

Technical Appendix B

Physicochemical Properties for TRI Chemicals and Chemical Categories

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1 Introduction

To predict the fate and transport of the reportable TRI chemicals and chemical categories, the RSEI model relies on a chemical database called that contains physicochemical properties and estimates of chemical removal efficiencies at incinerators and at publicly owned treatment works (POTWs). The physicochemical properties in the database include rates of chemical decay in air and water; organic carbon-water, octanol-water, and soil-water partition coefficients (K_{oc} , K_{ow} , and K_d , respectively); water solubilities; bioconcentration factors; Henry's Law constants (K_H); and molecular weights. To evaluate the effects of treatment and disposal, the model also requires incinerator destruction and removal efficiencies (DREs) as well as removal efficiencies for POTWs, including estimates of the percent of chemical removed due to volatilization, biodegradation, and sorption to sludge within a POTW. However, not all of the properties included in the model are currently used for modeling.

The sources of values in this database were originally documented in November, 1992. Since that time, the data have been significantly updated, with several new sources being used. The most significant new data sources are the experimental and estimation databases from Syracuse Research Corporation (PHYSROP, CHEMFATE, and the EPI Suite) and the RREL Treatability Database Version 5.0, maintained by the U.S. EPA Risk Reduction Engineering Laboratory (U.S. EPA, 1994). Table B-1 lists each parameter, its field name in the chemical database and the main data sources or estimation methods used to obtain chemical-specific values.

Table B-1. Physicochemical Properties and Data Sources

Property	Field Name	Main Data Source(s)
Rate of Chemical Decay in Air	AirDecay	AOPWIN (SRC) PHYSROP (SRC)
Organic Carbon-Water Partition Coefficient (K_{oc})	Koc	CHEMFATE (SRC) Lyman et al. (1990) PCKOC (SRC)
Rate of Chemical Decay in Water	H2ODecay	HYDROWIN (SRC)
Log of Octanol-Water Partition Coefficient ($\log K_{ow}$)	LogKow	PHYSROP (SRC)
Soil-Water Partition Coefficient (K_d)	Kd	Gerritse et al. (1982)
Water Solubility	WaterSolubility	PHYSROP (SRC)
Total Removal Efficiency for POTWs	POTWPartition(Removal)	RREL (U.S. EPA, 1994) STPWIN (SRC)
Within-POTW Sorption to Sludge	POTWPartition(Sludge)	EFDB (SRC) STPWIN (SRC)
Within-POTW Volatilization to Air	POTWPartition(Volatil)	EFDB (SRC) STPWIN (SRC)
Within-POTW Biodegradation	POTWPartition(Biod)	EFDB (SRC) STPWIN (SRC)
Incinerator Destruction and Removal Efficiency	IncineratorDRE	Assumed

Property	Field Name	Main Data Source(s)
Bioconcentration Factor	BCF	CHEMFATE(SRC) Lyman et al. (1990)
Henry's Law Constant	Henrys	PHYSPROP(SRC)
Molecular Weight	Molecular Weight	PHYSPROP(SRC)

2 Physicochemical Properties of Chemicals Included in the RSEI Model

This Appendix describes the methods used to update the chemical database and provides the sources for all of the data. Values for the physicochemical parameters for the TRI chemicals and chemical categories are provided in a separate spreadsheet that can be found on the [RSEI website](#). Explanations for the reference codes and full citations for the data sources can be found on the “Notes” page of the spreadsheet. The following sections discuss the data sources and special issues for each physicochemical parameter presented. The methods for treating chemical categories are also presented, followed by a summary of the resolution of certain TRI reporting issues which affect the exposure modeling.

2.1 Rate of Chemical Decay in Air (hr^{-1})

This parameter describes how fast a chemical degrades in air, primarily due to photooxidation by hydroxyl radicals. The daughter products of photodegradation are not modeled further; that is, it is assumed that all chemicals are photodegraded into nontoxic compounds. The main source for decay rates is SRC’s Atmospheric Oxidation Program (AOPWIN), which estimates the second-order rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. For the RSEI model, a concentration of hydroxyl radicals of 1.5×10^6 molecules/ cm^3 is used to convert the second-order rate constant provided in AOPWIN to a first-order rate constant. Furthermore, the rate is divided by a factor of two to reflect an assumed average day length of 12 hours:

$$\text{AirDecay}(\text{hr}^{-1}) = \text{AOPWINestimate} \left(\frac{\text{cm}^3}{\text{molecule}} * \text{sec} \right) * 1.5 * 10^6 \left(\frac{\text{molecules}}{\text{cm}^3} \right) * 3600 \frac{\text{sec}}{\text{hr}} * 1/2$$

For details on the methodology used in AOPWIN, see Meylan and Howard (1993).

2.2 Organic Carbon-Water Partition Coefficient (K_{oc} , in units of L/kg)

K_{oc} is “the ratio of the amount of chemical adsorbed per unit weight of organic carbon (oc) in the soil or sediment to the concentration of the chemical in solution at equilibrium” (Lyman et al., 1990; p. 4-1). K_{oc} provides an indication of the extent to which a chemical partitions between solid and solution phases in soil, or between water and sediment in aquatic systems. The K_{oc} values have units of L/kg.

Several sources were used for K_{oc} values. CHEMFATE, part of SRC’s Environmental Fate Database, is an online database that presents experimental and estimated values for various parameters. CHEMFATE was the preferred data source. If an appropriate value from CHEMFATE was not available, regression equations from Lyman et al. (1990) were used to estimate K_{oc} . If a solubility value was available, the following equation (Eq. 4-5 in Lyman et al., 1990) was used to estimate K_{oc} :

$$\log(K_{oc}) = -0.55 \log(S) + 3.64$$

Note that in this equation, solubility (S) must be entered in units of milligrams per liter (mg/L). In total, 261 chemicals were used to obtain this regression equation, which has an r^2 of 0.71. Solubility values ranged between approximately 5×10^{-4} mg/L to 1,000,000 mg/L.

If a solubility value was not available, or it did not fall within the range of solubility values used to develop the regression equation, then another equation, based on $\log(K_{ow})$, was used. If a $\log(K_{ow})$ value was available, Eq. 4-8 in Lyman et al. (1990) was used to estimate K_{oc} :

$$\log(K_{ov}) = 0.544 \log(K_{ow}) + 1.377$$

Fifty chemicals were used to obtain this regression equation, which has an r^2 of 0.74. Values of $\log(K_{ow})$ ranged between approximately -3 and 6.6.

If a $\log(K_{ow})$ value was not available, or it did not fall within the range of $\log(K_{ow})$ values used to develop the regression equation, then CHEMFATE or SRC's estimation program PCKOC was used. PCKOC uses an estimation method based on a first-order molecular conductivity index and a series of statistically derived fragment contribution factors for polar compounds to predict K_{oc} values. For details on the methodology used in this program, see Meylan et al. (1992).

2.3 Rate of Chemical Decay in Water (hr^{-1})

The primary source of water decay rates was SRC's estimation program HYDROWIN, which was developed for EPA. The program estimates abiotic hydrolysis rate constants and half-lives for esters, carbamates, epoxides, halomethanes, and selected alkyl halides. For the RSEI model, the half-life estimated for a pH of 7 was converted to a rate using the following equation:

$$k = -\ln(0.5)/t_{1/2}$$

For some chemicals, HYDROWIN stated that "Even at low pH, the hydrolysis rate is very fast: $t_{1/2} < 10$ minutes." For these chemicals, a first-order decay rate of 4.2/hr was used.

For details on the methodology used in HYDROWIN, see Mill et al. (1987). A few decay rates were obtained from the Office of Pesticide Program's OneLiner database, as included in PIRANHA (U.S. EPA, 1991).

For a few chemicals which do not undergo hydrolysis, a water decay rate was estimated based on information in CHEMFATE on photodegradation. Twelve hours of sunlight per day were assumed, and thus the rates provided in CHEMFATE for photodegradation in water were halved to estimate an average rate over a 24 hour period.

2.4 Log of Octanol-Water Partition Coefficient ($\log(K_{ow})$, unitless)

$\log(K_{ow})$ describes a chemical's lipophilic or hydrophobic properties. It is the ratio of a chemical's concentration in the octanol phase to its concentration in the aqueous phase of a two-phase system at equilibrium. It has been strongly correlated with environmental fate and transport parameters such as K_{oc} and BCF and therefore is often used to estimate values for those two parameters.

The primary source for values of $\log(K_{ow})$ was SRC's PHYSPROP database, which contains experimental and estimated values. A few values were estimated using SRC's program KOWWIN. KOWWIN uses a fragment constant methodology, in which a compound's structure is divided into functional fragments, and the coefficients for all groups are summed to obtain the compound's coefficient. Coefficients for individual fragments are derived from multiple regressions of more than 2400 reliably measured values. For details on the methodology used, see Meylan and Howard (1995). Note that the parameter $\log(K_{ow})$ has no units because it is the ratio of two concentrations.

2.5 Soil-Water Partition Coefficient (K_d , in units of L/kg)

In the RSEI chemical database, explicit values for this parameter are provided only for inorganic compounds. Organic compounds are modeled by combining chemical-specific K_{oc} values, as listed in the chemical database, with an estimate of the fraction of organic carbon, f_{oc} , to obtain a soil-water partition coefficient. For all the metals except aluminum, K_d values were estimated from column studies by Gerritse et al. (1982) using sand with an f_{oc} value of 0.0355 g/g, a cation exchange capacity of 0.22 meq/g, zero clay content, and a solution pH of 5.¹ The median of the range of K_d values for each metal was taken, assuming a log-normal distribution. For classes of inorganic compounds, the same values were used as for the elemental inorganic compound. For aluminum, the K_d value is based on Langmuir isotherm data presented in Bodek et al. (1988). The K_d values presented have units of L/kg.

2.6 Water Solubility (mg/L)

Water solubility values were primarily obtained from SRC's PHYSPROP database. The water solubility values have units of mg/L.

2.7 POTW Removal Efficiencies and Within-POTW Partitioning Percentages

The POTW removal efficiency and the three within-POTW partitioning percentages describe the fate of chemicals during treatment at POTWs. The 'POTW Partition Removal' is the total POTW removal efficiency, or the total percentage of the chemical removed by the POTW (influent concentration minus effluent concentration divided by influent concentration). The three within-POTW partitioning percentages describe the fate of the total amount of chemical removed by the POTW; the chemical may be removed by sorbing to sludge (POTW Partition Sludge), by volatilizing into the air (POTW Partition Volatil) or by being biodegraded by microorganisms (POTW Partition Biodeg). Note that the within-POTW partitioning percentages sum to 100 percent.

¹The assumption that the waste in landfills is similar to the above conditions results in a conservative estimate of the leachate concentration of metals, because low clay content and relatively low pH tend to increase the mobility of metals.

POTW removal efficiencies were available from the RREL Treatability Database maintained by the U.S. EPA Risk Reduction Engineering Laboratory (U.S. EPA, 1994). For any given chemical, the RREL Treatability Database provides a list of removal efficiencies published in the scientific literature. Each value is characterized by the technology used, the type of influent, and the scale of the experiment. For all values associated with activated sediment and full scale experiments, a geometric mean was derived and used as the POTW removal efficiency. Within-POTW partitioning values for most organic chemicals were supplied by David Lynch of the Exposure Assessment Branch of Office of Pollution Prevention and Toxics. Inorganic chemicals, except for ammonia, were assumed to partition 100 percent to sludge.

For those chemicals without data provided by David Lynch, SRC's STPWIN program was used to estimate total removal efficiency and within-POTW partitioning values. Details on the methodology used in STPWIN can be found in Clark et al. (1995). One value was obtained from Howard et al. (1991).

2.8 Bioconcentration Factor (BCF, in units of L/kg)

Bioconcentration factors (BCFs) are used to describe the equilibrium concentrations of chemicals in aquatic organisms living in contaminated water. The BCF is defined as the ratio of the chemical concentration in the organism (mg/kg) to that in the surrounding water (mg/L). Many experimental and estimated BCF values were obtained from SRC's CHEMFATE database. If an appropriate BCF value from CHEMFATE was not available, regression equations from Lyman et al. (1990) were used to estimate BCF values, as described below.

If a $\log(K_{ow})$ value was available for a chemical and was within the range used to develop the regression equation (0.90 to 6.9), Eq. 5-2 in Lyman et al. (1990) was used to estimate a BCF:

$$\log BCF = 0.76 \log (K_{ow}) - 0.23$$

Two hundred and fifty-five chemicals used this regression equation, which has an r^2 of 0.823.

If a $\log(K_{ow})$ value was not available, or it did not fall within the range of values used to develop the regression equation, then another equation, based on water solubility, was used. If a water solubility value was available and within the range of 0.001 to 50,000 mg/L, Eq. 5-3 in Lyman et al. (1990) was used to estimate a BCF:

$$\log BCF = 2.791 - 0.564 \log (S)$$

Thirty-nine chemicals were used to obtain this regression equation, which has an r^2 of 0.49.

If the above two equations could not be applied to estimate BCF values, then Chemfate or SRC's BCFWIN program was used.

2.9 Incinerator Destruction/Removal Efficiencies

This parameter describes the percentage of a chemical removed or destroyed during combustion in an incinerator. We assume that the typical municipal waste combustor destruction/removal efficiency for organics is 99 percent. This assumption ignores the fact that chemicals of concern,

such as dioxins, may be formed during the incineration process. The exceptions to the 99 percent removal assumption are PCBs and dioxin and dioxin-like compounds, both of which are assumed to have a DRE of 99.9999 percent, as required by TSCA regulation.

For incinerator destruction/removal efficiencies for inorganic chemicals, values were taken from multiple hearth sludge incinerator studies, as reported in U.S. EPA, 1992.

2.10 Henry's Law Constant (atm·m³/mol)

The Henry's Law constant is defined as the ratio of a chemical concentration in air (often expressed as a partial pressure with units of atmospheres) to the chemical concentration in water (often expressed as moles per cubic meter) under equilibrium conditions. This constant is used to model volatilization from off-site landfills. The primary source for this parameter is SRC's PHYSPROP database. The units of the Henry's Law constants are atm·m³/mol.

2.11 Maximum Contaminant Level (mg/L)

Maximum Contaminant Levels (MCLs) are enforceable standards for chemicals in drinking water and are to be set as close to the Maximum Contaminant Level Goals (MCLGs), which are based on health effects, as is feasible. MCLs are based upon the availability of analytical methods, treatment technologies, and costs for achieving various levels of removal. MCLs have not been set for most TRI chemicals. For those chemicals that do have MCLs, the RSEI model limits the concentrations in drinking water so that they cannot exceed the appropriate MCLs.

2.12 Molecular Weight (g/mol)

The molecular weight is not specifically used in the RSEI model, but values are provided as part of the physicochemical database. The primary source for molecular weights is SRC's PHYSPROP database.

3 Chemical Categories

EPA's annual 'Reporting Form R and Instructions' describes the reporting requirements for several categories that combine similar chemicals into one release report. For these categories, facilities are not required to report the pounds released of each individual chemical in the category, but only the total pounds released for the entire category. Because it is not known in what proportion individual chemicals within each category are released, professional judgment was used to assign surrogate values for the various physicochemical properties to each category. In most cases, the most toxic chemical of each category, based on the calculated toxicity weight, was selected, and the toxicity and physicochemical data for that chemical were assigned to the entire chemical category. In these cases, the actual risk for the chemical category would be less than or equal to the modeled risk.

The rest of this section describes the decisions made for each chemical category. Note that a chemical category does not have a CAS number in the chemical database; instead, it has a three digit number preceded by an 'N.'²

3.1 Metal/Metalloid Compounds

Metal/metalloid compounds are reported separately in TRI, but in RSEI each compound category is combined with the metal/metalloid elemental form. The physicochemical properties from the elemental form are used to represent the combined category. Table B-2 shows the metal compound categories included in TRI. Most categories include any unique chemical substance that contains the metal as part of that chemical's infrastructure. Any additional restrictions are noted in the table.

² The only exception is the category polychlorinated biphenyls (PCBs), which has been assigned a CAS number. Physicochemical data are readily available for this category, and therefore this category is not discussed further here.

Table B-2. Metal Categories

CAS Number	Name	Exclusions
N010	Antimony compounds	None.
N020	Arsenic compounds	None.
N040	Barium compounds	Does not include Barium sulfate (CAS# 7727-43-7).
N050	Beryllium compounds	None.
N078	Cadmium compounds	None.
N090	Chromium compounds	None.
N096	Cobalt compounds	None.
N100	Copper compounds	Does not include copper phthalocyanine compounds that are substituted with only hydrogen, and/or chlorine, and/or bromine.
N420	Lead compounds	None.
N450	Manganese compounds	None.
N458	Mercury compounds	None.
N495	Nickel compounds	None.
N725	Selenium compounds	None.
N740	Silver compounds	None.
N760	Thallium compounds	None.
N770	Vanadium compounds	None.
N982	Zinc compounds	None.

3.2 Chlorophenols

Of the 19 chlorophenols which have the formula $C_6OHCl_xH_{(5-x)}$, where $x = 1$ to 5 , toxicity data were available for six. Pentachlorophenol (CAS# 87-86-5) had the highest toxicity value, so that chemical was used as a surrogate for the category for both toxicity and physicochemical data.

3.3 Cyanide Compounds

This category includes only chemicals that can be represented by the formula $X^{y+}(CN^-)_y$, where $X = H^+$ or any other ion where a formal dissociation may occur, for example, KCN or $Ca(CN)_2$. Because cyanide compounds in a gaseous state exhibit markedly different properties than compounds in solution, two surrogate compounds were used for toxicity scores and physicochemical data for the chemical category. For the inhalation toxicity score, the air decay rate, and the Henry's Law constant, the properties of hydrogen cyanide, the most toxic gaseous compound, were used. For the oral exposure pathway, toxicity data were collected for metal cyanide compounds, the most toxic group of nongaseous cyanide compounds. Copper cyanide ($Cu(CN)_2$) was found to be the most toxic metal cyanide compound. Thus, for the oral toxicity

score and for all physicochemical properties other than the air decay rate and the Henry's Law constant, the properties of (Cu(CN)₂) were used for this chemical category.

3.4 Diisocyanates

This category only includes those chemicals listed in Table B-3. At this time, toxicity and physicochemical data have not been obtained or estimated for this category.

Table B-3. Members of Diisocyanates Category

CAS Number	Chemical
822-06-0	1,6-Hexamethylene diisocyanate
101-68-8	Methylene bis(phenylisocyanate) (MDI) and polymeric MDI
38661-72-2	1,3-Bis(methylisocyanate)-cyclohexane
10347-54-3	1,4-Bis(methylisocyanate)-cyclohexane
2556-36-7	1,4-Cyclohexane diisocyanate
134190-37-7	Diethyldiisocyanatobenzene
4128-73-8	4,4'-Diisocyanatodiphenyl ether
75790-87-3	2,4'-Diisocyanatodiphenyl sulfide
91-93-0	3,3'-Dimethoxybenzidine-4,4'-diisocyanate
91-97-4	3,3'-Dimethyl-4,4'-diphenylene diisocyanate
139-25-3	3,3'-Dimethyldiphenylmethane-4,4'-diisocyanate
4098-71-9	Isophorone diisocyanate
75790-84-0	4-Methyldiphenylmethane-3,4-diisocyanate
5124-30-1	1,1-Methylene bis(4-isocyanatocyclohexane)
3173-72-6	1,5-Naphthalene diisocyanate
123-61-5	1,3-Phenylene diisocyanate
104-49-4	1,4-Phenylene diisocyanate
9016-87-9	Polymeric diphenylmethane diisocyanate
16938-22-0	2,2,4-Trimethylhexamethylene diisocyanate
15646-96-5	2,4,4-Trimethylhexamethylene diisocyanate

3.5 Dioxin and Dioxin-like Compounds

This category includes manufacturing and the processing or otherwise use of dioxin and dioxin-like compounds if the dioxin and dioxin-like compounds are present as contaminants in a chemical and if they were created during the manufacture of that chemical. Of the 17 congeners reportable under this category and shown below in Table B-4, physicochemical data were available only for TCDD (2,3,7,8-Tetrachlorodibenzo-p-dioxin), which was used as a surrogate for the entire category. However, POTW removal rates were not available, so dioxin transfers to POTWs are not currently modeled in RSEI. Fugitive and stack air releases, direct releases to water and transfers off-site to incineration are modeled. The incineration destruction removal efficiency is assumed to be 99.9999, as required by TSCA.

Table B-4. Members of the Dioxin and Dioxin-like Compounds Category

CAS	Dioxin and Dioxin-like Compounds Name
01746-01-6	2,3,7,8-Tetrachlorodibenzo- p-dioxin
40321-76-4	1,2,3,7,8-Pentachlorodibenzo- p-dioxin
39227-28-6	1,2,3,4,7,8-Hexachlorodibenzo- p-dioxin
57653-85-7	1,2,3,6,7,8-Hexachlorodibenzo- p-dioxin
19408-74-3	1,2,3,7,8,9-Hexachlorodibenzo- p-dioxin
35822-46-9	1,2,3,4,6,7,8-Heptachlorodibenzo- p-dioxin
03268-87-9	1,2,3,4,6,7,8,9-Octachlorodibenzo- p-dioxin
51207-31-9	2,3,7,8-Tetrachlorodibenzofuran
57117-41-6	1,2,3,7,8-Pentachlorodibenzofuran
57117-31-4	2,3,4,7,8-Pentachlorodibenzofuran
70648-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran
57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran
72918-21-9	1,2,3,7,8,9-Hexachlorodibenzofuran
60851-34-5	2,3,4,6,7,8-Hexachlorodibenzofuran
67562-39-4	1,2,3,4,6,7,8-Heptachlorodibenzofuran
55673-89-7	1,2,3,4,7,8,9-Heptachlorodibenzofuran
39001-02-0	1,2,3,4,6,7,8,9-Octachlorodibenzofuran

3.6 Ethylenebisdithiocarbamic (EBDC) Acids, Salts, and Esters

This category contains any unique chemical substance that contains an EBDC or an EBDC salt as a part of that chemical's infrastructure. According to EPA's 1998 Status of Pesticides in Registration, Reregistration, and Special Review (The Rainbow Report), chemicals regulated in the category EBDCs include maneb, mancozeb, metiram, nabam, zineb, and amobam. Maneb, metiram, nabam, and zineb are separately reported in TRI. Toxicity data were available for four compounds (mancozeb, maneb, metiram, and zineb); of these, metiram had the highest toxicity weight. Therefore, metiram was selected as the surrogate for both toxicity and physicochemical data.

3.7 Glycol Ethers

This category includes chemicals that can be represented by the formula $R-(OCH_2CH_2)_n-OR'$ where $n = 1, 2, \text{ or } 3$; $R = \text{alkyl } C_7 \text{ or less, or, } R = \text{phenyl or alkyl substituted phenyl}$; $R' = H, \text{ or alkyl } C_7 \text{ or less}$; or, OR' consists of carboxylic acid ester, sulfate, phosphate, nitrate, or sulfonate. Eight common glycol ethers were identified: ethylene glycol monobutyl ether (CAS#111-76-2), dipropylene glycol monomethyl ether (CAS#34590-94-8), ethylene glycol diethyl ether (CAS#629-14-1), ethylene glycol monoethyl ether acetate (CAS#11-15-9), ethylene glycol monoethyl ether (CAS#110-80-5), monomethyl ether acetate (CAS#110-49-6), ethylene glycol monomethyl ether (CAS#109-86-4), and propylene glycol monomethyl ether (CAS#107-98-2). Of these, four chemicals had available toxicity data. Ethylene glycol monomethyl ether had the highest toxicity weight of the four and therefore was used as a surrogate for the category for both the toxicity data and the physicochemical data.

3.8 Nicotine and Salts

This category includes any unique chemical substance that contains nicotine or a nicotine salt as part of that chemical's infrastructure. Nicotine was selected as a surrogate for both toxicity and physicochemical values. However, no toxicity values were available for nicotine.

3.9 Nitrate Compounds

This category only includes compounds that are water dissociable and are reportable only when in an aqueous solution. Toxicity data for nitrate were available from IRIS; however, at this time, physicochemical data have not been determined for this category.

3.10 Polybrominated Biphenyls (PBBs)

This category includes chemicals that can be represented by the formula $C_{12}Br_xH_{(10-x)}$, where $x = 1 \text{ to } 10$. Toxicity data for a PBB mixture were available from HEAST. However, no physicochemical data was available for PBB mixtures. According to the Consumer Product Safety Commission, hexabromobiphenyl (CAS#36355-01-8) was the major component in the most widely used mixture of PBBs. Therefore, this chemical was selected as a surrogate for the entire class for physicochemical data.

3.11 Polychlorinated Alkanes

This category includes chemicals that can be represented by the formula $C_xH_{2x+2-y}Cl_y$, where $x = 10$ to 13 and $y = 3$ to 12 , and the average chlorine content ranges from 40 to 70 percent, with the limiting molecular formulas $C_{10}H_{19}Cl_3$ and $C_{13}H_{16}Cl_{12}$. At this time, toxicity and physicochemical data have not been determined for this category.

3.12 Polycyclic Aromatic Compounds (PACs)

There are 21 members of this class listed in the Form R instructions as reportable under TRI, as shown in Table B-5. Of these 21 chemicals, only benzo(a)pyrene (CAS# 50-32-8) and benzo(j,k)fluorene (CAS#206-44-0) had available toxicity data. The toxicity weight for benzo(j,k)fluorene (tox weight = 13) is approximately 1,000-fold lower than that for benzo(a)pyrene (tox weight = 15,000). However, absent information on the composition of the total PAC emissions, the model uses a conservative approach and uses the benzo(a)pyrene value to represent the group. This chemical was selected as a surrogate for the entire class for physicochemical data. For toxicity data, the toxicity of this group is assumed to be 18% of the toxicity for benzo(a)pyrene. This approach follows that used in EPA's National-Scale Air Toxics Assessment (NATA) evaluation for polycyclic organic matter (POM).

Table B-5. Members of Polycyclic Aromatic Compounds Category

CAS Number	Chemical
56-55-3	Benz(a)anthracene
205-99-2	Benzo(b)fluoranthene
205-82-3	Benzo(j)fluoranthene
207-08-9	Benzo(k)fluoranthene
189-55-9	Benzo(rst)pentaphene
218-01-9	Benzo(a)phenanthrene
50-32-8	Benzo(a)pyrene
226-36-8	Dibenzo(a,h)acridine
224-42-0	Dibenzo(a,j)acridine
53-70-3	Dibenz(a,h)anthracene
194-59-2	7H-Dibenzo(c,g)carbazole
5385-75-1	Dibenzo(a,e)fluoranthene
192-65-4	Dibenzo(a,e)pyrene
189-64-0	Dibenzo(a,h)pyrene
191-30-0	Dibenzo(a,l)pyrene
57-97-6	7,12-Dimethylbenz(a)anthracene
193-39-5	Indenol[1,2,3-cd]pyrene

CAS Number	Chemical
3697-24-3	5-Methylchrysene
5522-43-0	1-Nitropyrene
206-44-0	Benzo(j,k)fluorene
56-49-5	3-Methylcholanthrene

3.13 Strychnine and salts

This category includes any unique chemical substance that contains strychnine or a strychnine salt as part of that chemical's infrastructure. Strychnine (CAS#57-24-9) was used as a surrogate for both toxicity and physicochemical data for this category.

3.14 Warfarin and salts

This category includes any unique chemical substance that contains warfarin or a warfarin salt as part of that chemical's infrastructure. Warfarin (CAS# 81-81-2) was used as a surrogate for both toxicity and physicochemical data for this category.

4 Summary of Resolution of Certain TRI Reporting Issues

In March 1996, several reporting issues pertaining to the TRI chemicals ammonia, ammonium sulfate, and mineral acids were resolved. These issues and the corresponding modifications or recommendations which were agreed upon are summarized below.

4.1 Ammonia and Ammonium Sulfate

Effective for the 1994 reporting year, only the ammonia or a fraction of the water-dissociable portion of ammonia in a compound will be reportable to TRI. This includes anhydrous ammonia, aqueous ammonia, and ammonia from water-dissociable ammonium salts and other sources (the latter includes ammonium sulfate). The total quantity of ammonia is calculated, but only 10% of this quantity counts towards threshold levels for reporting and it is this 10% which is actually reported. To re-calculate the original quantity of ammonia, one must multiply the reported quantity of releases and transfers (e.g., POTW) to water and land by 10 (air emissions are reported at 100%).

Because of these reporting changes, comparisons should not be made between ammonia reporting before 1995 and after 1995.

4.2 Mineral Acids

Mineral acids include sulfuric and hydrochloric acid. The Agency has made the decision to modify reporting to include only the more highly toxic exposures to aerosol releases of certain of these acids. The acid aerosols include mists, vapors, gas, fog and other airborne forms of any particle size. For sulfuric acid, this change in reporting takes place in 1994, while for hydrochloric acid the change takes place for reporting year 1995. The very high decay rate in water of these acids will greatly reduce any risk-based impacts associated with releases or transfers to water.

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