36 C	0.04 C	2 E	0.001 E
Diesel emissions			1.43E-03 I				52 N	5.2 N					
Diethyl phthalate	84662	8.00E-01 I					29000 N	2900 N	1100 N	1E+06 N	63000 N	520 E	110 E
Diethylene glycol, monobutyl ether	112345		5.71E-03 H				210 N	21 N					
Diethylene glycol, monoethyl ether	111900	2.00E+00 H					73000 N	7300 N	2700 N	1E+06 N	160000 N		
Diethylforamide	617845	1.10E-02 H					400 N	40 N	15 N	22000 N	860 N		
Di(2-ethylhexyl)adipate	103231	6.00E-01 I		1.20E-03 I			56 C	5.2 C	2.6 C	4800 C	530 C		
Diethylstilbestrol	56531			4.70E+03 H			0.00001 C	1E-06 C	7E-07 C	0.0012 C	0.00014 C		
Difenzoquat (Avenge)	43222486	8.00E-02 I					2900 N	290 N	110 N	160000 N	6300 N		
Diflubenzuron	35367385	2.00E-02 I					730 N	73 N	27 N	41000 N	1600 N		
1,1-Difluoroethane	75376		1.14E+01 I			☒	69000 N	42000 N					
Diisopropyl methylphosphonate (DIMP)	1445756	8.00E-02 I					2900 N	290 N	110 N	160000 N	6300 N		
Dimethipin	55290647	2.00E-02 I					730 N	73 N	27 N	41000 N	1600 N		
Dimethoate	60515	2.00E-04 I					7.3 N	0.73 N	0.27 N	410 N	16 N		
3,3'-Dimethoxybenzidine	119904			1.40E-02 H			4.8 C	0.45 C	0.23 C	410 C	46 C		
Dimethylamine	124403		5.71E-06 W				0.21 N	0.021 N					
2,4-Dimethylaniline hydrochloride	21436964			5.80E-01 H			0.12 C	0.011 C	0.0054 C	9.9 C	1.1 C		
2,4-Dimethylaniline	95681			7.50E-01 H			0.09 C	0.0083 C	0.0042 C	7.6 C	0.85 C		
N-N-Dimethylaniline	121697	2.00E-03 I					73 N	7.3 N	2.7 N	4100 N	160 N		
3,3'-Dimethylbenzidine	119937			9.20E+00 H			0.0073 C	0.00068 C	0.00034 C	0.62 C	0.069 C	29 C	0.00039 C
N,N-Dimethylformamide	68122	1.00E-01 H	8.57E-03 I				3700 N	31 N	140 N	200000 N	7800 N		
1,1-Dimethylhydrazine	57147			2.60E+00 W	3.50E+00 W		0.026 C	0.0018 C	0.0012 C	2.2 C	0.25 C		
1,2-Dimethylhydrazine	540738			3.70E+01 W	3.70E+01 W		0.0018 C	0.00017 C	0.00009 C	0.15 C	0.017 C		
2,4-Dimethylphenol	105679	2.00E-02 I					730 N	73 N	27 N	41000 N	1600 N	5400 S	3 E
2,6-Dimethylphenol	576261	6.00E-04 I					22 N	2.2 N	0.81 N	1200 N	47 N		
3,4-Dimethylphenol	95658	1.00E-03 I					37 N	3.7 N	1.4 N	2000 N	78 N		
Dimethyl phthalate	131113	1.00E+01 H					370000 N	37000 N	14000 N	1E+06 N	780000 N	1600 E	1200 E
Dimethyl terephthalate	120616	1.00E-01 I					3700 N	370 N	140 N	200000 N	7800 N		
1,2-Dinitrobenzene	528290	4.00E-04 H					15 N	1.5 N	0.54 N	820 N	31 N		
1,3-Dinitrobenzene	99650	1.00E-04 I					3.7 N	0.37 N	0.14 N	200 N	7.8 N		
1,4-Dinitrobenzene	100254	4.00E-04 H					15 N	1.5 N	0.54 N	820 N	31 N		
4,6-Dinitro-o-cyclohexyl phenol	131895	2.00E-03 I					73 N	7.3 N	2.7 N	4100 N	160 N		

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2,4-Dinitrophenol	51285	2.00E-03 I					73 N	7.3 N	2.7 N	4100 N	160 N	360 N	0.1 E
Dinitrotoluene mixture				6.80E-01 I			0.099 C	0.0092 C	0.0046 C	8.4 C	0.94 C		
2,4-Dinitrotoluene	121142	2.00E-03 I					73 N	7.3 N	2.7 N	4100 N	160 N	120 S	0.2 E
2,6-Dinitrotoluene	606202	1.00E-03 H					37 N	3.7 N	1.4 N	2000 N	78 N	370 S	0.1 E
Dinoseb	88857	1.00E-03 I					37 N	3.7 N	1.4 N	2000 N	78 N		
di-n-Octyl phthalate	117840	2.00E-02 H					730 N	73 N	27 N	41000 N	1600 N	1000000 S	1000000 E
1,4-Dioxane	123911			1.10E-02 I			6.1 C	0.57 C	0.29 C	520 C	58 C		
Diphenamid	957517	3.00E-02 I					1100 N	110 N	41 N	61000 N	2300 N		
Diphenylamine	122394	2.50E-02 I					910 N	91 N	34 N	51000 N	2000 N		
1,2-Diphenylhydrazine	122667			8.00E-01 I	7.70E-01 I		0.084 C	0.0081 C	0.0039 C	7.2 C	0.8 C		
Diquat	8 007	2.20E-03 I					80 N	8 N	3 N	4500 N	170 N		
Direct black 38	1937377			8.60E+00 H			0.0078 C	0.00073 C	0.00037 C	0.67 C	0.074 C		
Direct blue 6	2602462			8.10E+00 H			0.0083 C	0.00077 C	0.00039 C	0.71 C	0.079 C		
Direct brown 95	16071866			9.30E+00 H			0.0072 C	0.00067 C	0.00034 C	0.62 C	0.069 C		
Disulfoton	298044	4.00E-05 I					1.5 N	0.15 N	0.054 N	82 N	3.1 N		
1,4-Dithiane	505293	1.00E-02 I					370 N	37 N	14 N	20000 N	780 N		
Diuron	330541	2.00E-03 I					73 N	7.3 N	2.7 N	4100 N	160 N		
Dodine	2439103	4.00E-03 I					150 N	15 N	5.4 N	8200 N	310 N		
Endosulfan	115297	6.00E-03 I					220 N	22 N	8.1 N	12000 N	470 N	1 S	3 E
Endothall	145733	2.00E-02 I					730 N	73 N	27 N	41000 N	1600 N		
Endrin	72208	3.00E-04 I					11 N	1.1 N	0.41 N	610 N	23 N	16 S	0.4 E
Epichlorohydrin	106898	2.00E-03 H	2.86E-04 I	9.90E-03 I	4.20E-03 I		6.8 C	1 N	0.32 C	580 C	65 C		
1,2-Epoxybutane	106887		5.71E-03 I				210 N	21 N					
Ethephon (2-chloroethyl phosphonic acid)	16672870	5.00E-03 I					180 N	18 N	6.8 N	10000 N	390 N		
Ethion	563122	5.00E-04 I					18 N	1.8 N	0.68 N	1000 N	39 N		
2-Ethoxyethanol acetate	111159	3.00E-01 A					11000 N	1100 N	410 N	610000 N	23000 N		
2-Ethoxyethanol	110805	4.00E-01 H	5.71E-02 I				15000 N	210 N	540 N	820000 N	31000 N		
Ethyl acrylate	140885			4.80E-02 H			1.4 C	0.13 C	0.066 C	120 C	13 C		
EPTC (S-Ethyl dipropylthiocarbamate)	759944	2.50E-02 I					910 N	91 N	34 N	51000 N	2000 N		
Ethyl acetate	141786	9.00E-01 I					33000 N	3300 N	1200 N	1E+06 N	70000 N		
Ethylbenzene	100414	1.00E-01 I	2.86E-01 I			☒	1300 N	1000 N	140 N	200000 N	7800 N	260 E	3
Ethylene cyanohydrin	109784	3.00E-01 H					11000 N	1100 N	410 N	610000 N	23000 N		
Ethylene diamine	107153	2.00E-02 H					730 N	73 N	27 N	41000 N	1600 N		
Ethylene glycol	107211	2.00E+00 I					73000 N	7300 N	2700 N	1E+06 N	160000 N		
Ethylene glycol, monobutyl ether	111762		5.71E-03 H				210 N	21 N					
Ethylene oxide	75218			1.02E+00 H	3.50E-01 H		0.066 C	0.018 C	0.0031 C	5.6 C	0.63 C		
Ethylene thiourea (ETU)	96457	8.00E-05 I		1.19E-01 H			0.57 C	0.053 C	0.027 C	48 C	5.4 C		
Ethyl ether	60297	2.00E-01 I				☒	1200 N	730 N	270 N	410000 N	16000 N		
Ethyl methacrylate	97632	9.00E-02 H					3300 N	330 N	120 N	180000 N	7000 N		

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Ethyl p-nitrophenyl phenylphosphorothioate	2104645	1.00E-05 I					0.37 N	0.037 N	0.014 N	20 N	0.78 N		
Ethylnitrosourea	759739			1.40E+02 W			0.00048 C	0.00005 C	0.00002 C	0.041 C	0.0046 C		
Ethylphthalyl ethyl glycolate	84720	3.00E+00 I					110000 N	11000 N	4100 N	1E+06 N	230000 N		
Express	10120	8.00E-03 I					290 N	29 N	11 N	16000 N	630 N		
Fenamiphos	22224926	2.50E-04 I					9.1 N	0.91 N	0.34 N	510 N	20 N		
Fluometuron	2164172	1.30E-02 I					470 N	47 N	18 N	27000 N	1000 N		
Fluoride	7782414	6.00E-02 I					2200 N	220 N	81 N	120000 N	4700 N		
Fluoridone	59756604	8.00E-02 I					2900 N	290 N	110 N	160000 N	6300 N		
Flurprimidol	56425913	2.00E-02 I					730 N	73 N	27 N	41000 N	1600 N		
Flutolanil	66332965	6.00E-02 I					2200 N	220 N	81 N	120000 N	4700 N		
Fluvalinate	69409945	1.00E-02 I					370 N	37 N	14 N	20000 N	780 N		
Folpet	133073	1.00E-01 I		3.50E-03 I			19 C	1.8 C	0.9 C	1600 C	180 C		
Fomesafen	72178020			1.90E-01 I			0.35 C	0.033 C	0.017 C	30 C	3.4 C		
Fonofos	944229	2.00E-03 I					73 N	7.3 N	2.7 N	4100 N	160 N		
Formaldehyde	50000	2.00E-01 I			4.55E-02 I		7300 N	0.14 C	270 N	410000 N	16000 N		
Formic Acid	64186	2.00E+00 H					73000 N	7300 N	2700 N	1E+06 N	160000 N		
Fosetyl-al	39148248	3.00E+00 I					110000 N	11000 N	4100 N	1E+06 N	230000 N		
Furan	110009	1.00E-03 I					37 N	3.7 N	1.4 N	2000 N	78 N		
Furazolidone	67458			3.80E+00 H			0.018 C	0.0016 C	0.00083 C	1.5 C	0.17 C		
Furfural	98011	3.00E-03 I	1.43E-02 A				110 N	52 N	4.1 N	6100 N	230 N		
Furium	531828			5.00E+01 H			0.0013 C	0.00013 C	0.00006 C	0.11 C	0.013 C		
Furmecyclox	60568050			3.00E-02 I			2.2 C	0.21 C	0.11 C	190 C	21 C		
Glufosinate-ammonium	77182822	4.00E-04 I					15 N	1.5 N	0.54 N	820 N	31 N		
Glycidaldehyde	765344	4.00E-04 I	2.86E-04 H				15 N	1 N	0.54 N	820 N	31 N		
Glyphosate	1071836	1.00E-01 I					3700 N	370 N	140 N	200000 N	7800 N		
Haloxyfop-methyl	69806402	5.00E-05 I					1.8 N	0.18 N	0.068 N	100 N	3.9 N		
Harmony	79277273	1.30E-02 I					470 N	47 N	18 N	27000 N	1000 N		
HCH (alpha)	319846			6.30E+00 I	6.30E+00 I		0.011 C	0.00099 C	0.0005 C	0.91 C	0.1 C	0.9 E	0.0004 E
HCH (beta)	319857			1.80E+00 I	1.80E+00 I		0.037 C	0.0035 C	0.0018 C	3.2 C	0.35 C	16 E	0.002 E
HCH (gamma) Lindane	58899	3.00E-04 I		1.30E+00 H			0.052 C	0.0048 C	0.0024 C	4.4 C	0.49 C	4.2 C	0.006 E
HCH-technical	608731			1.80E+00 I	1.79E+00 I		0.037 C	0.0035 C	0.0018 C	3.2 C	0.35 C		
Heptachlor	76448	5.00E-04 I		4.50E+00 I	4.55E+00 I	☒	0.0023 C	0.0014 C	0.0007 C	1.3 C	0.14 C	0.3 E	0.06 E
Heptachlor epoxide	1024573	1.30E-05 I		9.10E+00 I	9.10E+00 I	☒	0.0012 C	0.00069 C	0.00035 C	0.63 C	0.07 C	1 E	0.03 E
Hexabromobenzene	87821	2.00E-03 I				☒	12 N	7.3 N	2.7 N	4100 N	160 N		
Hexachlorobenzene	118741	8.00E-04 I		1.60E+00 I	1.61E+00 I	☒	0.0066 C	0.0039 C	0.002 C	3.6 C	0.4 C	1 E	0.8 E
Hexachlorobutadiene	87683	2.00E-04 H		7.80E-02 I	7.70E-02 I	☒	0.14 C	0.081 C	0.04 C	73 C	8.2 C	1 E	0.1 E
Hexachlorocyclopentadiene	77474	7.00E-03 I	2.00E-05 H			☒	0.15 N	0.073 N	9.5 N	14000 N	550 N	2 E	10 E
Hexachlorodibenzo-p-dioxin mixture	19408743			6.20E+03 I	4.55E+03 I		0.00001 C	1E-06 C	5E-07 C	0.0009 C	0.0001 C		
Hexachloroethane	67721	1.00E-03 I		1.40E-02 I	1.40E-02 I	☒	0.75 C	0.45 C	0.23 C	410 C	46 C	49 E	0.2 E

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Hexachlorophene	70304	3.00E-04 I					11 N	1.1 N	0.41 N	610 N	23 N		
Hexahydro-1,3,5-trinitro-1,3,5-triazine	121824	3.00E-03 I		1.10E-01 I			0.61 C	0.057 C	0.029 C	52 C	5.8 C		
1,6-Hexamethylene diisocyanate	822060		2.86E-06 I				0.1 N	0.01 N					
n-Hexane	110543	6.00E-02 H	5.71E-02 I			X	350 N	210 N	81 N	120000 N	4700 N	32 N	13 N
Hexazinone	51235042	3.30E-02 I					1200 N	120 N	45 N	67000 N	2600 N		
Hydrazine, hydrazine sulfate	302012			3.00E+00 I	1.71E+01 I		0.022 C	0.00037 C	0.0011 C	1.9 C	0.21 C		
**Hydrogen chloride	7647010		5.71E-03 I				210 N	21 N					
**Hydrogen sulfide	7783064	3.00E-03 I	2.85E-04 I				110 N	1 N	4.1 N	6100 N	230 N		
Hydroquinone	123319	4.00E-02 H					1500 N	150 N	54 N	82000 N	3100 N		
Imazalil	35554440	1.30E-02 I					470 N	47 N	18 N	27000 N	1000 N		
Imazaquin	81335377	2.50E-01 I					9100 N	910 N	340 N	510000 N	20000 N		
Iprodione	36734197	4.00E-02 I					1500 N	150 N	54 N	82000 N	3100 N		
**Iron	7439896	3.00E-01 E					11000 N	1100 N	410 N	610000 N	23000 N		
Isobutanol	78831	3.00E-01 I				X	1800 N	1100 N	410 N	610000 N	23000 N		
Isophorone	78591	2.00E-01 I		9.50E-04 I			71 C	6.6 C	3.3 C	6000 C	670 C	3400 E	0.2 E
Isopropalin	33820530	1.50E-02 I					550 N	55 N	20 N	31000 N	1200 N		
Isopropyl methyl phosphonic acid	1832548	1.00E-01 I					3700 N	370 N	140 N	200000 N	7800 N		
Isoxaben	82558507	5.00E-02 I					1800 N	180 N	68 N	100000 N	3900 N		
Kepone	143500			1.80E+01 E			0.0037 C	0.00035 C	0.00018 C	0.32 C	0.035 C		
Lactofen	77501634	2.00E-03 I					73 N	7.3 N	2.7 N	4100 N	160 N		
Linuron	330552	2.00E-03 I					73 N	7.3 N	2.7 N	4100 N	160 N		
Lithium	7439932	2.00E-02 E					730 N	73 N	27 N	41000 N	1600 N		
Londax	83056996	2.00E-01 I					7300 N	730 N	270 N	410000 N	16000 N		
Malathion	121755	2.00E-02 I					730 N	73 N	27 N	41000 N	1600 N		
Maleic anhydride	108316	1.00E-01 I					3700 N	370 N	140 N	200000 N	7800 N		
Maleic hydrazide	123331	5.00E-01 I					18000 N	1800 N	680 N	1E+06 N	39000 N		
Malononitrile	109773	2.00E-05 H					0.73 N	0.073 N	0.027 N	41 N	1.6 N		
Mancozeb	8018017	3.00E-02 H					1100 N	110 N	41 N	61000 N	2300 N		
Maneb	12427382	5.00E-03 I					180 N	18 N	6.8 N	10000 N	390 N		
Manganese and compounds	7439965	5.00E-03 I	1.43e-05 I				180 N	0.052 N	6.8 N	10000 N	390 N		
Mephosfolan	950107	9.00E-05 H					3.3 N	0.33 N	0.12 N	180 N	7 N		
Mepiquat chloride	24307264	3.00E-02 I					1100 N	110 N	41 N	61000 N	2300 N		
**Mercuric chloride	7487947	3.00E-04 I					11 N	1.1 N	0.41 N	610 N	23 N		
Mercury (inorganic)	7439976	3.00E-04 H	8.57E-05 H				11 N	0.31 N	0.41 N	610 N	23 N	7 E	3 E
Mercury (methyl)	22967926	1.00E-04 I					3.7 N	0.37 N	0.14 N	200 N	7.8 N		
Merphos	150505	3.00E-05 I					1.1 N	0.11 N	0.041 N	61 N	2.3 N		
Merphos oxide	78488	3.00E-05 I					1.1 N	0.11 N	0.041 N	61 N	2.3 N		
Metalaxyl	57837191	6.00E-02 I					2200 N	220 N	81 N	120000 N	4700 N		
Methacrylonitrile	126987	1.00E-04 I	2.00E-04 A				3.7 N	0.73 N	0.14 N	200 N	7.8 N		

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Methamidophos	10265926	5.00E-05 I					1.8 N	0.18 N	0.068 N	100 N	3.9 N		
Methanol	67561	5.00E-01 I					18000 N	1800 N	680 N	1E+06 N	39000 N		
Methidathion	950378	1.00E-03 I					37 N	3.7 N	1.4 N	2000 N	78 N		
Methomyl	16752775	2.50E-02 I					910 N	91 N	34 N	51000 N	2000 N		
Methoxychlor	72435	5.00E-03 I					180 N	18 N	6.8 N	10000 N	390 N	41 S	62 E
2-Methoxyethanol acetate	110496	2.00E-03 A					73 N	7.3 N	2.7 N	4100 N	160 N		
2-Methoxyethanol	109864	1.00E-03 H	5.71E-03 I				37 N	21 N	1.4 N	2000 N	78 N		
2-Methoxy-5-nitroaniline	99592			4.60E-02 H			1.5 C	0.14 C	0.069 C	120 C	14 C		
Methyl acetate	79209	1.00E+00 H					37000 N	3700 N	1400 N	1E+06 N	78000 N		
Methyl acrylate	96333	3.00E-02 A					1100 N	110 N	41 N	61000 N	2300 N		
2-Methylaniline hydrochloride	636215			1.80E-01 H			0.37 C	0.035 C	0.018 C	32 C	3.5 C		
2-Methylaniline	95534			2.40E-01 H			0.28 C	0.026 C	0.013 C	24 C	2.7 C		
Methyl chlorocarbonate	79221	1.00E+00 W					37000 N	3700 N	1400 N	1E+06 N	78000 N		
4-(2-Methyl-4-chlorophenoxy) butyric acid	94815	1.00E-02 I					370 N	37 N	14 N	20000 N	780 N		
2-Methyl-4-chlorophenoxyacetic acid	94746	5.00E-04 I					18 N	1.8 N	0.68 N	1000 N	39 N		
2-(2-Methyl-14-chlorophenoxy)propionic acid	93652	1.00E-03 I					37 N	3.7 N	1.4 N	2000 N	78 N		
Methylcyclohexane	108872		8.57E-01 H				31000 N	3100 N				60 S	1500 N
Methylene bromide	74953	1.00E-02 A				☒	61 N	37 N	14 N	20000 N	780 N		
Methylene chloride	75092	6.00E-02 I	8.57E-01 H	7.50E-03 I	1.64E-03 I	☒	4.1 C	3.8 C	0.42 C	760 C	85 C	7 E	0.01 E
4,4'-Methylene bis(2-chloroaniline)	101144	7.00E-04 H		1.30E-01 H	1.30E-01 H		0.52 C	0.048 C	0.024 C	44 C	4.9 C		
4,4'-Methylenebisbenzeneamine	101779			2.50E-01 W			0.27 C	0.025 C	0.013 C	23 C	2.6 C		
4,4'-Methylene bis(N,N'-dimethyl)aniline	101611			4.60E-02 I			1.5 C	0.14 C	0.069 C	120 C	14 C		
4,4'-Methylenediphenyl isocyanate	101688		5.71E-06 I			☒	0.035 N	0.021 N					
Methyl ethyl ketone	78933	6.00E-01 I	2.86E-01 I			☒	1900 N	1000 N	810 N	1E+06 N	47000 N		
Methyl hydrazine	60344			1.10E+00 W			0.061 C	0.0057 C	0.0029 C	5.2 C	0.58 C		
Methyl isobutyl ketone	108101	8.00E-02 H	2.29E-02 A				2900 N	84 N	110 N	160000 N	6300 N		
Methyl methacrylate	80626	8.00E-02 H					2900 N	290 N	110 N	160000 N	6300 N		
2-Methyl-5-nitroaniline	99558			3.30E-02 H			2 C	0.19 C	0.096 C	170 C	19 C		
Methyl parathion	298000	2.50E-04 I					9.1 N	0.91 N	0.34 N	510 N	20 N	28 S	0.041 N
2-Methylphenol (o-cresol)	95487	5.00E-02 I					1800 N	180 N	68 N	100000 N	3900 N	12000 S	6 E
3-Methylphenol (m-cresol)	103394	5.00E-02 I					1800 N	180 N	68 N	100000 N	3900 N		
4-Methylphenol (p-cresol)	106445	5.00E-03 H					180 N	18 N	6.8 N	10000 N	390 N		
Methyl styrene (mixture)	25013154	6.00E-03 A	1.14E-02 A			☒	60 N	42 N	8.1 N	12000 N	470 N	100 N	1 N
Methyl styrene (alpha)	98839	7.00E-02 A				☒	430 N	260 N	95 N	140000 N	5500 N	8.8 S	7.5 N
Methyl tertbutyl ether (MTBE)	1634044	5.00E-03 E	8.57E-01 I			☒	180 N	3100 N	6.8 N	10000 N	390 N		
Metolaclor (Dual)	51218452	1.50E-01 H					5500 N	550 N	200 N	310000 N	12000 N		
Metribuzin	21087649	2.50E-02 I					910 N	91 N	34 N	51000 N	2000 N		
Mirex	2385855	2.00E-04 I		1.80E+00 W			0.037 C	0.0035 C	0.0018 C	3.2 C	0.35 C		
Molinate	2212671	2.00E-03 I					73 N	7.3 N	2.7 N	4100 N	160 N		

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Molybdenum	7439987	5.00E-03 I					180 N	18 N	6.8 N	10000 N	390 N		
Monochloramine	10599903	1.00E-01 I					3700 N	370 N	140 N	200000 N	7800 N		
Naled	300765	2.00E-03 I					73 N	7.3 N	2.7 N	4100 N	160 N		
2-Naphthylamine	91598			1.30e+02 E			0.00052 C	0.00005 C	0.00002 C	0.044 C	0.0049 C		
Napropamide	15299997	1.00E-01 I					3700 N	370 N	140 N	200000 N	7800 N		
Nickel refinery dust					8.40E-01 I			0.0075 C					
Nickel and compounds	7440020	2.00E-02 I					730 N	73 N	27 N	41000 N	1600 N	6900 E	21 E
Nickel subsulfide	12035722				1.70E+00 I			0.0037 C					
Nitrapyrin	1929824	1.50E-03 W					55 N	5.5 N	2 N	3100 N	120 N		
Nitrate	14797558	1.60E+00 I					58000 N	5800 N	2200 N	1E+06 N	130000 N		
Nitric Oxide	10102439	1.00E-01 W					3700 N	370 N	140 N	200000 N	7800 N		
Nitrite	14797650	1.00E-01 I					3700 N	370 N	140 N	200000 N	7800 N		
2-Nitroaniline	88744	6.00E-05 W	5.71E-05 H				2.2 N	0.21 N	0.081 N	120 N	4.7 N		
3-Nitroaniline	99092	3.00E-03 O					110 N	11 N	4.1 N	6100 N	230 N		
4-Nitroaniline	100016	3.00E-03 O					110 N	11 N	4.1 N	6100 N	230 N		
Nitrobenzene	98953	5.00E-04 I	5.71E-04 A			☒	3.4 N	2.1 N	0.68 N	1000 N	39 N	110 E	0.09 E
Nitrofurantoin	67209	7.00E-02 H					2600 N	260 N	95 N	140000 N	5500 N		
Nitrofurazone	59870			1.50E+00 H	9.40E+00 H		0.045 C	0.00067 C	0.0021 C	3.8 C	0.43 C		
Nitrogen dioxide	10102440	1.00E+00 W					37000 N	3700 N	1400 N	1E+06 N	78000 N		
Nitroguanidine	556887	1.00E-01 I					3700 N	370 N	140 N	200000 N	7800 N		
4-Nitrophenol	100027	6.20E-02 O					2300 N	230 N	84 N	130000 N	4800 N		
2-Nitropropane	79469		5.71E-03 I		9.40E+00 H		210 N	0.00067 C					
N-Nitrosodi-n-butylamine	924163			5.40E+00 I	5.60E+00 I		0.012 C	0.0011 C	0.00058 C	1.1 C	0.12 C		
N-Nitrosodiethanolamine	1116547			2.80E+00 I			0.024 C	0.0022 C	0.0011 C	2 C	0.23 C		
N-Nitrosodiethylamine	55185			1.50E+02 I	1.51E+02 I		0.00045 C	0.00004 C	0.00002 C	0.038 C	0.0043 C		
N-Nitrosodimethylamine	62759			5.10E+01 I	4.90E+01 I		0.0013 C	0.00013 C	0.00006 C	0.11 C	0.013 C		
N-Nitrosodiphenylamine	86306			4.90E-03 I			14 C	1.3 C	0.64 C	1200 C	130 C	29 C	0.2 E
N-Nitroso di-n-propylamine	621647			7.00E+00 I			0.0096 C	0.00089 C	0.00045 C	0.82 C	0.091 C	0.014 C	0.00002 E
N-Nitroso-N-methylethylamine	10595956			2.20E+01 I			0.0031 C	0.00028 C	0.00014 C	0.26 C	0.029 C		
N-Nitrosopyrrolidine	930552			2.10E+00 I	2.13E+00 I		0.032 C	0.0029 C	0.0015 C	2.7 C	0.3 C		
m-Nitrotoluene	99081	1.00E-02 H				☒	61 N	37 N	14 N	20000 N	780 N	460 S	0.42 N
o-Nitrotoluene	88722	1.00E-02 H				☒	61 N	37 N	14 N	20000 N	780 N	460 S	0.42 N
p-Nitrotoluene	99990	1.00E-02 H				☒	61 N	37 N	14 N	20000 N	780 N	460 S	0.42 N
Norflurazon	27314132	4.00E-02 I					1500 N	150 N	54 N	82000 N	3100 N		
NuStar	85509199	7.00E-04 I					26 N	2.6 N	0.95 N	1400 N	55 N		
Octabromodiphenyl ether	32536520	3.00E-03 I					110 N	11 N	4.1 N	6100 N	230 N		
Octahydro-1357-tetranitro-1357-tetrazocine	2691410	5.00E-02 I					1800 N	180 N	68 N	100000 N	3900 N		
Octamethylpyrophosphoramide	152169	2.00E-03 H					73 N	7.3 N	2.7 N	4100 N	160 N		
Oryzalin	19044883	5.00E-02 I					1800 N	180 N	68 N	100000 N	3900 N		

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Oxadiazon	19666309	5.00E-03 I					180 N	18 N	6.8 N	10000 N	390 N		
Oxamyl	23135220	2.50E-02 I					910 N	91 N	34 N	51000 N	2000 N		
Oxyfluorfen	42874033	3.00E-03 I					110 N	11 N	4.1 N	6100 N	230 N		
Paclobutrazol	76738620	1.30E-02 I					470 N	47 N	18 N	27000 N	1000 N		
Paraquat	1910425	4.50E-03 I					160 N	16 N	6.1 N	9200 N	350 N		
Parathion	56382	6.00E-03 H					220 N	22 N	8.1 N	12000 N	470 N	110 S	3.9 N
Pebulate	1114712	5.00E-02 H					1800 N	180 N	68 N	100000 N	3900 N		
Pendimethalin	40487421	4.00E-02 I					1500 N	150 N	54 N	82000 N	3100 N		
Pentabromo-6-chloro cyclohexane	87843			2.30E-02 H			2.9 C	0.27 C	0.14 C	250 C	28 C		
Pentabromodiphenyl ether	32534819	2.00E-03 I					73 N	7.3 N	2.7 N	4100 N	160 N		
Pentachlorobenzene	608935	8.00E-04 I				X	4.9 N	2.9 N	1.1 N	1600 N	63 N	570 N	48 N
Pentachloronitrobenzene	82688	3.00E-03 I		2.60E-01 H		X	0.041 C	0.024 C	0.012 C	22 C	2.5 C		
Pentachlorophenol	87865	3.00E-02 I		1.20E-01 I			0.56 C	0.052 C	0.026 C	48 C	5.3 C	7.9 C	0.2 E
Permethrin	52645531	5.00E-02 I					1800 N	180 N	68 N	100000 N	3900 N		
Phenmedipham	13684634	2.50E-01 I					9100 N	910 N	340 N	510000 N	20000 N		
Phenol	108952	6.00E-01 I					22000 N	2200 N	810 N	1E+06 N	47000 N	21000 S	49 E
m-Phenylenediamine	108452	6.00E-03 I					220 N	22 N	8.1 N	12000 N	470 N		
p-Phenylenediamine	106503	1.90E-01 H					6900 N	690 N	260 N	390000 N	15000 N		
Phenylmercuric acetate	62384	8.00E-05 I					2.9 N	0.29 N	0.11 N	160 N	6.3 N		
2-Phenylphenol	90437			1.94E-03 H			35 C	3.2 C	1.6 C	3000 C	330 C		
Phorate	298022	2.00E-04 H					7.3 N	0.73 N	0.27 N	410 N	16 N		
Phosmet	732116	2.00E-02 I					730 N	73 N	27 N	41000 N	1600 N		
**Phosphine	7803512	3.00E-04 I	8.57E-05 H				11 N	0.31 N	0.41 N	610 N	23 N		
**Phosphoric acid	7664382	I	2.86E-03				100 N	10 N					
Phosphorus (white)	7723140	2.00E-05 I					0.73 N	0.073 N	0.027 N	41 N	1.6 N		
p-Phthalic acid	100210	1.00E+00 H					37000 N	3700 N	1400 N	1E+06 N	78000 N		
Phthalic anhydride	85449	2.00E+00 I	3.43E-02 H				73000 N	130 N	2700 N	1E+06 N	160000 N		
Picloram	1918021	7.00E-02 I					2600 N	260 N	95 N	140000 N	5500 N		
Pirimiphos-methyl	29232937	1.00E-02 I					370 N	37 N	14 N	20000 N	780 N		
Polybrominated biphenyls		7.00E-06 H		8.90E+00 H			0.0076 C	0.0007 C	0.00035 C	0.64 C	0.072 C		
Polychlorinated biphenyls (PCBs)	1336363			7.70E+00 I			0.0087 C	0.00081 C	0.00041 C	0.74 C	0.083 C		
Aroclor 1016	12674112	7.00E-05 I					2.6 N	0.26 N	0.095 N	140 N	5.5 N		
Aroclor 1254	11097691	2.00E-05 I					0.73 N	0.073 N	0.027 N	41 N	1.6 N		
Polychlorinated terphenyls (PCTs)				4.50E+00 E			0.015 C	0.0014 C	0.0007 C	1.3 C	0.14 C		
Polynuclear aromatic hydrocarbons												110000 S	
Acenaphthene	83329	6.00E-02 I					2200 N	220 N	81 N	120000 N	4700 N	120 S	200 E
Anthracene	120127	3.00E-01 I					11000 N	1100 N	410 N	610000 N	23000 N	6.8 S	4300 E
Benz[a]anthracene	56553			7.30E-01 E	6.10E-01 E		0.092 C	0.01 C	0.0043 C	7.8 C	0.88 C	27 S	0.7 E
Benzo[b]fluoranthene	205992			7.30E-01 E	6.10E-01 E		0.092 C	0.01 C	0.0043 C	7.8 C	0.88 C	23 S	4 E

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Benzo[k]fluoranthene	207089			7.30E-02 E	6.10E-02 E		0.92 C	0.1 C	0.043 C	78 C	8.8 C		4 E
Benzo[a]pyrene	50328			7.30E+00 I	6.10E+00 W		0.0092 C	0.001 C	0.00043 C	0.78 C	0.088 C	11 S	4 E
Carbazole	86748			2.00E-02 H			3.4 C	0.31 C	0.16 C	290 C	32 C	11 S	0.5 E
Chrysene	218019			7.30E-03 E	6.10E-03 E		9.2 C	1 C	0.43 C	780 C	88 C	3.6 S	1 E
Dibenz[ah]anthracene	53703			7.30E+00 E	6.10E+00 E		0.0092 C	0.001 C	0.00043 C	0.78 C	0.088 C	7.2 S	11 E
Fluoranthene	206440	4.00E-02 I					1500 N	150 N	54 N	82000 N	3100 N	68 S	980 E
Fluorene	86737	4.00E-02 I					1500 N	150 N	54 N	82000 N	3100 N	89 S	160 E
Indeno[1,2,3-cd]pyrene	193395			7.30E-01 E	6.10E-01 E		0.092 C	0.01 C	0.0043 C	7.8 C	0.88 C	280 S	35 E
Naphthalene	91203	4.00E-02 W					1500 N	150 N	54 N	82000 N	3100 N	180 S	30 E
Pyrene	129000	3.00E-02 I					1100 N	110 N	41 N	61000 N	2300 N	56 S	1400 E
Prochloraz	67747095	9.00E-03 I		1.50E-01 I			0.45 C	0.042 C	0.021 C	38 C	4.3 C		
Profluralin	26399360	6.00E-03 H					220 N	22 N	8.1 N	12000 N	470 N		
Prometon	1610180	1.50E-02 I					550 N	55 N	20 N	31000 N	1200 N		
Prometryn	7287196	4.00E-03 I					150 N	15 N	5.4 N	8200 N	310 N		
Pronamide	23950585	7.50E-02 I					2700 N	270 N	100 N	150000 N	5900 N		
Propachlor	1918167	1.30E-02 I					470 N	47 N	18 N	27000 N	1000 N		
Propanil	709988	5.00E-03 I					180 N	18 N	6.8 N	10000 N	390 N		
Propargite	2312358	2.00E-02 I					730 N	73 N	27 N	41000 N	1600 N		
Propargyl alcohol	107197	2.00E-03 I					73 N	7.3 N	2.7 N	4100 N	160 N		
Propazine	139402	2.00E-02 I					730 N	73 N	27 N	41000 N	1600 N		
Propham	122429	2.00E-02 I					730 N	73 N	27 N	41000 N	1600 N		
Propiconazole	60207901	1.30E-02 I					470 N	47 N	18 N	27000 N	1000 N		
Propylene glycol	57556	2.00E+01 H					730000 N	73000 N	27000 N	1E+06 N	1000000 N		
Propylene glycol, monoethyl ether	52125538	7.00E-01 H					26000 N	2600 N	950 N	1E+06 N	55000 N		
Propylene glycol, monomethyl ether	107982	7.00E-01 H	5.71E-01 I				26000 N	2100 N	950 N	1E+06 N	55000 N		
Propylene oxide	75569		8.57E-03 I	2.40E-01 I	1.29E-02 I		0.28 C	0.49 C	0.013 C	24 C	2.7 C		
Pursuit	81335775	2.50E-01 I					9100 N	910 N	340 N	510000 N	20000 N		
Pydrin	51630581	2.50E-02 I					910 N	91 N	34 N	51000 N	2000 N		
Pyridine	110861	1.00E-03 I					37 N	3.7 N	1.4 N	2000 N	78 N		
Quinalphos	13593038	5.00E-04 I					18 N	1.8 N	0.68 N	1000 N	39 N		
Quinoline	91225			1.20E+01 H			0.0056 C	0.00052 C	0.00026 C	0.48 C	0.053 C		
Resmethrin	10463868	3.00E-02 I					1100 N	110 N	41 N	61000 N	2300 N		
Ronnel	299843	5.00E-02 H					1800 N	180 N	68 N	100000 N	3900 N		
Rotenone	83794	4.00E-03 I					150 N	15 N	5.4 N	8200 N	310 N		
Savey	78587050	2.50E-02 I					910 N	91 N	34 N	51000 N	2000 N		
Selenious Acid	7783008	5.00E-03 I					180 N	18 N	6.8 N	10000 N	390 N		
Selenium	7782492	5.00E-03 I					180 N	18 N	6.8 N	10000 N	390 N		3 E
Selenourea	630104	5.00E-03 H					180 N	18 N	6.8 N	10000 N	390 N		
Sethoxydim	74051802	9.00E-02 I					3300 N	330 N	120 N	180000 N	7000 N		

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Contaminant	CAS	RfDo mg/kg/d	RfDi mg/kg/d	CPSo kg·d/mg	CPSi kg·d/mg	VOC	Risk-Based Concentrations: Tap Water µg/L	Ambient Air µg/m3	Fish mg/kg	Soil Ingestion: Industrial mg/kg	Soil Ingestion: Residential mg/kg	Soil Screening Levels-Transfers from Soil to: Air mg/kg	Soil Screening Levels-Transfers from Soil to: Groundwater mg/kg
Silver and compounds	7440224	5.00E-03 I					180 N	18 N	6.8 N	10000 N	390 N		
Simazine	122349	5.00E-03 I		1.20E-01 H			0.56 C	0.052 C	0.026 C	48 C	5.3 C		
Sodium azide	26628228	4.00E-03 I					150 N	15 N	5.4 N	8200 N	310 N		
Sodium diethyldithiocarbamate	148185	3.00E-02 I		2.70E-01 H			0.25 C	0.023 C	0.012 C	21 C	2.4 C		
Sodium fluoroacetate	62748	2.00E-05 I					0.73 N	0.073 N	0.027 N	41 N	1.6 N		
Sodium metavanadate	13718268	1.00E-03 H					37 N	3.7 N	1.4 N	2000 N	78 N		
Strontium, stable	7440246	6.00E-01 I					22000 N	2200 N	810 N	1E+06 N	47000 N		
Strychnine	57249	3.00E-04 I					11 N	1.1 N	0.41 N	610 N	23 N		
Styrene	100425	2.00E-01 I	2.86E-01 I			☒	1600 N	1000 N	270 N	410000 N	16000 N	1400 E	2 E
Systhane	88671890	2.50E-02 I					910 N	91 N	34 N	51000 N	2000 N		
2,3,7,8-TCDD (dioxin)	1746016			1.56E+05 H	1.16E+05 H		4E-07 C	5E-08 C	C	4E-05 C	4E-06 C		
Tebuthiuron	34014181	7.00E-02 I					2600 N	260 N	95 N	140000 N	5500 N		
Temephos	3383968	2.00E-02 H					730 N	73 N	27 N	41000 N	1600 N		
Terbacil	5902512	1.30E-02 I					470 N	47 N	18 N	27000 N	1000 N		
Terbufos	13071799	2.50E-05 H					0.91 N	0.091 N	0.034 N	51 N	2 N		
Terbutryn	886500	1.00E-03 I					37 N	3.7 N	1.4 N	2000 N	78 N		
1,2,4,5-Tetrachlorobenzene	95943	3.00E-04 I				☒	1.8 N	1.1 N	0.41 N	610 N	23 N	91 N	0.69 N
1,1,1,2-Tetrachloroethane	630206	3.00E-02 I		2.60E-02 I	2.59E-02 I	☒	0.41 C	0.24 C	0.12 C	220 C	25 C		
1,1,2,2-Tetrachloroethane	79345			2.00E-01 I	2.03E-01 I	☒	0.052 C	0.031 C	0.016 C	29 C	3.2 C	0.4 E	0.001 E
Tetrachloroethylene (PCE)	127184	1.00E-02 I		5.20E-02 E	2.03E-03 E	☒	1.1 C	3.1 C	0.061 C	110 C	12 C	11 E	0.04 E
2,3,4,6-Tetrachlorophenol	58902	3.00E-02 I					1100 N	110 N	41 N	61000 N	2300 N		
p,a,a,a-Tetrachlorotoluene	5216251			2.00E+01 H		☒	0.00053 C	0.00031 C	0.00016 C	0.29 C	0.032 C		
Tetrachlorovinphos	961115	3.00E-02 I		2.40E-02 H			2.8 C	0.26 C	0.13 C	240 C	27 C		
Tetraethyldithiopyrophosphate	3689245	5.00E-04 I					18 N	1.8 N	0.68 N	1000 N	39 N		
Tetraethyl lead	78002	1.00E-07 I					0.0037 N	0.00037 N	0.00014 N	0.2 N	0.0078 N	0.00068 N	0.000034 N
**1,1,1,2-Tetrafluoroethane	811972	I	2.29E+01			☒	140000 N	84000 N					
Thallic oxide	1314325	7.00E-05 W					2.6 N	0.26 N	0.095 N	140 N	5.5 N		
Thallium													0.4 E
Thallium acetate	563688	9.00E-05 I					3.3 N	0.33 N	0.12 N	180 N	7 N		
Thallium carbonate	6533739	8.00E-05 I					2.9 N	0.29 N	0.11 N	160 N	6.3 N		
Thallium chloride	7791120	8.00E-05 I					2.9 N	0.29 N	0.11 N	160 N	6.3 N		
Thallium nitrate	10102451	9.00E-05 I					3.3 N	0.33 N	0.12 N	180 N	7 N		
Thallium selenite	12039520	9.00E-05 W					3.3 N	0.33 N	0.12 N	180 N	7 N		
Thallium sulfate	7446186	8.00E-05 I					2.9 N	0.29 N	0.11 N	160 N	6.3 N		
Thiobencarb	28249776	1.00E-02 I					370 N	37 N	14 N	20000 N	780 N		
2-(Thiocyanomethylthio)-benzothiazole	21564170	3.00E-02 H					1100 N	110 N	41 N	61000 N	2300 N		
Thiofanox	39196184	3.00E-04 H					11 N	1.1 N	0.41 N	610 N	23 N		
Thiophanate-methyl	23564058	8.00E-02 I					2900 N	290 N	110 N	160000 N	6300 N		
Thiram	137268	5.00E-03 I					180 N	18 N	6.8 N	10000 N	390 N		

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Contaminant	CAS	RfDo mg/kg/d	RfDi mg/kg/d	CPSo kg·d/mg	CPSi kg·d/mg	VOC	Risk-Based Concentrations: Tap Water µg/L	Ambient Air µg/m3	Fish mg/kg	Soil Ingestion: Industrial mg/kg	Soil Ingestion: Residential mg/kg	Soil Screening Levels-Transfers from Soil to: Air mg/kg	Groundwater mg/kg
Tin and compounds		6.00E-01 H					22000 N	2200 N	810 N	1E+06 N	47000 N		
Toluene	108883	2.00E-01 I	1.14E-01 I			☒	750 N	420 N	270 N	410000 N	16000 N	520 E	5 E
Toluene-2,4-diamine	95807			3.20E+00 H			0.021 C	0.002 C	0.00099 C	1.8 C	0.2 C		
Toluene-2,5-diamine	95705	6.00E-01 H					22000 N	2200 N	810 N	1E+06 N	47000 N		
Toluene-2,6-diamine	823405	2.00E-01 H					7300 N	730 N	270 N	410000 N	16000 N		
p-Toluidine	106490			1.90E-01 H			0.35 C	0.033 C	0.017 C	30 C	3.4 C		
Toxaphene	8001352			1.10E+00 I	1.12E+00 I		0.061 C	0.0056 C	0.0029 C	5.2 C	0.58 C	5 E	0.04 E
Tralomethrin	66841256	7.50E-03 I					270 N	27 N	10 N	15000 N	590 N		
Triallate	2303175	1.30E-02 I					470 N	47 N	18 N	27000 N	1000 N		
Triasulfuron	82097505	1.00E-02 I					370 N	37 N	14 N	20000 N	780 N		
1,2,4-Tribromobenzene	615543	5.00E-03 I				☒	30 N	18 N	6.8 N	10000 N	390 N		
Tributyltin oxide (TBTO)	56359	3.00E-05 I					1.1 N	0.11 N	0.041 N	61 N	2.3 N		
2,4,6-Trichloroaniline hydrochloride	33663502			2.90E-02 H			2.3 C	0.22 C	0.11 C	200 C	22 C		
2,4,6-Trichloroaniline	634935			3.40E-02 H			2 C	0.18 C	0.093 C	170 C	19 C		
1,2,4-Trichlorobenzene	120821	1.00E-02 I	5.71e-02 H			☒	190 N	210 N	14 N	20000 N	780 N	240 E	2 E
1,1,1-Trichloroethane	71556	9.00E-02 W	2.86E-01 W			☒	1300 N	1000 N	120 N	180000 N	7000 N	980 E	0.9 E
1,1,2-Trichloroethane	79005	4.00E-03 I		5.70E-02 I	5.60E-02 I	☒	0.19 C	0.11 C	0.055 C	100 C	11 C	0.8 E	0.01 E
Trichloroethylene (TCE)	79016	6.00E-03 E		1.10E-02 W	6.00E-03 E	☒	1.6 C	1 C	0.29 C	520 C	58 C	3 E	0.02 E
Trichlorofluoromethane	75694	3.00E-01 I	2.00E-01 A			☒	1300 N	730 N	410 N	610000 N	23000 N	790 N	13 N
2,4,5-Trichlorophenol	95954	1.00E-01 I					3700 N	370 N	140 N	200000 N	7800 N	8200 S	120 E
2,4,6-Trichlorophenol	88062			1.10E-02 I	1.09E-02 I		6.1 C	0.57 C	0.29 C	520 C	58 C	150 C	0.06 E
2,4,5-Trichlorophenoxyacetic acid	93765	1.00E-02 I					370 N	37 N	14 N	20000 N	780 N		
2-(2,4,5-Trichlorophenoxy)propionic acid	93721	8.00E-03 I					290 N	29 N	11 N	16000 N	630 N		
1,1,2-Trichloropropane	598776	5.00E-03 I				☒	30 N	18 N	6.8 N	10000 N	390 N	13 N	0.14 N
1,2,3-Trichloropropane	96184	6.00E-03 I		7.00e+00 I		☒	0.0015 C	0.00089 C	0.00045 C	0.82 C	0.091 C	0.00003 C	6.000E-06 C
1,2,3-Trichloropropene	96195	5.00E-03 H				☒	30 N	18 N	6.8 N	10000 N	390 N		
1,1,2-Trichloro-1,2,2- trifluoroethane	76131	3.00E+01 I	8.57E+00 H			☒	59000 N	31000 N	41000 N	1E+06 N	1000000 N	2400 S	3100 N
Tridiphane	58138082	3.00E-03 I					110 N	11 N	4.1 N	6100 N	230 N		
Triethylamine	121448		2.00E-03 I				73 N	7.3 N					
Trifluralin	1582098	7.50E-03 I		7.70E-03 I			8.7 C	0.81 C	0.41 C	740 C	83 C		
**1,2,4-Trimethylbenzene	95636	5.00e-02 E				☒	300 N	180 N	68 N	100000 N	3900 N		
**1,3,5-Trimethylbenzene	108678	5.00e-02 E				☒	300 N	180 N	68 N	100000 N	3900 N	98 S	0.26 M
Trimethyl phosphate	512561			3.70E-02 H			1.8 C	0.17 C	0.085 C	150 C	17 C		
1,3,5-Trinitrobenzene	99354	5.00E-05 I					1.8 N	0.18 N	0.068 N	100 N	3.9 N		
Trinitrophenylmethylnitramine	479458	1.00E-02 H					370 N	37 N	14 N	20000 N	780 N		
2,4,6-Trinitrotoluene	118967	5.00E-04 I		3.00E-02 I			2.2 C	0.21 C	0.11 C	190 C	21 C		
Uranium (soluble salts)	7440611	3.00E-03 I					110 N	11 N	4.1 N	6100 N	230 N		
Vanadium	7440622	7.00E-03 H					260 N	26 N	9.5 N	14000 N	550 N		
Vanadium pentoxide	1314621	9.00E-03 I					330 N	33 N	12 N	18000 N	700 N		

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Contaminant	CAS	RfDo mg/kg/d	RfDi mg/kg/d	CPSo kg·d/mg	CPSi kg·d/mg	V O C	Risk-Based Concentrations: Tap Water µg/L	Ambient Air µg/m3	Fish mg/kg	Soil Ingestion: Industrial mg/kg	Soil Ingestion: Residential mg/kg	Soil Screening Levels-Transfers from Soil to: Air mg/kg	Groundwater mg/kg
Vanadium sulfate	36907423	2.00E-02 H					730 N	73 N	27 N	41000 N	1600 N		
Vernam	1929777	1.00E-03 I					37 N	3.7 N	1.4 N	2000 N	78 N		
Vinclozolin	50471448	2.50E-02 I					910 N	91 N	34 N	51000 N	2000 N		
Vinyl acetate	108054	1.00E+00 H	5.71E-02 I				37000 N	210 N	1400 N	1E+06 N	78000 N	370 E	8
Vinyl bromide	593602		8.57E-04 I			☒	5.2 N	3.1 N				2 N	0.018 N
Vinyl chloride	75014			1.90E+00 H	3.00E-01 H	☒	0.019 C	0.021 C	0.0017 C	3 C	0.34 C	0.002 E	0.01 E
Warfarin	81812	3.00E-04 I					11 N	1.1 N	0.41 N	610 N	23 N	0.046 N	1800 N
m-Xylene	108323	2.00E+00 H	2.00E-01 W			☒	1400 N	730 N	2700 N	1E+06 N	160000 N	950 S	240 M
o-Xylene	9.55E+04	2.00E+00 H	2.00E-01 W			☒	1400 N	730 N	2700 N	1E+06 N	160000 N	730 S	1.50E+02 M
p-Xylene	1.06E+05		8.57E-02 W			☒	520 N	310 N				1000 S	2.20E+02 M
Xylene (mixed)	1.33E+06	2.00E+00 I				☒	12000 N	7300 N	2700 N	1E+06 N	160000 N	320 E	7.40E+01 E
Zinc	7.44E+06	3.00E-01 I					11000 N	1100 N	410 N	610000 N	23000 N		4.20E+04 E
Zinc phosphide	1.31E+06	3.00E-04 I					11 N	1.1 N	0.41 N	610 N	23 N		
Zineb	1.21E+07	5.00E-02 I					1800 N	180 N	68 N	100000 N	3900 N		

DERIVATION OF CONSTRUCTION WORKER SOIL INGESTION SCREENING CONCENTRATION

The construction worker soil ingestion screening concentration has been derived using the same basic approach as the industrial soil screening value, except that a construction worker soil ingestion rate has been utilized and a one year exposure duration was assumed for construction activities related to site redevelopment. A target hazard quotient of 1 is the basis of the screening concentration. Since a one year exposure is considered a subchronic exposure scenario, a subchronic Reference Dose (RfD) for mercury has been employed. However, the conservative screening value is based on the subchronic RfD for methyl mercury (0.0001 mg/kg/day), the mercury species with the lowest RfD. The USEPA has adopted the chronic RfD as the subchronic RfD as well. The calculation of the soil ingestion screening concentration for the construction worker is shown in Table B-1.

The construction worker soil ingestion rate (118 mg soil per day) has been calculated based on a series of assumptions previously made by the USEPA. The soil ingestion rate represents a recalculation of work previously conducted by Hawley, with an updated skin soil adherence rate. The soil ingestion rate has been calculated as follows. Hawley has assumed that an adult working outdoors ingests twice daily a quantity of soil corresponding to one-half the covering of the inside surface of the fingers and thumbs of both hands. According to USEPA (1992), the inside surface of the fingers and thumbs of both hands is 14% of the surface area of the hands or 118 cm^2 and the upper bound estimate of soil adherence rate is 1.0 mg/cm^2. Based on this information, the daily soil intake rate is: 2 x 0.5 (118 cm^2) x 1.0 mg soil/cm2 = 118 mg soil / day.

Hawley, J.K., 1985. Assessment of Health Risk from Exposure to Contaminated Soil, Risk Analysis, Vol.
5, No. 4, pp.289-302.

USEPA, 1992. Dermal Exposure Assessment: Principles and Applications, Interim Report, EPA/600/8-91/011B, January

TABLE B-1 - DERIVATION OF CONSTRUCTION WORKER SOIL INGESTION SCREENING CONCENTRATION

CONSTRUCTION WORKER SCENARIO	UN ITS	VALUE	
SOIL INGESTION RATE	MG/DAY	118	
FREQUENCY OF EXPOSURE	DAYS/WK	5	
DURATION OF EXPOSURE	WEEKS	50	
FRACTION OF SOIL INGESTION AT SITE	NA	0.5	
BODYWEIGHT	KG	70	
RELATIVE ABSORPTION FACTOR	NA	1	
UNITS CONVERSION FACTOR (CF1)	KG/MG	1.00E-06	
UNITS CONVERSION FACTOR (CF2)	DAY/WK	7.00E+00	
ORAL RfD	MG/KG/DAY	1.00E-04	METHYL MERCURY
TARGET HAZARD INDEX	NA	1.00E+00	

TARGET CONCENTRATION (SOIL INGESTION)	MG/KG	166

TARGET SOIL CONC (INGESTION ONLY) = TARGET HI X RfD X BW X DURATION X CF2 / (SOIL INGESTION RATE X FREQUENCY X DURATION X RELATIVE ABSORPTION FACTOR X FRACTION FROM SITE X CF1)

ATTACHMENT C

MERCURY SPECIATION AND BIOAVAILABILITY TESTING BACKGROUND INFORMATION AND TECHNIQUES

TECHNICAL BACKGROUND AND RATIONALE

MERCURY SPECIATION

Mercury can occur in soils as elemental mercury in liquid or vapor form, organic mercury compounds, mercuric chloride, or one of several different mineral species, including mercuric oxides, carbonates, and sulfides. In general, organic mercury, mercuric chloride, and elemental mercury in the vapor phase are very soluble and bioavailable, mercuric oxides and carbonates are less soluble, and liquid elemental mercury and mercuric sulfides are insoluble and non-bioavailable. Furthermore, mercury speciation may vary with depth in soils. The chemical form of mercury controls its mobility in the soil, its bioavailability when ingested, and its response to specific remedial actions. Therefore, an understanding of mercury speciation in soils at the Ames Street site will be critical for determining the bioavailability of mercury, evaluating risk, and selecting appropriate remedial actions.

The importance of mercury speciation can be illustrated with two examples. If a soil contains only organic mercury compounds, which generally are highly soluble, the mercury is likely to be highly bioavailable. In addition, a relatively simple technology—such as soil washing—may be a viable means of remediating the soil. In contrast, if all the mercury is present as insoluble mercuric sulfide, the bioavailability will be low and will result in a less stringent site-specific cleanup standard for soil across the site. However, due to the same physical properties, mercuric sulfide may be more difficult to remove from the soils, and a more aggressive remedial technology may be required to meet the cleanup standard.

Mercury speciation in soils can be evaluated using three general methods:

- Sequential extractions
- Electron microprobe analysis
- Heavy mineral separations.

Recently, several investigators have focused on developing sequential extraction procedures to quantitatively evaluate the speciation of mercury in soils (Revis et al. 1989; Miller 1993; Sakamoto et al. 1992). Application of the procedures of each investigator to the same samples from Oak Ridge, Tennessee showed mercury occurring predominantly as elemental mercury and mercuric sulfide minerals (Barnett et al. 1994). However, the relative proportions of the two species did not agree among procedures, indicating that the extractions were either not fully effective in removing specific mercury compounds or not fully specific in extracting individual mercury species. This problem is common to sequential extraction methods (Belzile et al. 1989). All the extraction techniques gave similar levels of organic mercury in soils. However, the method of Miller (1993), developed by the EPA, generally found much less elemental mercury and mercuric sulfide

than the other two extraction procedures. The method of Sakamoto et al. (1992) tended to have poor recovery for elemental mercury. The method of Revis et al. (1993) showed higher recoveries of mercuric sulfide and elemental mercury, but it does not include a procedure for mercuric oxides and carbonates (acid-soluble mercury). Given the drawbacks of all the methods, a procedure combining the most effective aspects of each is likely to produce the most reliable results.

Electron microprobe analysis is a mineralogical technique that provides direct visual evidence of the mercury phases present in soil. The microprobe is used to determine the distribution of the specific mercury-bearing phases in the soil and can be used to qualitatively, rather than quantitatively, confirm the visible amounts of these phases. Microprobe analysis is particularly useful for documenting the morphology and composition of the metal-bearing grains and photographing these relations. This information can then be used to assess the bioavailability of the metal in the soil (Davis et al. 1993). The microprobe technique, however, is not without limitations. It is difficult to quantitatively determine the entire mass of mercury in the soil, because some phases may be distributed throughout the soil at low concentrations that are difficult to quantify. Also, it may be difficult to detect mercury-bearing phases in soils with very low levels of mercury. Finally, in preparing the samples for microprobe analysis, some of the organic and elemental mercury may be lost due to volatilization, potentially skewing the results.

Heavy mineral separation of mercury-bearing phases from soil is an additional mineralogical technique to provide information on the distribution of mercury species in the soil. This technique involves grinding a soil sample and mixing in a high-density liquid such as methylene iodide (specific gravity 3.325). In this liquid, silicate minerals and organic materials will float, and heavy mercury-bearing phases will settle out, along with other heavy minerals. This heavy mineral concentrate can then be analyzed visually, by microprobe, and by x-ray diffraction to detect mercury-bearing phases. The results of heavy mineral separations provide visual confirmation of the mercury speciation results. More importantly, mineral separations provide conclusive evidence of the presence or absence of significant concentrations of all mercury phases in site soils.

The interpretation of mercury speciation data will focus on determining the internal consistency and applicability of the sequential extraction results. Total mercury concentrations will be compared to the sum of the individual mercury species determined in each soil. Also, duplicate analyses will be compared. Speciation results from soils spiked with known quantities of mercury species will be evaluated to determine the portion of mercury re-extracted by the speciation procedures. Once the sequential extraction data are analyzed, these results will be compared to microprobe and heavy mineral separation data, to evaluate whether the different speciation techniques provide consistent results. If the results are different, the discrepancies will be evaluated in light of the known limitations of the analytical methods, to develop a realistic assessment of the distribution of mercury species in soils from the Ames Street site.

MERCURY BIOAVAILABILITY

In humans, an orally administered dose of a compound is seldom completely absorbed, and differences in the extent of absorption of orally administered compounds exist among different exposure media. For most compounds, the toxicity values derived by the U.S. Environmental Protection Agency (EPA) are not adjusted to absorbed dose (i.e., the dose response evaluation is based on the administered dose). This procedure can lead to errors in assessing the risks of exposure to a particular chemical in a medium other than the one used in the toxicity or epidemiology studies on which the toxicity values are based. For example, the EPA's oral toxicity value, or reference dose (RfD), for inorganic mercury was derived from studies in which mercuric chloride dissolved in water was administered to laboratory animals. Because it is likely that most of the mercury at the Ames Street site is present in forms that are less soluble than mercuric chloride, absorption of mercury from ingested site soils will be reduced compared to mercuric chloride. If these differences in mercury bioavailability are not accounted for, risks associated with ingestion of mercury in site soils will be overestimated. The adjustment factor to correct for differences in absorption from different exposure media is termed the bioavailability adjustment factor (BAF). This fractional value is used to adjust the dose or intake so that it is expressed in the same terms as the doses used to generate the toxicity values.

Substantial evidence exists that mercury solubility and bioavailability vary with mercury species. Studies in rodents suggest that 10 to 20 percent of mercuric chloride is absorbed from single oral doses. Several studies comparing tissue levels in rodents after single or repeated doses of mercuric chloride and mercuric sulfide have concluded that mercuric sulfide is very poorly absorbed. In 1993, the EPA reviewed available studies on the toxicity and bioavailability of mercuric sulfide in response to a petition for a provisional mercuric sulfide reference dose for an Oak Ridge, Tennessee, site. At that time, the EPA concluded that insufficient information was available to derive a separate RfD for mercuric sulfide, but they did note that comparison of relative tissue levels of mercury in animal studies suggested that mercuric sulfide was 30 to 80 times less bioavailable than mercuric chloride. Thus, a relative BAF of 1/30 to 1/80 (0.03–0.01) may be appropriate when

applying toxicity values for mercuric chloride to mercuric sulfide. Little or no information is available on the oral absorption of other mercury compounds or elemental mercury relative to mercuric chloride; however, other mercury species are likely to be more bioavailable than mercuric sulfide. The bioavailability of mercury species in soil may be further reduced due to interactions with soil constituents. Thus, site-specific BAFs will vary, depending on the mix of mercury species present at the site and the composition of other soil constituents. Because a variety of mercury species may be present in soils at the Ames Street site, site-specific mercury BAF(s) will be determined based on a study of site soil samples.

For the purpose of this study, bioaccessible mercury is defined as the fraction of mercury that is soluble in the gastrointestinal (GI) tract and is available for absorption, while bioavailability is defined as the fraction of mercury that is absorbed into the bloodstream. Because mercury in soil must be solubilized in order to become bioavailable, mercury bioaccessibility is a precursor to, and provides an upper-bound estimate of, mercury bioavailability.

The PTI *in vitro* test has been utilized to assay the bioavailability of lead and arsenic in soils, and has been validated in several animal models (Ruby et al. 1993, 1995; Appendix A, Attachment D). For this study, the standard PTI *in vitro* test has been modified to provide a test system appropriate for mercury bioaccessibility evaluation (see Methodology section, below).

In vitro assays similar to the PTI test have been employed at several other sites to estimate site-specific bioavailability of mercury in soil. At the Almaden Quick Silver County Park in Los Gatos, California, the form of mercury present in site soils, which resulted from mining and ore processing (predominantly mercuric sulfide), was experimentally measured to be from 0.03 to 9.4 percent as soluble as mercuric chloride, in a simulated gastrointestinal environment (CDM 1992). The Los Gatos site samples were tested using a leaching procedure designed to emulate the human gastrointestinal system. Two-hundred milligrams (mg) of sample (sieved to <2 mm) was added to 480 milliliters (mL) of a pH-2.5 solution of dilute hydrochloric acid (HCl) in 500-mL bottles, and the bottles were agitated for 4 hours to simulate conditions in the human stomach. The human intestine was emulated by adjusting the pH of the solution to 6.5 using sodium hydroxide, and agitating for an additional 4 hours. At the end of the simulated stomach and intestinal phases, aliquots of the solutions were filtered (0.45 μm) and analyzed for their mercury content. Based on the results of this *in vitro* assay, the Santa Clara County Parks and Recreation Department and California state regulatory authorities agreed to use a BAF of 0.3 for the Los Gatos site.

An *in vitro* procedure nearly identical to the one above was used to evaluate the solubility of mercury in soil samples collected at Oak Ridge National Laboratory in Tennessee (Barnett and Turner 1995). The experimental procedure was altered in that the soil samples were pulverized after sieving, and only the <180-μm size fraction was subjected to the leaching procedure. For 19 of the 20 samples, the mercury in soils was determined to be from 0.3

to 14.2 percent soluble (average of 3.2 percent). One sample, the only sample with detectable mercury vapor in the sample headspace, contained 45.9 percent soluble mercury by this *in vitro* method. Mercuric chloride was determined to be 100 percent soluble in the *in vitro* test system. Based on these analyses, the EPA accepted a site-specific BAF of 0.1 for mercury in soils (DOE 1995).

METHODOLOGY

OVERVIEW

Mercury speciation analysis will be conducted on selected soil samples to determine the forms of mercury present. The speciation data will indicate the predicted solubility of mercury in the soil samples and will provide a mechanistic explanation for the estimated bioavailability of mercury from the Ames Street site soils. An *in vitro* test that replicates human gastrointestinal tract chemistry and function will be performed on selected samples following speciation to determine the fraction of mercury in soil samples that is soluble and available for absorption in the gastrointestinal tract (i.e., the fraction that is bioaccessible). Because the bioaccessible fraction of mercury provides an upper-bound estimate on the bioavailability of ingested mercury, the *in vitro* test data for the Ames Street site soil samples can be used to develop conservative site-specific BAF(s). The resulting BAF(s) can then be used to adjust the soil mercury intake estimates and to develop revised site-specific soil remediation goals.

MERCURY SPECIATION ANALYSIS

As described above, both sequential extractions and mineralogical techniques for determining the speciation of mercury in soils are not without limitations. In order to address these limitations, PTI will conduct a coupled study of mercury speciation that combines sequential extractions and mineralogical techniques. The use of more than one method will allow for data cross-checking and validation, which will increase the reliability of study results. Also, the combined approach will allow for better quantification of mercury species distribution, especially organic and elemental mercury in soils, and the mineralogical photographs will provide visual evidence of mercury distribution.

Total mercury concentrations will be measured in all of the soil samples. Speciation analysis will then be conducted on selected samples with total mercury concentration >10 mg/kg. Prior to speciation analysis, mercury in the headspace of the sample bottles will be determined in the laboratory at room temperature using a Jerome mercury vapor analyzer, Model 431X. Speciation analysis will be performed on dry samples. Because of the volatile nature of mercury, the samples will be air dried at room temperature, instead of oven dried. The speciation analysis will first be performed using a sequential extraction procedure, whereby samples are extracted with chloroform to analyze for organic mercury, and then treated with 0.1 M H_2SO_4 to extract mercuric oxide and carbonate minerals. The remaining sample will be analyzed for total mercury (i.e., elemental mercury + mercuric sulfide) and then heated to extract elemental mercury. Mercuric sulfide will be the concentration of total mercury left after heating. Elemental mercury will be determined by subtracting the mercuric sulfide concentration from the total mercury concentration prior to

heating. In addition to the sequential extractions, speciation will be determined by microprobe and heavy mineral separations. These results will provide corroborative visual evidence of various mercury phases in site soils. Quality assurance and quality control (QA/QC) procedures will be implemented, including collection and analysis of sample duplicates, spiked soils, and sample blanks. The results of the various mercury speciation studies will be used to identify samples for further *in vitro* studies to assess mercury bioavailability.

IN VITRO BIOAVAILABILITY TESTING

The *in vitro* procedure is described in detail in the SAP (Appendix A). Extracts from the *in vitro* procedure will be submitted to Columbia Analytical Services (Kelso, Washington) for mercury analysis. Analytical methods and laboratory quality assurance measures are described below. The *in vitro* test results for selected Ames Street site samples will be used to develop a site-specific BAF for mercury, based on the average fraction of mercury solubilized from the soils, corrected for recovery of mercuric chloride in the assay. Multiple BAFs may be developed for different areas of the site or different mercury forms in soil, based on the speciation data, if the testing results support this approach to data interpretation.

QA/QC procedures will be implemented by spiking two stomach solution samples. Instead of adding a soil sample to the reaction vessel, a known amount of an aqueous solution of reagent-grade mercuric chloride ($HgCl_2$) will be added as a spike. The QA/QC procedure will then follow the *in vitro* test method as described in the SAP (Appendix A). The samples will be spiked with a low concentration of $HgCl_2$, relative to total soil mercury concentrations. The duplicate spike solutions will be evaluated to determine recovery of mercuric chloride in the *in vitro* test.

MERCURY SPECIATION ANALYSIS

SAMPLE PREPARATION

Based on the total mercury results, samples will be selected from locations at the Ames Street site for speciation analysis. The samples selected must contain enough mercury (i.e., > 10 mg/kg) to perform the speciation analyses and to quantify the spatial distribution of mercury in Ames Street site soil. Speciation will be performed to determine organic mercury, mercury oxide, elemental mercury, and mercuric sulfide. Personnel at the PTI laboratory in Boulder, Colorado will perform the sequential extractions.

MERCURY VAPOR ANALYSIS

To measure the headspace mercury in the 16-oz soil sampling bottles, attach the Jerome Model 431X mercury vapor analyzer to the septum. If the Jerome Model 431X mercury vapor analyzer reads the upper detection limit of 1 mg/m^3, then a Jerome Dilution Module can be used. This device will dilute the headspace mercury so that a percentage of mercury vapor can be detected. After reading the headspace mercury, the samples will be air dried.

SPECIATION EXTRACTION METHODS

The methods of Revis et al. (1989) and Sakamoto et al. (1992) will be followed for the extraction of mercury species from the Ames Street site soils. Modifications have been made to both procedures in order to combine the two methods.

The PTI laboratory will be set up to perform extractions of mercury species. All procedures will be performed under a vapor hood. Sample extracts for each mercury species will be sent to Columbia Analytical Services (CAS) for mercury analyses.

Organic Mercury and Acid-Soluble Mercury

Sakamoto et al. (1992) developed a method for differential determination of organic mercury and acid-soluble mercury, which includes mercury(I) oxide, mercury(II) oxide, mercury carbonates, and mercuric chloride, based on the successive extraction of these mercury compounds with chloroform and sulfuric acid. The mercury in each extract is determined by cold vapor atomic adsorption spectroscopy (CVAAS).

The method for extracting organic mercury from soils is as follows:

- Place 20 mL of chloroform and 1–5 g of sediment sample in a 50-mL glass centrifuge tube
- Stopper the tube and shake in a shaker for 2 minutes
- Centrifuge at 3000 rpm for 2 minutes
- Transfer the chloroform phase into a separatory funnel
- Repeat the extraction with another 20 mL of chloroform
- Add 3 mL of 0.01 M sodium thiosulfate solution to the combined chloroform extract in the separatory funnel and shake for 2 minutes
- Send the aqueous solution to CAS to determine the mercury concentration by CVAAS.

The method for extracting acid-soluble mercury from soils is as follows:

- After completion of the organic mercury extraction, leave the 50-mL glass centrifuge tube unstoppered to evaporate the residual chloroform to dryness
- Add 10 mL of 0.1 M sulfuric acid to the residue
- Stopper the centrifuge tube and shake it in the shaker for 2 minutes
- Centrifuge it at 3000 rpm for 2 minutes
- Send the supernatant to CAS to determine the mercury concentration by CVAAS

- Air dry and save the residue in the centrifuge tube for the elemental mercury extraction.

Elemental Mercury (Hg^0) and Mercuric Sulfide

To separate and determine elemental mercury (Hg^0) and mercuric sulfide (HgS), use the residue remaining after extracting organic mercury and mercury oxide, and follow the method of Revis et al. (1989):

- Send a residue split to CAS to determine ΣHg (i.e., Hg^0 + HgS) using CVAAS
- Thinly spread a 5-g sample of homogenized residue on a stainless steel tray
- Place the tray in a continuously aerated oven at 150 °C for 5 days
- Digest the sample with aqua regia acid
- Send the sample to CAS to determine ΣHg by CVAAS
- The amount of HgS in the sample is the amount of ΣHg after roasting.
- The amount of Hg^0 in the sample is the difference between the ΣHg prior to roasting and the amount of HgS after roasting.

MICROPROBE ANALYSIS

Polished sample "pucks" will be prepared at the Laboratory for Geological Studies, University of Colorado, Boulder, for electron microprobe analysis by embedding 4 grams of sample in epoxy within a sample mold, setting the mold to cure at room temperature, and grinding a flat surface on the sample side to expose as much sample as possible. Successive polishing steps will employ a 600-grit wet/dry abrasive paper stretched across a glass plate, 15-μm and 6-μm diamond on a cloth pad fixed to a steel lap, and finally 0.1-μm diamond on a felt pad fixed to a steel lap. All polishing steps will use kerosene to avoid dissolution of water-soluble Hg phases, and all polishing will be performed at low speeds to avoid plucking of the sample grains. Finally, sample pucks will be cleaned in an ultrasonic cleaner with isopropyl alcohol, air dried, and placed in a carbon coater, where a thin layer of carbon will be sputtered onto the surface of each puck.

Electron microprobe analysis (EMPA) will also be conducted at the Laboratory for Geological Studies, University of Colorado, Boulder, on a JEOL 8600 electron microprobe operating at 15 kV with a 20-nA specimen current and a 1-μm beam, according to the methods described in Attachment C, as adapted for mercury speciation. Quantitative mineralogic data will be collected using wavelength dispersive spectrometers and mineral standards, and corrected using Phi Rho Z parameters. The Hg-bearing particles will be identified using a combination of energy dispersive detection (EDS), wavelength dispersive detection (WDS), and backscatter electron image detection (BEI). Initially, spectra are generated for each grain that allow identification of all elements with an atomic mass greater than or equal to that of carbon. Subsequently, the elemental proportions are quantified using standards, and the mineral proportions are identified based on the equivalent weight of the oxide. Therefore, the identifications provide quantitative stoichiometric ratios from which the mineral identity can be calculated. The relations between Hg-bearing phases will be established from BEI images and WDS/EDS analyses as necessary. Representative BEI photomicrographs of identified phases and their associations will be produced, with scale bar, magnification, sample identification, and phase identification recorded on each photomicrograph.

Individual Hg-bearing particles will be analyzed (representing one point count each) until a minimum of 100 particles has been evaluated, or 5 hr of machine time has been spent on the analysis. Point counts will be made by traversing each sample from left to right and top to bottom in a grid pattern, with each vertical displacement moving only to the adjacent field of view. Magnification settings of 40 to 100× and 300 to 600× will be used; the latter magnification allows analysis of the smallest identifiable (1–2 μm) phases. The grain size of each Hg carrier will be determined by measuring the dimension of the long axis. Percent compositions of Hg phases in each sample will be determined by summing the total area of all Hg grains and dividing the area for each phase by the total area.

HEAVY MINERAL SEPARATIONS

Heavy minerals will be identified in the PTI laboratory in Boulder, Colorado by shaking 5 g of ground and sieved soil in 100 mL of methylene iodide (specific gravity 3.325) in a separatory funnel. The samples will be allowed to settle until the liquid clears. The heavy fraction will be dispensed into a beaker and triple washed with acetone. The heavy fraction will be collected, then examined and photographed under a binocular microscope. This heavy fraction will also be analyzed by powder x-ray diffraction at the Laboratory for Geological Studies, University of Colorado, Boulder. Finally, the heavy mineral fraction will be analyzed by electron microprobe in a fashion similar to the bulk soil samples. Results of this visual observation of mercury species in soils will be tabulated and used to assist in evaluating the sequential extraction mercury speciation.

ANALYTICAL PROCEDURES

Sample extracts will be shipped on ice under strict chain of custody, in accordance with SOP-5, to CAS and the PTI laboratory in Boulder, Colorado. Soil samples for total mercury analysis will be analyzed by CVAAS (Method 7471A, U.S. EPA 1991), which includes acid digestion. Sample results will be reported on a dry-weight basis. Aqueous-phase extracts will be analyzed for mercury by a similar CVAAS methodology (Method 7470A, U.S. EPA 1991). Samples also will be analyzed for total sulfides, total carbonates, and TOC.

IN VITRO BIOAVAILABILITY TESTING

SAMPLE PREPARATION

Selected soil samples will undergo the *in vitro* procedure to estimate relative mercury bioavailability. The samples will be prepared in PTI's Boulder, Colorado laboratory by air drying and sieving to <250 μm. The <250-μm size fraction has been selected for this study because this particle size has been observed to adhere to children's hands, and is the fraction of soil most likely to be ingested (Duggan and Inskip 1985).

A split of each sieved sample (<250 μm) also will be submitted for determination of total mercury and sulfur, and total organic carbon (TOC), by the analytical method described below.

IN VITRO TEST METHOD

The *in vitro* test is designed to determine the fraction of mercury that is solubilized and available for absorption in the gastrointestinal tract. Development of the test, and the rationale for selection of representative parameters, are described in detail in the literature included in Attachment D. The *in vitro* method was designed to replicate gastrointestinal-tract parameters for a human child, including stomach and small intestinal pH and chemistry, soil-to-solution ratio, stomach mixing, and stomach emptying rate. The method is implemented in two phases, simulating the passage of ingested soil from the acidic environment of the stomach to the near-neutral conditions of the small intestine.

Because of the concern for potential loss of volatile mercury from the reaction vessel, the *in vitro* test methodology used to estimate the bioavailability of arsenic and lead has been altered for mercury bioavailability testing. The reaction will be carried out in a sealed container, to minimize potential loss of volatile mercury. Argon gas will be introduced into the reaction vessel at the beginning of the *in vitro* assay to purge it of atmospheric oxygen, to simulate the anoxic conditions present in the gastrointestinal tract. A gold trap will be placed on the inflowing argon gas to remove mercury from the inflowing gas.

The *in vitro* test will be conducted according to the following method (all chemicals from Sigma Chemical Company, unless otherwise noted):

- Prepare the stomach solution by adding the following compounds to 1 L of deionized water (stirred continually on a stir plate):

  1.25 g pepsin (50 mg, activity of 800–2,500 units/mg)
  0.50 g citrate (Fisher Chemical Co.)
  0.50 g malate (Aldrich Chemical Co.)
  420 μL lactic acid (synthetic syrup 85 percent w/w)
  500 μL acetic acid (97 percent w/w; Fisher Chemical Co.).

- Adjust the pH of the stomach solution to 2.5 by adding a measured volume of concentrated HCl.

- Add 150 mL of stomach solution to the 200-mL acrylic reaction vessel (see Attachment D).

- Sparge the stomach solution with argon for 5 minutes to remove oxygen.

- Measure the Eh of the stomach solution.

- Sparge the stomach solution with argon for an additional 2 minutes.

- Add 1.5 g of soil and seal the reaction vessel.

- Submerge the reaction vessel approximately half-way into a temperature-controlled water bath heated to maintain a constant 37 °C in the reaction vessel (Attachment D)

- Allow the soil/stomach solution to stand (no agitation) for 10 minutes.

- Stir the mixture with a plastic propeller stir rod mounted in a rheostat-controlled motor (Arrow Engineering Model 1750 motor on a rheostat setting of 2, resulting in approximately 150 rpm for the stir rod).

- Check the pH at 5-minute intervals, and readjust to pH 2.5 with HCl if necessary.

- Collect 5-mL samples at 30 and 60 minutes, using a stainless-steel hypodermic syringe to pierce the sampling septum. Centrifuge the 5-mL samples at

approximately 2500 xg for 25 minutes and decant the supernatant for analysis.

- At 1 hour, titrate the solution to pH 7.0 by adding a 5-in length of dialysis tubing containing approximately 1 g of $NaHCO_3$ to each reaction vessel. The dialysis tubing is added without exposing the reaction vessel to atmospheric oxygen.

- Allow the pH of the reaction vessel solution to increase slowly to 7.0 $\pm$0.2 before removing the dialysis bag.

- Dissolve 260 mg of bile salts and 75 mg of pancreatin in 10 mL of deionized water and inject the fluid into the reaction vessel through the septum.

- Using a stainless-steel hypodermic syringe, obtain 5 mL of intestinal-phase sample through the septum at 1.0 and 3.0 hours after the reaction fluid reaches equilibrium at pH 7. Centrifuge each sample at approximately 2500 xg for 25 minutes and decant the supernatant for analysis.

- Measure and record the concentration of mercury vapor in the headspace of the reaction flask by connecting a mercury vapor analyzer (Jerome Model 431X) to the reaction vessel, and opening the sealed sampling septum to allow air flow through the reaction vessel.

- After the final sample is collected, measure and record the pH and Eh of the flask contents.

- Measure and record the final volume of the flask contents in a graduated cylinder.

- Analyze each of the two stomach-phase and the two small-intestinal-phase samples for mercury concentration, by the analytical method described below.

IN VITRO TEST SYSTEM EVALUATION

Prior to analyzing samples for the purpose of developing a site-specific bioavailability adjustment factor (BAF), site soil samples will be evaluated using the *in vitro* test to determine the potential for loss of mercury during the test (e.g., from volatilization, or mercury adhering to the test cell walls). In a mass balance experiment, two site soil samples will be tested in triplicate in the assay. The absolute quantity of mercury recovered in the fluid, solid, and vapor phases from the reaction vessel after the assay is completed

(analytical procedures described below) will be compared to the quantity of mercury determined to be present in the soil sample before the *in vitro* assay (estimated from analysis of a split of the soil sample), to evaluate recovery of mercury from the test system.

ANALYTICAL PROCEDURES

All *in vitro* test samples will be shipped to CAS under strict chain of custody. Soil samples for total mercury analysis will be analyzed by CVAAS (Method 7471A, U.S. EPA 1991), which includes acid digestion. Sample results will be reported on a dry-weight basis. *In vitro* extracts will be analyzed for mercury by a similar CVAAS methodology (Method 7470A, U.S. EPA 1991).

QUALITY CONTROL PROCEDURES

MERCURY SPECIATION ANALYSIS

Quality Assurance and Quality Control (QA/QC) samples will be collected in accordance with SOP-6 to provide checks on sample collection and handling procedures, and analytical accuracy and precision. Field quality control will include field duplicates, external contamination blanks (ECBs), cross-contamination blanks (CCBs), and standard reference materials (SRMs). Laboratory quality control will include blank, spike, and duplicate samples. PTI laboratory control samples will be prepared as specified below.

IN VITRO TESTING

In vitro test quality control samples will include two soils that will be run through the procedure in triplicate. In addition, two *in vitro* tests with a soluble mercury spike will be performed to evaluate matrix spike recovery. Finally, a blank stomach solution spiked with a known amount of soluble mercury will be submitted as a blind laboratory control sample.

LABORATORY QUALITY CONTROL

The specific quality control procedures to be performed for the analyses of mercury and other metals are cited in U.S. EPA (1991). The laboratory quality control samples will include a preparation blank, laboratory control sample, laboratory duplicate, and matrix spike sample for each batch of 20 samples or each digestion group, whichever is more frequent.

For every 20 or fewer samples of a similar matrix analyzed by a particular method, the laboratory will submit a complete data package containing the following data and supporting information:

- A cover letter discussing the analytical procedures used and the problems encountered during sample analysis (if any).
- Sample log listing the identifying sample numbers and corresponding laboratory numbers (if applicable) for all samples included in the data package.
- Chain-of-custody forms for all samples included in the data package.
- Analyte concentrations with reporting units identified.

- The original raw laboratory data, bench sheets, and instrument printouts for all samples, including all laboratory quality control samples and blanks.

- Final dilution volumes, sample sizes, wet-to-dry ratios, and any other information—including formulas—required to derive the final reported sample concentration from the raw laboratory data.

- Final analytical results, with appropriate concentration units, for all *in vitro* and quality control *in vitro* samples, as well as laboratory quality control samples when required (i.e., laboratory method blanks, laboratory control samples [LCSs], and matrix spike samples).

- Instrument detection limits for each analyte in each package.

- A summary form indicating which method blanks are associated with each batch of samples for every analysis.

- Summarized recovery and/or relative percent difference (RPD) results for all laboratory quality assurance and quality control (QA/QC) checks, including all laboratory spike samples, calibration check samples, laboratory duplicate samples, method blanks, and LCSs for each analysis.

- Appropriate laboratory data qualification codes and their definitions.

- Summary forms for all initial and continuing instrument calibrations performed that apply to the project samples in each data package. These summaries must include the exact concentrations for the calibration standards and the acceptable linear calibration ranges for each instrument used. Some measure of the linearity of the initial calibration curve also must be determined and reported, as specified in the method.

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