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PART III: Brownfields

Chapter 8

DATABASE ANALYSIS OF STATE SURFACE SOIL REGULATORY GUIDANCE VALUES

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ABSTRACT

A 2001 study of Cleveland, Ohio brownfield surface soil contamination led to the examination of state regulatory guidance values for soils. Surface soils were of particular interest since these generally pose the greatest risk to human health at brownfield sites. This investigation initially focused on heavy metals, common contaminants at Cleveland brownfields. However, the observation of significant variability in guidance values applied to Cd, Cr, Cu, Pb, Ni, and Zn led to questions about other state-regulated components and ultimately to research examining the origins, magnitudes, and explanations for regulatory guidance value variability.

The results presented here are based on the compilation of an 18,776 state surface soil database assembled from regulatory guidance for organic, inorganic, and element contaminants. All values were captured electronically from internet sources. The structure of each guidance value dataset was then standardized in a database-compatible format. Chemical Abstract Service (CAS) registry numbers were added to each record if they were not already provided. Identification of all records by CAS number resolves the problem of chemical synonyms. All value datasets were then assembled into the ACCESS database S³GVD (State Surface Soil Guidance Value Database)

Statistical analysis is presented to characterize the nature and extent of variability in state surface soil guidance values. The organics, inorganics, and elements most and least commonly regulated and the range of guidance values are discussed. Log-scale Ordered Column Diagrams (LOCs) are used to explore the nature of individual chemical guidance value distributions.

Keywords: surface soil contamination, regulatory guidance values, database analysis

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1. INTRODUCTION

This manuscript describes the development and application of a database titled S3GVD (State Surface Soil Guidance Value Database) that contains data on current state regulatory guidance values used to determine significant levels of surface soil contamination. The database was assembled to help identify the extent of regulated contaminants and to explore the variability of the guidance “mass burden” values being applied. In this context, “current” means regulatory guidance that was available online via regulatory agency portals after January, 2006. The term “mass burden” refers to contamination levels specified in units of mg/kg. Measures in these units are sometimes referred to as “concentrations,” but we prefer to reserve the term “concentration” for contaminants defined as mass of solute per volume of liquid solvent. There are subtleties in the differences between the two that have implications for guidance values. For example, it is possible for a concentration to exceed 1,000,000 mg/l. This would be the case for a pure organic liquid with a density greater than water. However, it is not possible for a mass burden to exceed 1,000,000 mg/kg. No matter what it is made of, 1 kg is still 1,000,000 mg. If the chemical is a soil contaminant, mass burdens must be substantially less than this. This imposes a physical constraint of guidance values that is not always respected in regulation.

This manuscript describes how state guidance value datasets were identified, standardized, assembled, and vetted, and illustrates how S3GVD may be applied to examine the state of practice in regulatory surface soil contamination guidance.

This effort originated in a 2001 field survey of surface soil heavy metal contamination and implied health risks of brownfield soils of Cleveland, OH (Jennings et al. 2002a). Reconnaissance analysis indicated that many of these sites had high levels of Cd, Cr, Cu, Ni, Pb, and Zn. However, risk assessment was complicated by the fact that the State of Ohio was shifting from “background” guidance (values set at estimates of the naturally-occurring levels in uncontaminated soils) to health-based guidance (values set at estimates of the maximum contaminant mass burdens believed to maintain human health risk below a specified level in a predetermined exposure scenario). Ohio’s 1999 background standards for Cd, Cr, Ni, Pb, and Zn were 1.25, 22, 37, 33, and 90 mg/kg respectively (OEPA, 1999). Ohio’s 2002 health-based “Generic Remediation Standards (OEPA, 2002) raised these values to 35,120,000/230 (CrIII/CrT), 1,500, 400, and 23,000 mg/kg respectively (increased of up to 55,000%). This led to obvious questions about the applicability of the new standards, and to comparison between these and the guidance values used in other Midwestern states. The result was that, with the exception of Pb guidance, heavy metal regulatory guidance was found to differ by orders of magnitude, and these differences yielded significant changes in the implied risks (Petersen et al., 2006). Expansions of the basis of comparison ultimately led to an analysis of the heavy metal surface soil guidance available in all of the state, province, commonwealth, and territory environmental jurisdictions of North America (Jennings and Petersen 2006; Jennings and Ma 2006) and to a preliminary effort to examine the guidance for common organic pollutants (benzene, ethylbenzene, pentachlorophenol, phenol, naphthalene, tertachloroethylene, toluene, trichloroethylene, and xylenes) (Jennings, 2005). Results indicated that guidance value variability ranged from 4 to 6 orders of magnitude, but that organic compounds were difficult to compare because of differences in the way they were identified.

The analysis presented here was conducted to provide a more comprehensive assessment of the scope and variability in the U.S. regulatory guidance being applied to surface soil contamination. Database analysis was required to help manage the huge amount of data involved.

2. MATERIALS AND METHODS

2.1 Dataset Identification

Regulatory Guidance Value Datasets (GVDs) were identified by internet search. Many states provide more than one set of values because individual agencies or regulatory programs promulgate application-specific guidance. For example, Ohio provides guidance under both its Remedial Response and Voluntary Action programs. Delaware allows users to apply either “default” background standards or risk-based standards. Vermont allows users to apply alternatives such as guidance provided by EPA regions III, VI, or IX. Several states also list previous, current, and proposed GVDs and stage in changes over several years. Internet searches identified 80 GVDs. It is certainly possible that datasets were overlooked or that sets have been added or revised, but these 80 datasets provide a large sample of currently-available surface soil mass burden guidance.

Table 1 identifies the 80 regulatory guidance datasets identified. Detailed references (100+ web citations) are available for each (see Hanna, 2007), but have not been included here because of length restrictions. States are identified by their postal code abbreviation. The Guidance Value Designation column identifies the jurisdiction’s name for its guidance values. These vary from demonstrative designations such as “Soil Remediation Standards”, “Predetermined Soil Remediation Levels”, or “Soil Cleanup Value Standards” to less explicit identities such as “Soil Level”, “Remediation Objectives” or “Suggested Generic Soil Cleanup Levels”, but they all serve the same purpose. They identify contamination levels that are high enough to be of environmental or human health concern to warrant additional analysis. Many states provide guidance for a variety of site conditions (proximity to surface water bodies or potable groundwater), site uses (parks, residential, commercial, light industrial, heavy industrial), exposure types (ingestion, inhalation, dermal exposure) or exposure objects (child, indoor adult worker, outdoor adult worker, construction worker). The values selected were either generic values that apply to all sites, or residential, commercial, and industrial values that apply to surface soils where risk is dominated by inhalation, ingestion, or dermal contact. The final three columns of Table 1 summarize the number of guidance values found for organic, inorganic, and element contamination. Guidance values are characterized as element values if they specified mass burden for an element or elemental ion (e.g. Cr+3, Cr+6, Na+, Cl-, F-).

Table 1. Surface Soil RGD Identification, Type and Size Summary

RGD	State	Guidance Value Designation	O	I	E
1	Alabama (AL)	Preliminary Screening Values	165	9	22
2	Alaska (AK)	Cleanup Levels	108	2	15
3	Arizona (AZ)	Soil Remediation Standards, Soil Remediation Level (SRL)	492	41	26
4	Arizona (AZ)	Predetermined Soil Remediation Levels	519	19	30
5	Arkansas(AR)	Human Health Medium-Specific Screening Levels	388	44	28
6	California (CA)	Soil Level	34	3	19
7	California (CA)	Environmental Screening Levels	98	2	20
8	Colorado (CO)	Soil Cleanup Value Standards	19	0	6
9	Connecticut (CT)	Standards for Soil Remediation	151	3	22
10	Delaware (DE)	Default Background Remediation Standards	27	0	20
11	Delaware (DE)	Uniform Risk-Based Remediation Standards	363	37	30
12	Florida (FL)	Soil Cleanup Target Levels	373	11	28
13	Georgia (GA)	Risk Reduction Standards	394	143	19
14	Hawaii (HI)	Tier 1 Action Levels	17	0	2
15	Hawaii (HI)	Tier 1 Environmental Action Levels (EALs)	96	2	21
16	Idaho (ID)	Initial Default Target Levels	161	6	18
17	Illinois (IL)	Remediation Objectives	104	3	21
18	Indiana (IN)	Residential Closure Levels	122	3	14
19	Iowa (IA)	Statewide Standard for Soil	198	11	23
20	Kansas (KS)	Risk-Based Standards	157	4	15
21	Kentucky (KY)	Preliminary Remediation Goals	519	21	30
22	Louisiana (LA)	Screening Standards for Soil	124	5	16
23	Maine (ME)	Remedial Action Guidelines	40	1	13
24	Maryland (MD)	Uniform Numeric Risk-Based Standards Generic Numeric Cleanup Standards	122	2	20
25	Massachusetts (MA)	MCP Numerical Standards	99	2	16
26	Massachusetts (MA)	MCP Numerical Standards	95	1	16
27	Massachusetts (MA)	MCP Numerical Standards	95	1	16
28	Michigan (MI)	Risk-Based Screening Levels, Generic Cleanup Criteria and Screening Levels	227	3	29
29	Minnesota (MN)	Soil Reference Value	128	5	26
30	Mississippi (MS)	Target Remediation Goals	441	47	30
31	Missouri (MO)	Soil Target Concentrations	202	4	20
32	Montana (MT)	Preliminary Remediation Goals (Adjusted)	519	19	30
33	Montana (MT)	Risk-based Screening Level	25	0	0
34	Nebraska (NE)	Voluntary Cleanup Program Remediation Goals	521	28	30
35	Nevada (NV)	Interim Action Level	2	0	0
36	New Hampshire (NH)	Soil Standards	131	2	15

Table 1. Continued

RGD	State	Guidance Value Designation	O ⁽¹⁾	I ⁽²⁾	E ⁽³⁾
37	New Hampshire (NH)	Soil Standards	131	2	16
38	New Jersey (NJ)	Soil Cleanup Criteria	92	1	16
39	New Jersey (NJ)	Generic Soil Remediation Standards	117	2	17
40	New Mexico (NM)	Soil Screening Levels	175	8	24
41	New York (NY)	Recommended Soil Cleanup Objectives	95	1	23
42	New York (NY)	Recommended soil cleanup objectives for Gasoline and Fuel Oil Contaminated Soils	29	0	0
43	New York (NY)	Soil Cleanup Objectives	70	2	14
44	North Carolina (NC)	Soil Remediation Goals	248	6	17
45	North Dakota (ND)	Cleanup Action Level	1	0	0
46	Ohio (OH)	Generic Numerical Standards	105	2	18
47	Ohio (OH)	Residential Generic Cleanup Numbers (GNCs)	166	6	20
48	Oklahoma (OK)	Risk-Based Cleanup Levels	3	0	0
49	Oklahoma (OK)	Generic SSLs for Residential Scenario	92	2	15
50	Oklahoma (OK)	Medium Specific Screening Levels	388	41	28
51	Oregon (OR)	Soil Cleanup Level	64	1	11
52	Oregon (OR)	Residential Maximum Allowable Soil Concentration	64	1	11
53	Oregon (OR)	Preliminary Remediation Goals	520	18	30
54	Pennsylvania (PA)	Medium Specific Concentrations (MSC)	317	4	22
55.	Rhode Island (RI)	Direct Exposure Criteria	77	1	17
56.	South Carolina (SC)	Risk Based Screening Levels	77	1	17
57.	South Dakota (SD)	Action Level	6	0	0
58.	South Dakota (SD)	Look-up Table (sites without a water ingestion pathway)	6	0	0
59.	Tennessee (TN)	Preliminary Remediation Goals	519	19	30
60.	Texas (TX)	Protective Concentration Levels (PCLs)	590	12	30
61.	Texas (TX)	Surface/Air and Ingestion Standard (SAI)	588	10	30
62.	Texas (TX)	Risk-Based Screening Values (RBSVs)	588	10	30
63.	Utah (UT)	Risk-Based Corrective Action Screening Levels (SL)	9	0	0
64.	Utah (UT)	Recommended Cleanup Levels (RCLs)	9	0	1
65.	Vermont (VT)	Risk Based Concentration	293	25	27
67.	Vermont (VT)	Preliminary Remediation Goals	519	21	30
67.	Virginia (VA)	Risk Based Concentration	288	24	24
68.	Virginia (VA)	Soil Screening Level (SSL)	162	4	19
69.	Virginia (VA)	Risk-Based Concentration (RBC)	161	4	19
70.	Virginia (VA)	VRP Tier II Screening Concentration	163	4	19
71.	Washington (WA)	Soil Cleanup Levels	18	0	6
72.	Washington (WA)	Cleanup Levels	493	45	25
73.	West Virginia (WV)	De Minimis Standards for Soil	353	20	25

Table 1. Continued

RGD	State	Guidance Value Designation	O ⁽¹⁾	I ⁽²⁾	E ⁽³⁾
74.	West Virginia (WV)	Uniform Standards for Soil	495	42	0
75.	West Virginia (WV)	Natural Background	0	0	34
76.	Wisconsin (WI)	Suggested Generic Soil Cleanup Levels	18	0	0
77.	Wisconsin (WI)	Soil Cleanup Standards	7	0	5
78.	Wisconsin (WI)	Soil Screening Levels	8	0	0
79.	Wisconsin (WI)	Soil Screening Levels, Soil Screening Guidance	529	49	28
80.	Wyoming (WY)	Soil Cleanup Levels	522	19	30

Table Notes: RGD – Regulatory Guidance Database ; O – Number of Organic Guidance Values
I – Number of Inorganic Guidance Values; E – Number of Element Guidance Values

2.2 Guidance Value Database Standardization

All GVDs were edited into a standard format for incorporation into **S³GVD**. This required resolving several format issues including the issue of chemical name. Regulatory guidance almost always identifies contaminants by name. This poses a significant challenge to database analysis because there is little consistency in the way chemicals are named. Many organics are identified by their chemical structure, abbreviation, common name, or manufacturer's designation. This leads to three major data base analysis challenges.

2.2.1 Nomenclature versus common names

Organics such as toluene (C₇H₈) may be identified by the common name “toluene” or by the more descriptive nomenclature names of methylbenzene, monomethyl benzene, or phenylmethane. This is significant because a database search using any one of these names would yield incomplete results. Name variations also cause problems if guidance values are listed under multiple names. This inflates the apparent number of organics for which guidance is provided.

2.2.2 Name syntax

There are syntax variations by which nomenclature names may be listed. For example, the 1,1,1 version of the C₂H₃Cl₃ may be identified as (ethane, 1,1,1,-trichloro-), (1,1,1-trichloroethane), (trichloro-1,1,1-ethane), or (-trichloroethane) and the number of possible variations grows rapidly with structure complexity. Any of these name variations could be incorrectly interpreted as a unique chemical by database software.

2.2.3 Product Names

Organics such as Fluorene (C₁₃H₁₀; 2,2'-methylenebiphenyl), Lindane (C₆H₆Cl₆; 1,2,3,4,5,6-hexachlorocyclohexane), or Endosulfan (C₉H₆Cl₆O₃S; 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro,3-oxide) are often identified by a product name. The National Institute of Standards and Technology (NIST) records data for each of these under their product name rather than their chemical nomenclature.

To illustrate the potential magnitude of these problems, consider that NIST lists 86 synonyms for the common lawn and garden insecticide Dimpylate (C₁₂H₂₁N₂O₃PS) which is regulated in 31 states. Table 2 lists the 23 chemical nomenclature name variations listed in the NIST directory. Table 3 completes this list with 63 product names also listed by NIST. Considering the variations that can be created by capitalization and punctuation, there is a nearly unlimited number of name variations under which Dimpylate could be regulated.

One solution for the chemical name problem is to replace the names used by regulatory jurisdictions with a standard name for each contaminant. This was not done. There is no universal authority for determining "standard" names. Even in the NIST registry, chemicals are not consistently identified by nomenclature names and the punctuation used in nomenclature designations is not always consistent. Furthermore, even if names were standardized, database users might not recognize the contaminant by its standard name.

Table 2. Nomenclature Name Variation for Dimpylate, CAS No 333-41-5 (NIST, 2007)

No.	Nomenclature Name Variation
1	Phosphorothioic acid, O,O-diethyl O-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester
2	Phosphorothioic acid, O,O-diethyl O-(2-isopropyl-6-methyl-4-pyrimidinyl) ester
3	O,O-Diethyl-O-(2-isopropyl-4-methylpyrimidyl)thiophosphate
4	Diethyl 4-(2-isopropyl-6-methylpyrimidinyl)phosphorothionate
5	Isopropylmethylpyrimidyl diethyl thiophosphate
6	O-2-Isopropyl-4-methylpyrimidyl-O,O-diethyl phosphorothioate
7	O,O-Diethyl-O-(2-isopropyl-4-methyl-pyrimidin-6-yl)-monothiophosphat
8	O,O-Diethyl O-(2-isopropyl-4-methyl-6-pyrimidinyl) phosphorothioate
9	O,O-Diethyl O-(2-isopropyl-4-methyl-6-pyrimidyl) phosphorothioate
10	O,O-Diethyl O-(2-isopropyl-4-methyl-6-pyrimidyl) thionophosphate
11	O,O-Diethyl O-(2-isopropyl-6-methyl-4-pyrimidinyl)phosphorothioate
12	O,O-Diethyl O-(2-isopropyl-6-methyl-4-pyrimidinyl) phosphorothioate
13	O,O-Diethyl O-6-methyl-2-isopropyl-4-pyrimidinyl phosphorothioate
14	O,O-Diethyl 2-isopropyl-4-methylpyrimidyl-6-thiophosphate
15	O,O-Diethyl-O-(2-isopropyl-4-methyl-pyrimidin-6-yl)-monothiofosfaat
16	Phosphorothioate, O,O-diethyl O-6-(2-isopropyl-4-methylpyrimidyl)
17	Thiophosphate de O,O-diethyle et de O-2-isopropyl-4-methyl-6-pyrimidyle
18	4-Pyrimidinol, 2-isopropyl-6-methyl-, O-ester with O,O-diethyl phosphorothioate
19	O,O-Diethyl 2-isopropyl-6-methyl-4-pyrimidinylphosphorothioate
20	Diethyl 2-isopropyl-4-methyl-6-pyrimidinyl phosphorothionate
21	Phosphorothioic acid, O,O-diethyl 2-isopropyl-6-methyl-4-pyrimidinyl ester
22	o,o-Diethyl-O-(6-methyl-2-(1-methylethyl)-4-pyrimidinyl)phosphorothioate
23	o,o-Diethyl o-(2-isopropyl-6-methyl-4-pyrimidinyl) thiophosphate

Rather than standardize chemical names, a record was added (where it did not already exist) to identify each chemical by its Chemical Abstract Service registry number (CAS number). CAS numbers are unique numbers containing up to 9 digits that identify every substance that has been registered with the American Chemical Society. The CAS registry contains information on more than 31 million substances and is believed to be the most comprehensive database of this type in the world (ACS, 2005). The CAS numbers themselves have no chemical significance, but each is unique and the final digit in the sequence may be used in a validity test of the number. CAS numbers should be written with a hyphen in front of the third-from-last and last number in the digit sequence. For example, the CAS No. for Lindane is 58-89-9. Several states use CAS numbers, but some omit hyphens. Omitted hyphens were replaced. This avoided problems such as 58899 and 58-89-9 being identified as different classifications by database software. CAS numbers were added to all records in each guidance value dataset that did not already contain them. Several resources were used for this. The NIST web site (NIST, 2007) is very helpful, but requires that one know the CAS number to find a chemical. Several other resources were used to identify CAS numbers for chemicals regulated only by name. *Chemexper* (2006), proved to be most helpful. This provides information on most chemicals currently being manufactured. *PubChem* (NCBE 2006) maintained by the National Center for Biotechnology Information and the *Substance Registry System* (USEPA, 2006) maintained by the Environmental Protection Agency were also used to identify CAS numbers for chemicals not listed in *Chemexper*.

Table 3. Product Name Variation for Dimpylate, CAS No. 333-41-5, (NIST, 2007)

No.	Name	No.	Name	No	Name e
24	Diazinone	45	AG-500	66	Bassadinon
25	Antigal	46	Basudin 10 G	67	Disonex
26	Basudin	47	Bazuden	68	Agridin 60
27	Bazudin	48	Dazzel	69	Antlak
28	Ciazinon	49	Diazajet	70	Diagran
29	Dacutox	50	Diazide	71	Diazinon AG 500
30	Dassitox	51	Diazitol	72	Diaterr-fos
31	Dianon	52	Diazol	73	Diazinon liquid
32	Dicid	53	Dipofene	74	Diethyl dimpylatum
33	Dimpylat	54	Ektoband	75	Diziktol
34	Exodin	55	Geigy 24480	76	Dizinon
35	ENT 19,507	56	Nedcidol	77	Drawizon
36	Flytrol	57	Neocidol (oil)	78	Dyzol
37	G 301	58	Nucidol	79	Fezudin
38	G-24480	59	NCI-C08673	80	Kayazinon
39	Galesan	60	Oleodiazinon	81	Kayazol
40	Garden Tox	61	Nemacur	82	Knox Out 2FM
41	Neocidol	62	Basudin 5G	83	Neocidol veterinary powder
42	Sarolex	63	Nipsan	84	Spectracide 25EC
43	Spectracide	64	Knox-out	85	Root guard
44	Alfa-Tox	65	Meodinon	86	Diazinon

In addition to adding CAS numbers, records were added to identify the data source, the dates of origin and electronic capture, and a code to distinguish organic, inorganic, and element guidance. Records were also reordered into a consistent format, but efforts were made to maintain the format and precision of all numerical information. In some instances, this led to questions about the true value of the guidance. Some states compute values from formula and coefficients stored in on-line spreadsheets. The results are displayed using a format set in the spreadsheet, but the actual values are stored to much higher precision. When these values are copied, the whole computation (to many significant figures) is preserved, so it can be displayed to any desired precision. For this analysis, the displayed precision was assumed to be the intended accuracy.

2.3 Database Verification

Once GVDs were standardized, each was imported into S3GVD. This resulted in a database of 18,776 guidance value records. A series of verification protocols were then applied to detect and help resolve inconsistencies.

One method of checking for consistencies was to sort all database records by CAS number and then examine the names associated with all identical CAS numbers. When names appeared that were not synonyms, the original state documentation was consulted. If discrepancies existed between state-supplied names and CAS numbers, the name was assumed to be correct.

Inconsistencies were also sought by sorting the database by chemical name and verifying that each unique name was associated with the appropriate CAS number. Because of the use of synonyms, this resulted in more name groups than CAS numbers, but helped identify name/number associations that were not consistent.

As a final check, an inverse CAS registry was used to identify chemical structure and verify CAS numbers for each unique contaminant name group.

The verification test sequence yielded a diminishing number of inconsistencies. Most of these were typographical or syntax errors in chemical names or CAS numbers. In the final verification test, only 3 inconsistencies were detected out of 18,776 records (an error rate of 0.016%), but it is possible that errors remain. It is also likely that states have added new contaminants or updated existing values since the dataset was captured. S3GVD should be updated frequently to accommodate the evolution of regulatory guidance.

2.4 Log Ordered Column Diagrams

Jennings and Petersen 2006 applied Log Ordered Column Diagrams (LOCDs) to illustrate the variability of regulatory guidance values for residential soils. Jennings, and Ma (2007) extended this method to include the use of the fuzzy mode (\tilde{M}) to help identify “common” ranges in guidance value distributions. These approaches will be applied here. Furthermore, to help serve as a basis of comparison for the whole value distribution, consider the following:

Let x be a lognormally distributed random variable that has a probability of 0.998 of falling within the number range $[1 - 100,000]$. This random variable would have a mean (μ_L) of 2.50 and a standard deviation (σ_L) of 0.809.

Generate 50 random samples of x , (50 x_i realizations) by using a normal random number generator to generate values of $\log(x)$. Order these realizations from highest to lowest.

Repeat “ii” several (N) times and average the results.

Plot the results as a LOCD.

The results of this process are illustrated in Fig. 1. Given a sufficiently large value of N, what will emerge is a column diagram approximation of the cumulative distribution function (CDF) of x . The results of Fig. 1 were calculated from 10 realizations. This is an easily anticipated result, but is noteworthy because of a few of its properties. Note that the arithmetic mean (in this case 1,568) is substantially higher than 10^{μ_L} ($10^{2.564}=366$) and the median. Also note that there is no mode. However, one should also note that the “nice” version of Fig. 1 only emerges in the average after realizations are averaged. Figure 2 illustrates a LOCD of one single realization. In Fig. 2 the parent distribution is not as easily detected.

Finally, consider that it is possible (but unlikely) to randomly generate a number set with a non-trivial mode. In the example of Fig.3, a mode was created by rounding off values in the neighborhood of 300 to one significant figure. This can be extended to a “fuzzy mode” by extending the range by some percent of the mode. Jennings and Ma (2007) found that 10% was a reasonable extension based on the way regulatory guidance values are calculated and rounded.

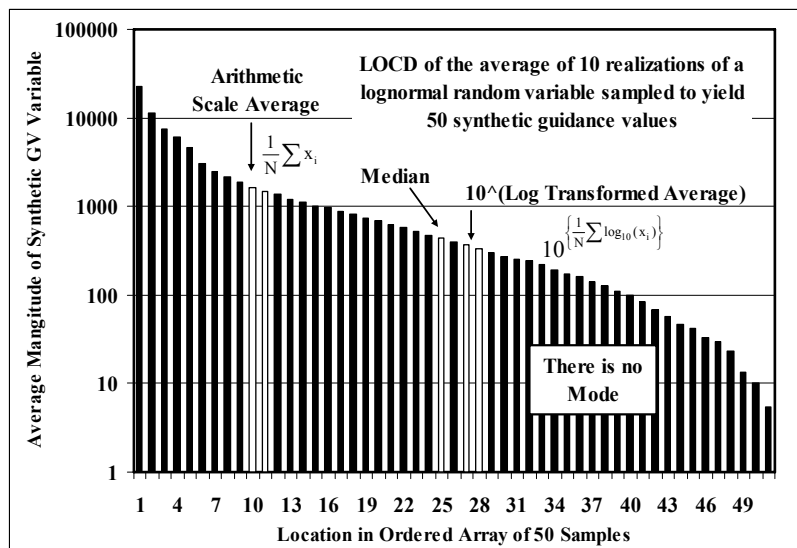


Figure 1. LOCD of the Average of 10 Realizations Each of 50 Ranked, Lognormal Random Numbers

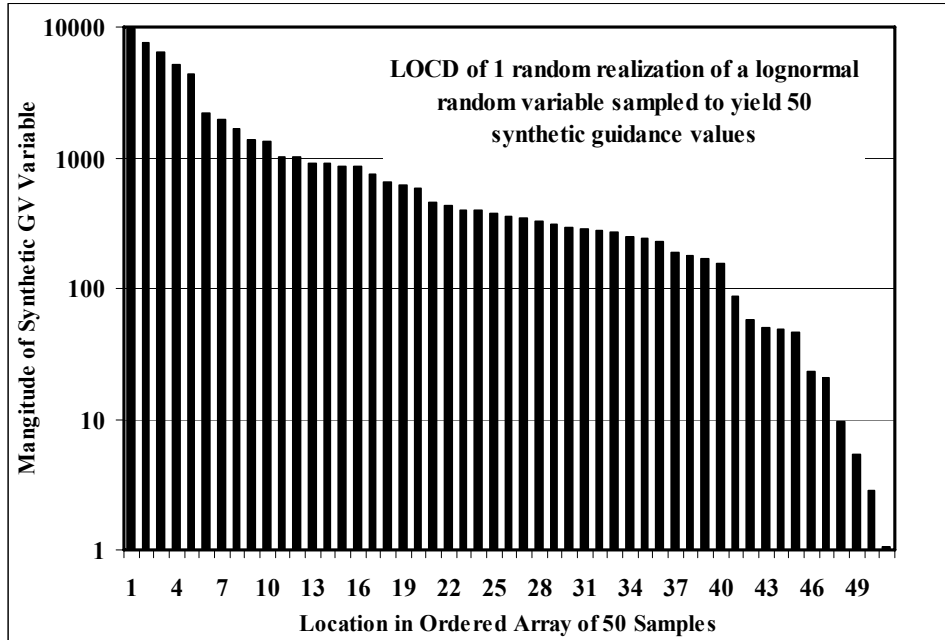


Figure 2. LOCD of 1 Realization of 50 Ranked Lognormal Random Numbers

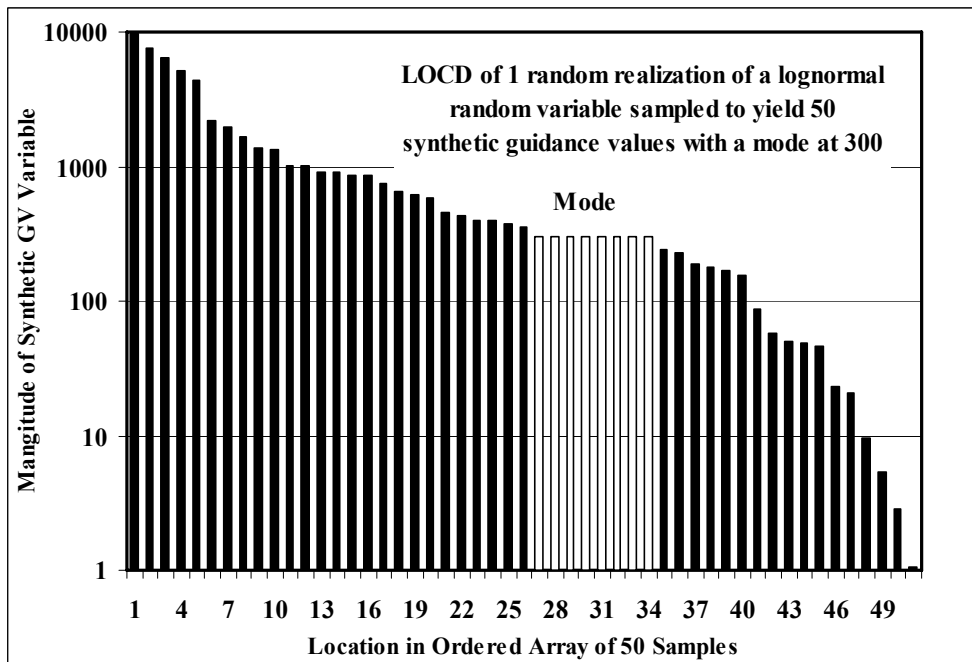


Figure 3. LOCD of 1 Realization of 50 Lognormally Random Numbers with a Synthetic Mode

Fig. 3 provides a useful (but not particularly complementary) basis by which to compare the value distributions of regulatory guidance values.

Figure 5 presents a histogram of the data of Fig. 4 using an interval size of approximately $\sigma/4$. The number of values in national superfund or by EPA region guidance have been indicated. It seems likely (but not apparent) that these numbers have influenced the size of state GVDs.

One obvious question one might ask is which state has the most (or least) conservative guidance. This is easy to answer for any one compound, but more difficult to characterize across the whole array of regulated compounds. One method of approaching the question is to examine the extremes of the guidance values for each compound, and to count the number of times a state's guidance falls at a compound extreme. The resulting counts are summarized in Table 5.

Note that counts have been provided for the number of times a state's guidance value is at the compound extreme, and the number of times this occurs for compounds with 10 or more guidance values. This second statistic was selected because some states provide guidance for unusual chemicals. When there is only 1 guidance value, the state's value is both a maximum and a minimum. When there are a few values, this need not be true, but the probability of a state's guidance value being at the compound extreme is still high. Furthermore, one must attempt to normalize these counts by the number of guidance values actually provided. States that provide few values will have few set at compound extremes even if they are all at extremes. Therefore, Table 5 presents the number of extreme values as a percentage of the state's total number of values.

By the measures of Table 5, one might suggest that MI, WA, TX, IN, and WV have the least conservative guidance values because more than 10% of their values are set at compound maxima. One might also suggest that AZ, WA, MI, IA, WV, and OR have the most conservative values because more than 10% of their values are set at compound minima. Clearly, both of these suggestions are imperfect because WA and MI appear on both lists, and either could correct if limited to a subset of regulated chemicals.

Rather than pursue additional general analysis, it seems more appropriate to explore the nature of the guidance provided for classes of compounds or for individual contaminants.

Table 4. Summary of *S³GVD* Attributes for Residential Surface Soils

Measure	Value
Total Number of Guidance Values (GVs)	18,776
Total Number of GVs for Organics	16,451
Total Number of GVs for Inorganics	891
Total Number of GVs for Elements	1,434
Total Number of States Represented	50
Maximum Number of Total State GVs (TX)	1888
Minimum Number of State Total GVs (ND)	1
Maximum Number of State Organics GVs (TX)	1766
Minimum Number of State Organics GVs (ND)	1
Maximum Number of State Inorganics GVs (GA)	143
Minimum Number of State Inorganics GVs (CO,ND,NV,SD,UT)	0
Maximum Number of State Element GVs (TX)	90
Minimum Number of State Element GVs (ND,NV,SD)	0
Average Number of GVs per state	376
Average Number of Organic GVs per state	329
Average Number of Inorganic GVs per state	18
Average Number of Element GVs per state	29
Total Number of Unique CAS Numbers	1221
Total Number of Unique Organic CAS Numbers	994
Total Number of Unique Inorganic CAS Numbers	178
Total Number of Unique Element CAS Numbers	49
Total Number of Distinct Elements	43
Average Number of Unique CAS GVs per State	291
Maximum Number of Unique CAS GVs per State	632
Minimum Number of Unique CAS GVs per State	1
Average Number of Unique Organic CAS GVs per State	291
Average Number of Unique Inorganic CAS GVs per State	178
Average Number of Unique Element CAS GVs per State	43

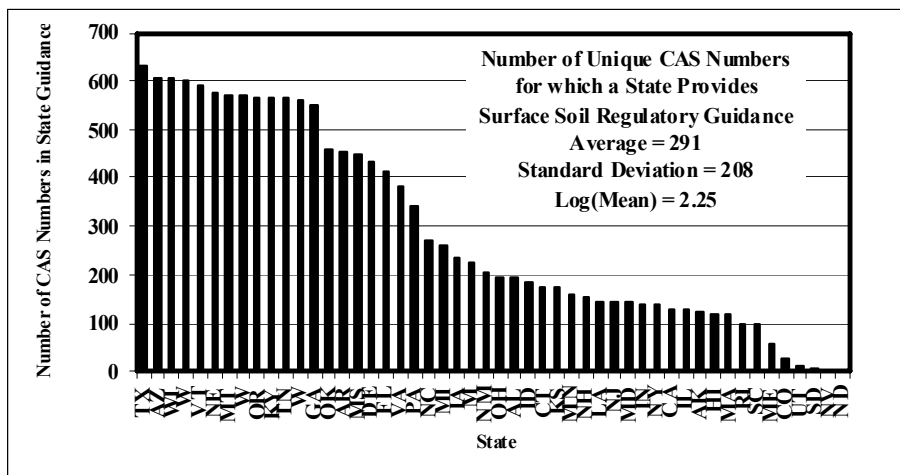


Figure 4. OCD of the Total Number of Unique CAS Numbers for which States Provide Surface Soil Regulatory Guidance Values

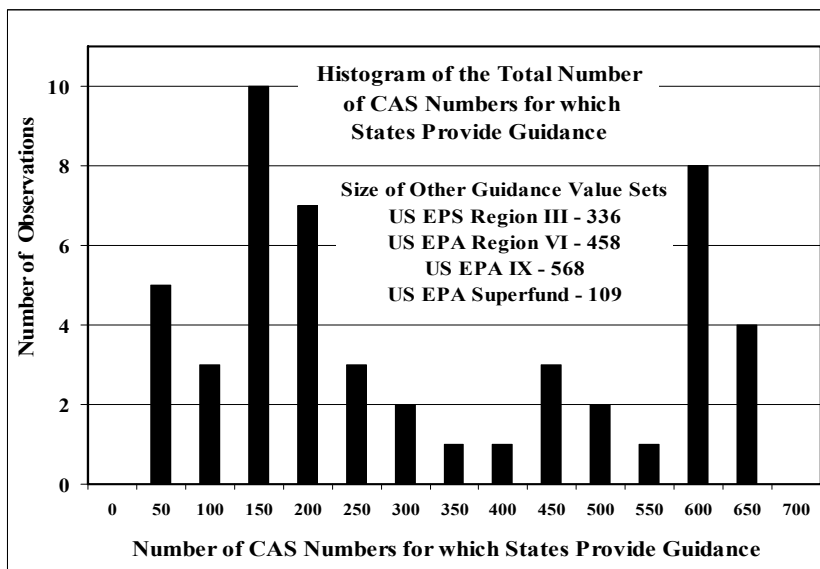


Figure 5. Histogram of the Total Number of CAS Numbers for which States Provide Guidance

2.5 Guidance Values for Organic Compounds S^3GVD

Guidance Values for Organic Compounds S^3GVD contains data on state regulatory guidance for 329 unique organic compound CAS designations. Selected data for the 100 most frequently regulated of these is presented in Table 5.

One useful statistic is the log₁₀ order of variation (LOV) computed as $\text{Log}_{10} \{(\text{maximum guidance value})/(\text{minimum guidance value})\}$. The average LOV of all 100 compounds is 4.44 (a factor of 27,500). The LOV of all 100 chemicals has a standard deviation of 1.11.

Figure 6 illustrates this average as a function of location in the ranked array of compounds. Note that variation is even higher for the most commonly regulated compounds. One possible explanation for this is that 4 of the 5 most commonly regulated compounds are the BTEX association (benzene, toluene, ethylbenzene, and xylenes) if dimethylbenzene is assumed to represent all (1,2- 1,3- and 1,4-dimethylbenzene). It seems likely that the range of values for these has been impacted by the differences between generic soil remediation regulation and underground storage tank programs.

Jennings and Hanna (2007) illustrated LOCD's for the top 10 organics of Table 6. Here, we will present LOCD of other compounds that illustrate the same basic features.

Figure 7 illustrates a LOCD of the residential surface soil guidance values for methylene chloride (CAS 75-09-2), the 12th most commonly regulated organic compound. Note that this has a LOV of more than 5 orders of magnitude. The fuzzy mode encompass 14 of the 64 regulatory values (22%), but appears quite far to the right in the distribution. There seem to be additional groups of similar values, but these appear closer than they are because of the log scale.

Figure 8 – 11 present LOCDs for 1,2-dichloroethane (CAS 107-06-2), 1,1,1-trichloroethane (CAS 71-55-6), Anthracene (CAS 120-12-7) and acetone (CAS 67-64-1) which are #13, #14, #17, and # 36 respectively on the list of the most regulated organics. Note that all of these are characterized by a high degree of variation (LOV>5). The fuzzy mode approach captures “typical” ranges with mixed success. The range captured for 1,2-dichloroethane only spans 8 of the 64 values (12.5%) and appears far to the right in the distribution. The range captured for Anthracene contains 21 of the 65 values (33%) but appears uncomfortably left (i.e. less conservative values) in the distribution.

Figure 12 presents a final example LOCD for hexachlorobenzene. This was selected as an example of an organic for which there appears to be more universal agreement on guidance value numbers. Note that hexachlorobenzene (#42 in Table 6) has a LOV of 2.35. The guidance value distribution of hexachlorobenzene also appears to be bi-fuzzy-modal. There is a fuzzy mode in the neighborhood of 0.3 mg/kg that captures 16 of the guidance values. There is also a fuzzy mode in the neighborhood of 0.4 that captures 14 guidance values. The ranges of these two modes do not overlap, but they are quite close. If the degree of fuzziness is expanded a bit, the modes would merge and capture 55% of the guidance values.

Table 5. Frequency of State Guidance Values at Compound Guidance Extremes

State	NGVUB	NGVUB>9	ΣGVs	% >9	State	NGVLB	NGVLB>9	ΣGV	%>9
TX	339	125	632	19.8	TX	240	29	632	4.6
WA	191	170	569	29.9	MT	213	199	569	35.0
GA	187	25	549	4.6	GA	202	34	549	6.2
MI	130	106	259	40.9	WI	124	93	608	15.3
WV	70	60	603	10.0	VA	108	49	382	12.8
AZ	46	36	608	5.9	ID	81	78	184	42.4
MS	40	8	450	1.8	DE	34	26	432	6.0
IA	32	23	232	9.9	NY	32	28	137	20.4
FL	31	25	412	6.1	MI	24	0	259	0.0
WI	29	7	608	1.2	OR	21	18	566	3.2
OR	20	16	566	2.8	CA	19	13	130	10.0
VA	19	18	382	4.7	AZ	16	5	608	0.8
IN	18	18	138	13.0	NC	15	2	271	0.7
VT	18	13	593	2.2	WA	14	1	569	0.2
MA	17	2	117	1.7	NH	12	2	154	1.3
NH	10	2	154	1.3	NE	10	8	574	1.4
OH	10	7	196	3.6	FL	9	0	412	0.0
KS	9	8	174	4.6	MS	9	1	450	0.2
NE	9	7	574	1.2	OK	8	3	460	0.7
KY	8	4	564	0.7	WY	8	7	562	1.2
TN	8	4	563	0.7	MA	8	4	117	3.4
MD	7	3	143	2.1	IA	7	1	232	0.4
OK	6	5	460	1.1	AL	7	6	192	3.1
AR	5	4	455	0.9	AR	5	1	455	0.2
CT	5	1	174	0.6	KS	5	4	174	2.3
ME	5	5	54	9.3	OH	4	3	196	1.5
CA	4	0	130	0.0	CT	4	2	174	1.1
DE	4	0	432	0.0	WV	4	0	603	0.0
MO	4	3	226	1.3	RI	3	3	95	3.2
NC	3	1	271	0.4	SC	3	3	95	3.2
NJ	3	3	144	2.1	NM	3	3	204	1.5
NM	3	3	204	1.5	VT	3	3	593	0.5
AL	1	0	192	0.0	KY	2	2	564	0.4
IL	1	1	128	0.8	MO	2	2	226	0.9
NY	1	0	137	0.0	CO	1	1	25	4.0
WY	1	1	562	0.2	MD	1	0	143	0.0
					ME	1	1	54	1.9
					TN	1	1	563	0.2
					ND	1	0	1	0.0
					NJ	1	1	144	0.7
					NV	1	0	2	0.0
					IN	1	1	138	0.7
					MD	1	0	143	0.0

NGVUB – No. of guidance values at upper bound
 NGVUB>9 – No. of guidance values at upper bound
 for CAS numbers with 10 or more values
 GV – Total number of state guidance values
 %>9 - % of guidance values at the indicated bound
 for CAS numbers with 10 or more values
 “LB” – lower bound

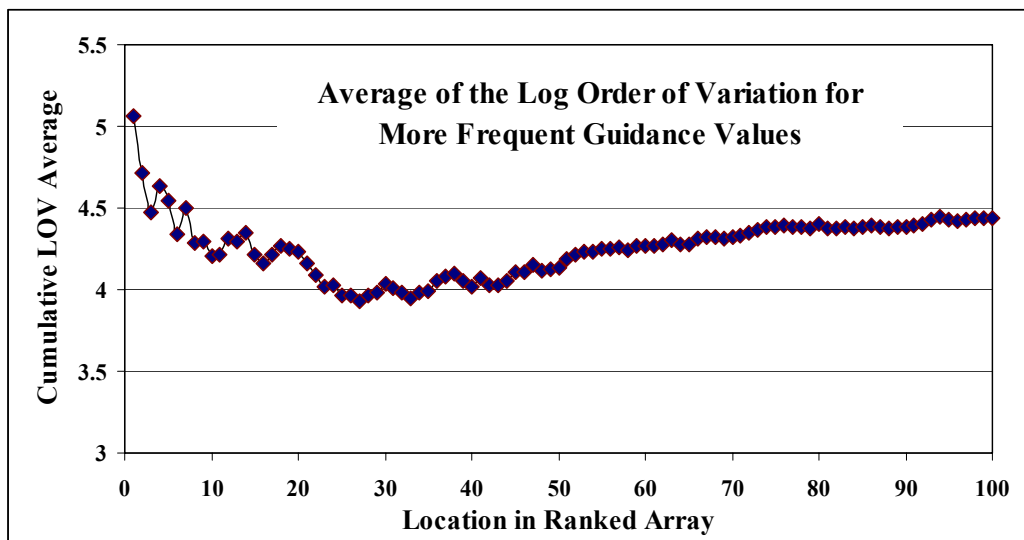


Figure 6. Average LOV as a Function of Position In the Ranked Array of The Most Frequently Regulated Organic Compounds

Table 6. Top 100 Organic Compounds for which Residential Surface Soil Guidance (mg/kg) is Provided

Rank	Freq.	CAS No.	Formulae	Name	Min	Max	LOV
1	76	91-20-3	C ₁₀ H ₈	Naphthalene	0.138	16000	5.06
2	74	108-88-3	C ₇ H ₈	Toluene	0.7	16000	4.36
3	74	71-43-2	C ₆ H ₆	Benzene	0.0178	180	4.00
4	73	1330-20-7	C ₈ H ₁₀	Dimethylbenzene	1.2	160000	5.12
5	72	100-41-4	C ₈ H ₁₀	Ethylbenzene	1	15000	4.18
6	69	50-32-8	C ₂₀ H ₁₂	Benzo[a]pyrene	0.00875	17.7	3.31
7	67	79-01-6	C ₂ HCl ₃	Trichloroethylene	0.00159	500	5.50
8	67	75-01-4	C ₂ H ₃ Cl	Chloroethene	0.0067	3.8	2.75
9	67	127-18-4	C ₂ Cl ₄	Tetrachloroethylene	0.0302	780	4.41
10	66	206-44-0	C ₁₆ H ₁₀	Fluoranthene	20	46000	3.36
11	66	83-32-9	C ₁₂ H ₁₀	Acenaphthene	2.2	41000	4.27
12	65	75-09-2	CH ₂ Cl ₂	Methylene chloride	0.0169	5010	5.47
13	65	107-06-2	C ₂ H ₄ Cl ₂	1,2-dichloroethane	0.00771	91	4.07
14	65	71-55-6	C ₂ H ₃ Cl ₃	1,1,1-trichloroethane	0.68	72000	5.02
15	65	56-55-3	C ₁₈ H ₁₂	Benz[a]anthracene	0.0875	20	2.36
16	65	129-00-0	C ₁₆ H ₁₀	Pyrene	13	29000	3.35
17	65	120-12-7	C ₁₄ H ₁₀	Anthracene	1.93	230000	5.08
18	64	67-66-3	CHCl ₃	Chloroform	0.00783	1200	5.19
19	64	56-23-5	CCl ₄	Carbon tetrachloride	0.012	96	3.90
20	64	108-90-7	C ₆ H ₅ Cl	Chlorobenzene	0.618	5000	3.91
21	64	53-70-3	C ₂₂ H ₁₄	Dibenz[a,h]anthracene	0.00875	5	2.76
22	64	193-39-5	C ₂₂ H ₁₂	o-phenylenepyrene	0.0875	32.8	2.57
23	64	205-99-2	C ₂₀ H ₁₂	Benz[e]acephenanthrylene	0.0875	20	2.36
24	64	218-01-9	C ₁₈ H ₁₂	Chrysene	0.1	2000	4.30
25	64	50-29-3	C ₁₄ H ₉ Cl ₅	1,1'(2,2,2-trichloroethylidene) bis[4-chlorobenzene]	0.188	57	2.48
26	64	86-73-7	C ₁₃ H ₁₀	Fluorene	3.71	27000	3.86
27	63	87-86-5	C ₆ HCl ₅ O	Pentachlorophenol	0.073	90	3.09
28	63	58-89-9	C ₆ H ₆ Cl ₆	Lindane	0.000896	80	4.95
29	63	156-60-5	C ₂ H ₂ Cl ₂	1,2-dichloroethene	0.19	5000	4.42
30	63	75-35-4	C ₂ H ₂ Cl ₂	1,1-dichloroethene	0.01	3910	5.59
31	63	207-08-9	C ₂₀ H ₁₂	Benzo[k]fluoranthene	0.1	200	3.30
32	63	60-57-1	C ₁₂ H ₈ Cl ₆ O	1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-1,4-endo-exo-5,8-dimethanonaphthalene	0.001	1.1	3.04
33	62	117-81-7	C ₂₄ H ₃₈ O ₄	Bis(2-ethylhexyl)phthalate	4	2800	2.85
34	62	72-20-8	C ₁₂ H ₈ Cl ₆ O	Endrin	0.00065	80	5.09
35	62	76-44-8	C ₁₀ H ₅ Cl ₇	Heptachlor	0.0002	5.6	4.45
36	61	67-64-1	C ₃ H ₆ O	Acetone	0.05	70400	6.15
37	61	75-34-3	C ₂ H ₄ Cl ₂	1,1-dichloroethane	0.2	15600	4.89
38	61	79-00-5	C ₂ H ₃ Cl ₃	1,1,2-trichloroethane	0.0141	1000	4.85
39	61	72-55-9	C ₁₄ H ₈ Cl ₄	P,p'-dde	0.188	45	2.38

Surface Soil Regulatory Guidance Values

Table 6. Continued

Rank	Freq.	CAS No.	Formulae	Name	Min	Max	LOV
40	61	72-54-8	C ₁₄ H ₁₀ Cl ₄	1,1-dichloro-2,2-bis(4-chlorophenyl)-ethane	0.266	95	2.55
41	60	108-95-2	C ₆ H ₆ O	Phenol	0.03	48000	6.20
42	60	118-74-1	C ₆ Cl ₆	Hexachlorobenzene	0.0399	8.9	2.35
43	60	95-50-1	C ₆ H ₄ Cl ₂	1,2-dichlorobenzene	1.1	7200	3.82
44	59	106-46-7	C ₆ H ₄ Cl ₂	1,4-dichlorobenzene	0.046	11000	5.38
45	59	124-48-1	CHBr ₂ Cl	Dibromochloroethane	0.00202	5000	6.39
46	59	156-59-2	C ₂ H ₂ Cl ₂	2,4-dichloroethene	0.193	3000	4.19
47	59	1634-04-4	C ₅ H ₁₂ O	2-methoxy-2-methylpropane	0.00667	8760	6.12
48	59	309-00-2	C ₁₂ H ₈ Cl ₆	Aldrin	0.00376	1	2.42
49	59	75-25-2	CHBr ₃	Tribromomethane	0.0292	1100	4.58
50	59	75-27-4	CHBrCl ₂	Bromodichloromethane	0.00268	110	4.61
51	59	78-93-3	C ₄ H ₈ O	1-butanone	0.00486	48000	6.99
52	59	88-06-2	C ₆ H ₃ Cl ₃ O	2,4,6-trichlorophenol	0.00436	1000	5.36
53	59	95-95-4	C ₆ H ₃ Cl ₃ O	2,4,5-trichlorophenol	0.1	23000	5.36
54	58	100-42-5	C ₈ H ₈	Styrene	1.83	16000	3.94
55	58	111-44-4	C ₄ H ₈ Cl ₂ O	Beta,beta'-dichloroethyl ether	4.06E-05	13	5.51
56	58	120-82-1	C ₆ H ₃ Cl ₃	1,2,4-trichlorobenzene	0.11	1800	4.21
57	58	120-83-2	C ₆ H ₄ Cl ₂ O	2,4-dichlorophenol	0.0217	660	4.48
58	58	67-72-1	C ₂ Cl ₆	Hexachloroethane	0.138	300	3.34
59	58	74-83-9	CH ₃ Br	Methyl bromide	0.000359	400	6.05
60	58	91-94-1	C ₁₂ H ₁₀ Cl ₂ N ₂	3,3'-dichloro-[1,1'-Biphenyl]-4,4' diamine	0.00183	25	4.14
61	57	1024-57-3	C ₁₀ H ₅ Cl ₇ O	Heptachlor epoxide	0.0003	4.39	4.17
62	57	105-67-9	C ₈ H ₁₀ O	2,4-dimethylphenol	0.174	11000	4.80
63	57	115-29-7	C ₉ H ₆ Cl ₆ O ₃ S	Encosulfan	0.0006	1400	6.37
64	57	72-43-5	C ₁₆ H ₁₅ Cl ₃ O ₂	Methoxychlor	8.8	1900	2.33
65	57	78-87-5	C ₃ H ₆ Cl ₂	1,2-dichloropropane	0.00933	140	4.18
66	57	84-66-2	C ₁₂ H ₁₄ O ₄	Diethyl phthalate	0.035	150000	6.63
67	56	79-34-5	C ₂ H ₂ Cl ₄	1,1,2,2-tetrachloroethane	0.000704	53	4.88
68	56	8001-35-2	C ₁₀ H ₁₅ Cl	Toxaphene	0.00042	20	4.68
69	56	87-68-3	C ₄ Cl ₆	1,1,2,3,4,4-hexachloro-1,3-Butadiene	0.0318	100	3.50
70	55	95-57-8	C ₆ H ₅ ClO	2-chlorophenol	0.0146	1400	4.98
71	54	106-93-4	C ₂ H ₄ Br ₂	1,2-dibromoethane	1.9E-05	1.6	4.93
72	54	121-14-2	C ₇ H ₆ N ₂ O ₄	1-methyl-2,4-dinitrobenzene	0.00029	160	5.74
73	54	51-28-5	C ₆ H ₄ N ₂ O ₅	2,4-dinitrophenol	0.00146	370	5.40
74	54	541-73-1	C ₆ H ₄ Cl ₂	1,3-dichlorobenzene	0.0188	7000	5.57
75	53	106-47-8	C ₆ H ₆ ClN	p-Chloroaniline	0.0119	730	4.79
76	53	630-20-6	C ₂ H ₂ Cl ₄	1,1,2,2-tetrachloroethane	0.0158	2300	5.16

Table 6. Continued

Rank	Freq.	CAS No.	Formulae	Name	Min	Max	LOV
77	52	1746-01-6	C ₁₂ H ₄ Cl ₄ O ₂	2,3,7,8-Tetrachlorodibenzo-p-dioxin	4.26E-07	0.001	3.37
78	52	319-84-6	C ₆ H ₆ Cl ₆	a-Lindane	0.00021	2.6	4.09
79	52	542-75-6	C ₃ H ₄ Cl ₂	1,3-dichloro-1-Propene	0.0023	26	4.05
80	52	75-00-3	C ₂ H ₅ Cl	Ethyl chloride	0.0191	31000	6.21
81	51	1336-36-3	(varies)	Polychlorinated biphenyls	0.07	14	2.30
82	50	108-10-1	C ₆ H ₁₂ O	Methyl isobutyl ketone	0.207	13000	4.80
83	50	95-48-7	C ₇ H ₈ O	2-methylphenol	0.1	7700	4.89
84	50	98-82-8	C ₉ H ₁₂	(1-methylethyl)-benzene	1.95	8000	3.61
85	49	108-60-1	C ₆ H ₁₂ C ₁₂ O	2,2'-oxybis[1-chloropropane	0.00908	3100	5.53
86	49	78-59-1	C ₉ H ₁₄ O	3,5,5-trimethyl-2-cyclohexen-1-one	0.14	16000	5.06
87	49	84-74-2	C ₁₆ H ₂₂ O ₄	Dibutyl phthalate	8.1	18000	3.35
88	48	319-85-7	C ₆ H ₆ Cl ₆	1,2,3,4,5,6-hexachloro (1a,2β,3a,4β,5a,6β)-cyclohexane	0.000751	5.4	3.86
89	48	77-47-4	C ₅ Cl ₆	1,2,3,4,5,5-hexachloro-1,3-cyclopentadiene	0.0117	1100	4.97
90	48	86-30-6	C ₁₂ H ₁₀ N ₂ O	N-nitroso-N-phenylbenzenamine	0.088	2200	4.40
91	48	98-95-3	C ₆ H ₅ NO ₂	Nitrobenzene	0.000347	100	5.46
92	47	106-44-5	C ₇ H ₈ O	4-methylphenol	0.021	910	4.64
93	47	131-11-3	C ₁₀ H ₁₀ O ₄	Dimethyl phthalate	0.035	100000 0	7.46
94	47	606-20-2	C ₇ H ₆ N ₂ O ₄	2-methyl-1,3-dinitrobenzene	0.000212	80	5.58
95	47	85-68-7	C ₁₉ H ₂₀ O ₄	Benzyl butyl ester phthalic acid	50	37000	2.87
96	46	96-12-8	C ₃ H ₅ Br ₂ Cl	1,2-dibromo-3-chloropropane	0.000975	4.1	3.62
97	45	117-84-0	C ₂₄ H ₃₈ O ₄	Di-n-octyl phthalate	0.3	151000	5.70
98	45	621-64-7	C ₆ H ₁₄ N ₂ O	n-nitroso-n-propyl-1-Propanamine	1.81E-05	1.71	4.98
99	45	75-69-4	CCl ₃ F	Trichloromonofluoromethane	0.41	24000	4.77
100	45	94-75-7	C ₈ H ₆ Cl ₂ O ₃	(2,4 Dichlorophenoxy) acetic acid	0.3	3000	4.00

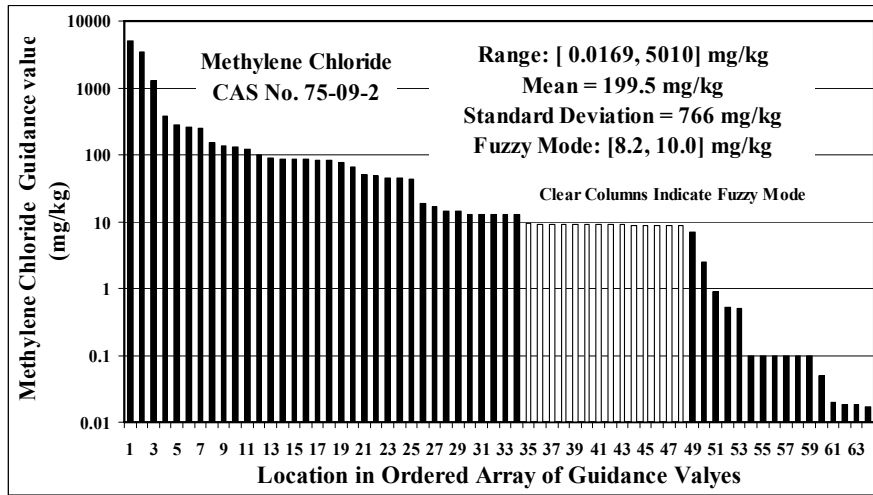


Figure 7. LOCD of Residential Surface Soil Regulatory Guidance Values for Methylene Chloride

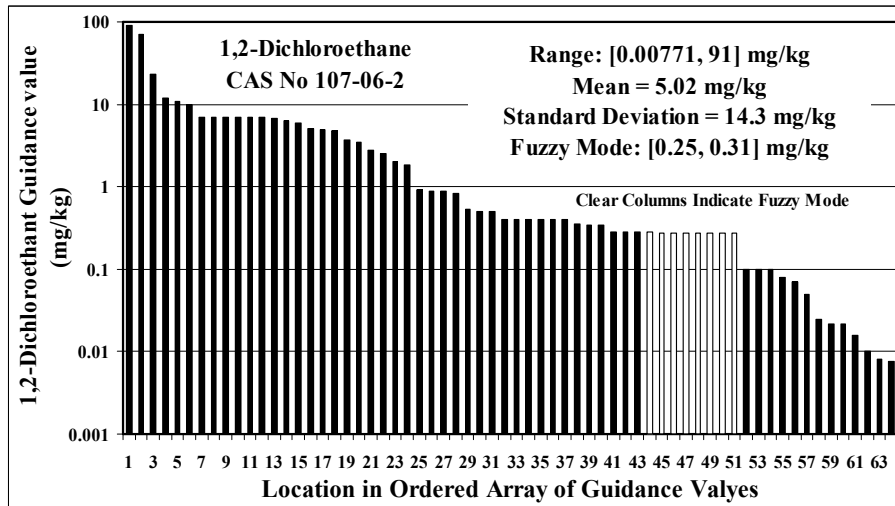


Figure 8. LOCD of Residential Surface Soil Regulatory Guidance Values for 1,2-Dichloroethane

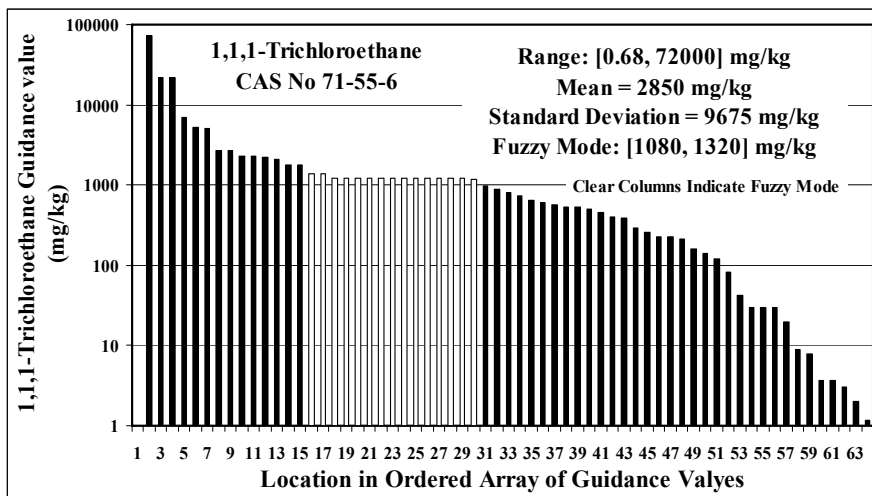


Figure 9. LOCD of Residential Surface Soil Regulatory Guidance Values for 1,1,1-Trichloroethane

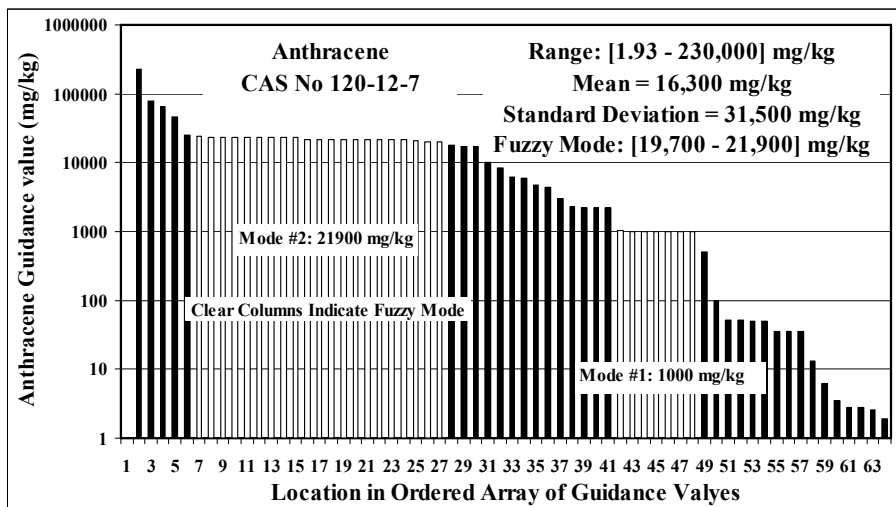


Figure 10. LOCD of Residential Surface Soil Regulatory Guidance Values for Anthracene

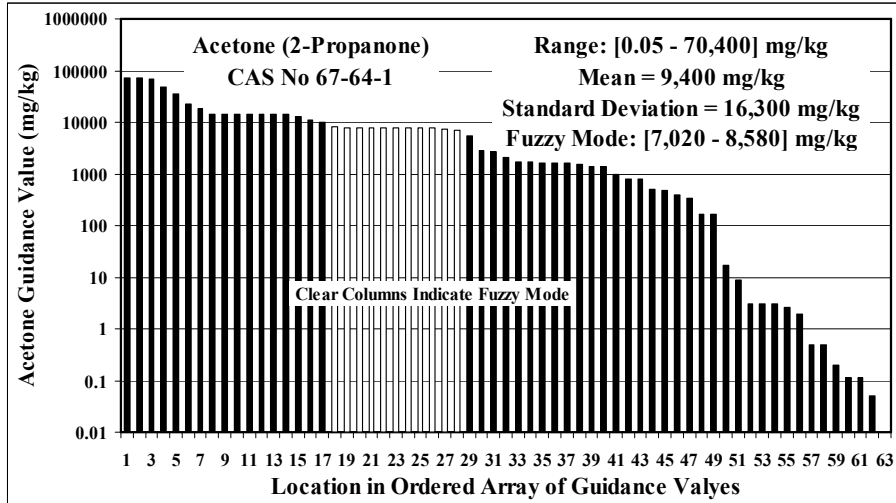


Figure 11. LOCD of Residential Surface Soil Regulatory Guidance Values for Acetone

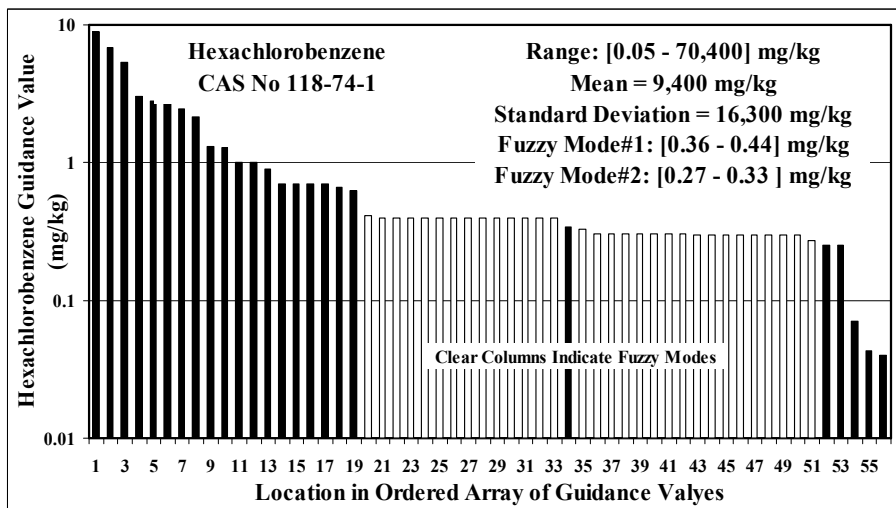


Figure 12. LOCD of Residential Surface Soil Regulatory Guidance Values for Hexachlorobenzene

All of the LOCDs of Fig. 7-12 seem to have strong similarities with the “small sample” synthetic log-normally distributed LOCD of Fig. 3.

2.6 Guidance Values for Inorganic Compounds - S^3GVD

Guidance Values for Inorganic Compounds S^3GVD contains regulatory guidance on 178 unique inorganic chemical CAS number designations, but only 60 of these have more than 1 guidance value, and only 38 have 10 or more guidance values. Information on the 20 most frequently regulated inorganics is summarized in Table 7, which lists the minimum and maximum residential value for each compound. The 158 inorganics not listed in Table 7, include:

- 23 sulfates – (e.g. dithallium sulfate, Tl_2SO_4 , CAS No. 7446-18-6)
- 22 chlorides (e.g. mercury dichloride, $HgCl_2$, CAS No.7487-94-7)
- 15 oxides (e.g. vanadium oxide, V_2O_5 , CAS No.1314-62-1)
- 11 cyanides (e.g. sodium cyanide, $NaCN$, CAS No.143-33-9)
- 10 nitrates or nitrites (e.g. mercury nitrate $Hg_2N_2O_6$, CAS No.7782-86-7)
- 10 arsenates or arsenites (e.g. lead hydrogen arsenate, $PbAsHO_4$, CAS No.7784-40-9),
- 8 chromates (e.g. sodium chromate, $CrNa_2O_4$, CAS No.7775-11-3) and
- 7 fluorides (e.g. zinc difluoride, ZnF_2 , CAS No.7783-49-5).

Table 7. Top 20 Inorganics for which Residential Surface Soil Guidance (mg/kg) is Provided

Rank	Frequency	CAS NO.	Formulae	Name	Min	Max	LOV
1	59	57-12-5	CN ⁻	Cyanide anion	0.0036	6900	6.28
2	49	75-15-0	CS ₂	Carbon disulfide	0.152	8000	4.72
3	32	74-90-8	CHN	Hydrogen cyanide	1.08	1600	3.17
4	30	7803-51-2	H ₃ P	Phosphine	1.83	59	1.51
5	29	7487-94-7	Hg Cl ₂	Mercury dichloride	0.011	383000	7.54
6	25	460-19-5	C ₂ N ₂	Cyanogen	0.43	3200	3.87
7	23	7601-90-3	HClO ₄	Perchloric acid	0.1	871000	6.94
8	22	506-77-4	CCIN	Cyanogen chloride	10	4000	2.60
9	20	7783-00-8	H ₂ O ₃ Se	Selenious acid	30.6	400	1.12
10	21	10599-90-3	H ₂ CIN	Chloramide	610	8000	1.12
11	20	1314-84-7	P ₂ Zn ₃	Zinc(II) diphosphide	2	26	1.11
12	20	506-68-3	CBrN	Cyanogen bromide	10	7200	2.86
13	19	14797-55-8	NO ₃ ⁻	NO ₃ anion	18.4	410000	4.35
14	18	14797-65-0	NO ₂ ⁻	Nitrogen oxide anion	1.84	130000	4.85
15	16	7773-06-0	H ₃ NO ₃ S·H ₃ N	Ammonium sulfamate	1220	16000	1.12
16	15	1309-64-4	O ₃ Sb ₂	Antimony trioxide	3	32	1.03
17	15	20859-73-8	AlP	Aluminum monophosphide	3.13	35	1.05
18	15	302-04-5	SCN ⁻	Thiocyanate	1.5	6110	3.61
19	14	7791-12-0	CITl	Thalium monochloride	0.6	20	1.52
20	14	13718-26-8	NaO ₃ V	Sodium vanadium(V) trioxide	6.11	80	1.12

On average, there is a variation of 3 orders of magnitude in the range of the 20 most commonly regulated inorganics. This falls to LOV=2 for the 60 CAS number designations with more than one guidance value if phosphoric acid (CAS No. 7664-38-2) is omitted. The guidance set for 7664-38-2 contains a value of 6.39×10^{33} mg/kg which is a physical impossibility and is believed to be an error in MS documentation. Readers should note, however, that physically impossible values (i.e. >1,000,000 mg/kg) are intentionally specified by some jurisdictions.

Figure 13 illustrates a LOCD of the guidance values for the most regulated inorganic compound (cyanide anion). The guidance values for cyanide anion vary over 6 orders of magnitude, but all but 2 values are contained within 3 orders of magnitude. If these guidance values are assumed to be log-normally distributed, then one would probably conclude that the lowest value is unlikely to belong to this population of numbers. The probability of observing a value as low as 0.368 mg/kg (the second lowest value) is about 0.003. One should observe a random value this low about once every 350 values. However the probability of observing a value of 0.0036 mg/kg (the lowest value) is approximately 1.7×10^{-6} (i.e. about once every 585,000 values). The fuzzy mode of the guidance value distribution spans 14 of the 59 guidance values, but is located near the high end of the distribution.

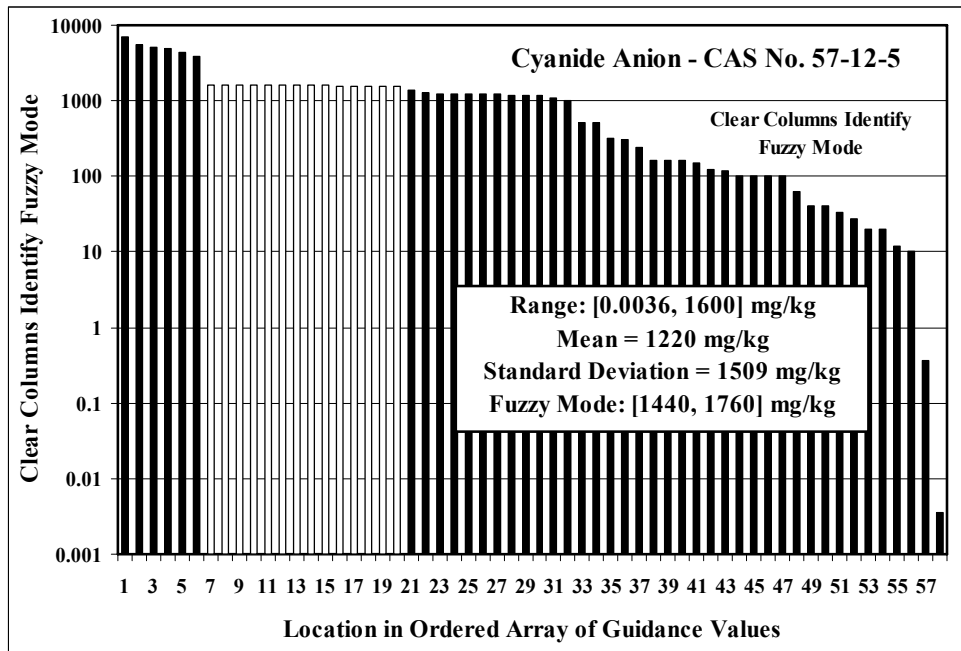


Figure 13. LOCD of Residential Surface Soil Regulatory Guidance Values for Cyanide Anion

Figure 14 illustrates a LOCD of the guidance for carbon disulfide (CS₂, CAS No. 75-15-0), the second most commonly regulated inorganic. The carbon disulfide guidance values are more evenly distributed (compared to Fig. 13) over 5 orders of magnitude. Although the fuzzy

mode spans a smaller percentage of the guidance values (9 of 49) it does appear to be more central in the value range.

Beyond cyanide and carbon disulfide, the numbers of and variability in guidance values is substantially lower than the numbers for organic compounds or elements. The LOV results for mercury dichloride ($HgCl_2$, CAS No. 7487-94-7) and perchloric acid ($HClO_4$, CAS No. 7601-90-3) are exceptions that are influenced by one unusual value. For mercury dichloride, no guidance value exceeds 100 mg/kg except for the extreme value of 383,000 mg/kg in the VA guidance. For perchloric acid, no value exceeds 55 mg/kg except for the extreme value of 871,000 mg/kg. Both of these values were based on an inhalation hazard, and both are substantially lower in alternative VA guidance value sets.

As a final example of the distributions of inorganic contaminant guidance values, Fig. 15 presents an arithmetic scale OCD for the residential soil guidance values of selenious acid (CAS No. 7783-00-8) for which there is only 1 order of magnitude in guidance value variation. For this case, the fuzzy mode captures 11 of the 20 guidance values.

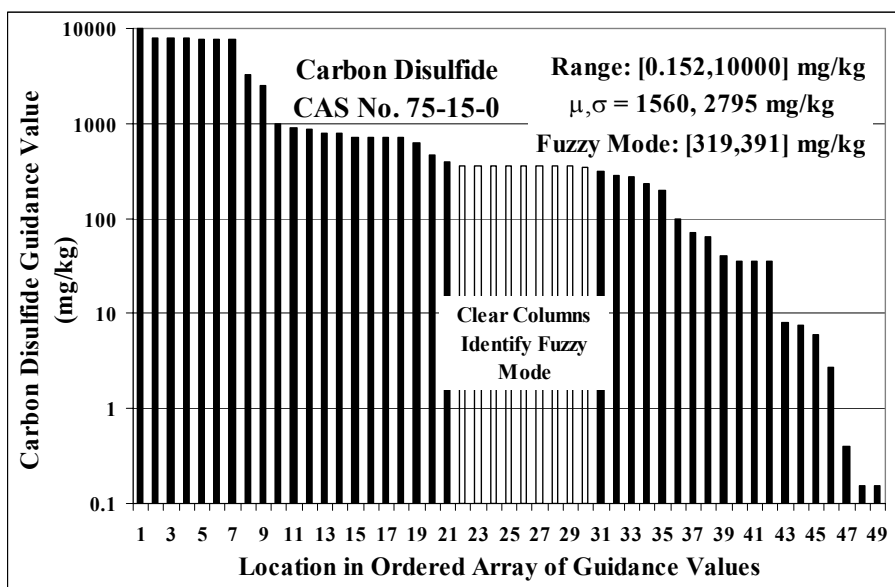


Figure 14. LOCD of Residential Surface Soil Regulatory Guidance Values for Carbon Disulfide

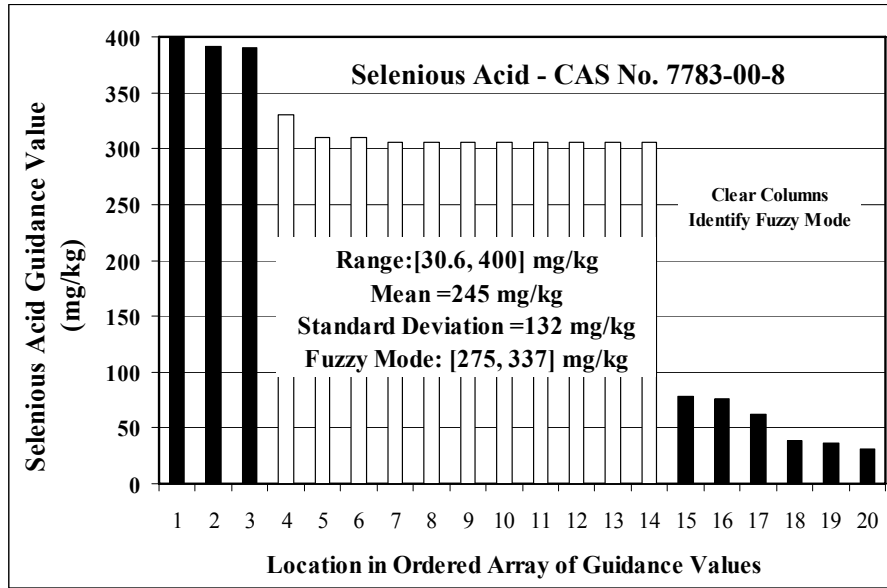


Figure 15. LOCD of Residential Surface Soil Regulatory Guidance Values for Selenious Acid

2.7 Guidance Values for Elements - S^3GVD

Guidance Values for Elements - S^3GVD also contains values for 49 element designations, but this total includes four different specifications for chromium (as Cr^{+3} , Cr^{+6} , $Cr(\text{total})$ and $Cr(\text{total as } 1:6 Cr^{+6}:Cr^{+3})$), and two specifications each for chlorine (Cl and Cl^-), fluorine (F and F^-), and sodium (Na and Na^+). If valance state differences are ignored, there are guidance values for 43 elements. The most common 32 of these are listed in Table 8. The remainder are made up of 3 guidance values each for magnesium and bismuth, 2 values each for calcium and potassium, and 1 value each for lanthanum, niobium, scandium, cerium, gallium, ytterbium, yttrium and zirconium. For the elements with 10 or more residential guidance values, there is an average LOV of 3.

A detailed analysis of the statistical properties of Cd, Cr, Cu, Pb, Ni, and Zn guidance values of North America may be found in Jennings and Petersen (2006) and Jennings and Ma (2007). Figures 16-21 complete the analysis of the top ten regulated elements (As, Be, Ag, Ba, Se, Sb).

Table 8. Top 30 Elements for which Residential Surface Soil Guidance (mg/kg) is Provided

Rank	Frequency	CAS No.	Element	Element	Min	Max	LOV
1	69	7440-38-2	As	Arsenic	0.004	30	3.88
2	68	7440-43-9	Cd	Cadmium	0.5	550	3.04
3	65	7440-02-0	Ni	Nickel	10	40000	3.60
4	64	7440-41-7	Be	Beryllium	0.002	680	5.53
5	63	7440-22-4	Ag	Silver	0.189	2500	4.12
6	63	7440-39-3	Ba	Barium	100	63000	2.80
7	62	7439-92-1	Pb	Lead	2	500	2.40
8	62	7440-66-6	Zn	Zinc	20	170000	3.93
9	62	7782-49-2	Se	Selenium	1	2600	3.41
10	60	7440-36-0	Sb	Antimony	3	180	1.78
11	57	7440-50-8	Cu	Copper	25	20000	2.90
12	56	7440-62-2	V	Vanadium	7.4	1500	2.31
13	55	18540-29-9	Cr(VI)	Chromium (VI)	1.8	2500	3.14
-----	53	16065-83-1	Cr(III)	Chromium (III)	36	790000	4.34
14	52	7439-97-6	Hg	Mercury	0.00509	100000	7.29
15	52	7440-28-0	Tl	Thallium	0.516	35	1.83
16	49	7439-96-5	Mn	Manganese	9.5	30000	3.50
17	41	7440-48-4	Co	Cobalt	10	15000	3.18
18	37	7782-41-4 ⁽¹⁾	F- or F	Fluorine anion	7.36	15000	3.31
-----	34	7440-47-3 ⁽²⁾	Cr (Total)	Total Chromium	10	59000	3.77
19	34	7429-90-5	Al	Aluminum	7600	150000	1.30
20	34	7440-42-8	B	Boron	1.6	51000	4.50
21	30	7439-98-7	Mo	Molybdenum	39	2600	1.82
22	29	7439-89-6	Fe	Iron	5.76	160000	4.44
23	29	7440-24-6	Sr	Strontium	4690	330000	1.85
24	29	7440-31-5	Sn	Tin	2000	93000	1.67
25	26	7723-14-0	P	Phosphorous	0.156	1000000	6.81
26	24	7439-93-2	Li	Lithium	136	5100	1.57
27	21	7440-61-1	U	Uranium	1.56	760	2.69
28	13	7782-50-5	Cl or Cl ⁻	Chlorine	12	20000	3.22
29	12	7440-32-6	Ti	Titanium	10000	38000000	3.58
30	8	7429-91-6	Dy	Dysprosium	782	16000	1.31

(1) or CAS No. 16984-48-8 (2) or Cr(total) based on an assumed Cr⁺⁶:Cr⁺³ ratio of 1:6

For As, Be, and Ag it is difficult to claim that the fuzzy mode bounds “typical” regulatory guidance values. For As, (see Fig. 16) the fuzzy mode bounds 21 of the 69 values, but these are clustered at the low end of the value distribution. For Ba and Ag, the reverse is true. The Be (see Fig. 17) fuzzy mode bounds 18 of the 64 values, but these are clustered near the high end of the value distribution.

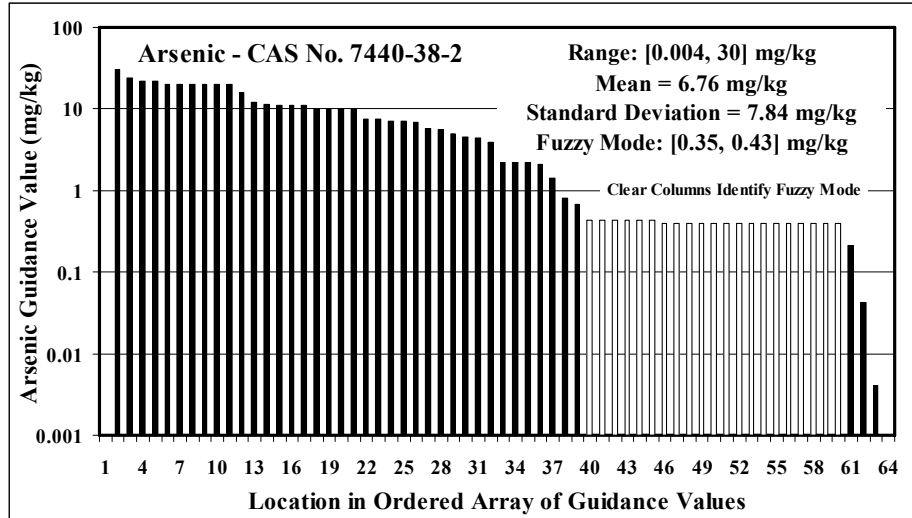


Figure 16. LOCD of Residential Surface Soil Regulatory Guidance Values for Arsenic

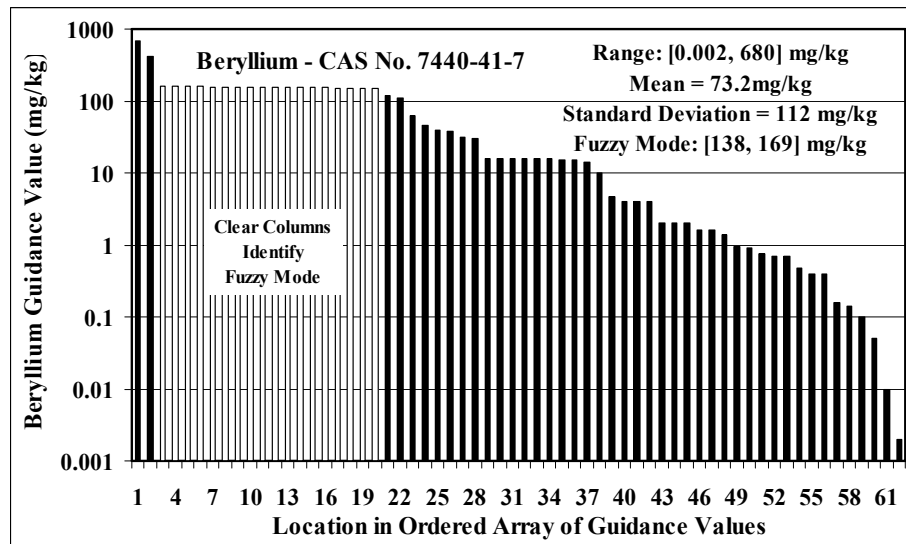


Figure 17. LOCD of Residential Surface Soil Regulatory Guidance Values for Beryllium

The Ag (See Fig. 18) fuzzy mode bounds 25 of the 63 values but these are also clustered near the high end of the distribution. This pattern is repeated for Se (29 of 62) (see Fig. 20) and Sb (24 of 60) (see Fig. 21). Only Ba (see Fig. 23) has a fuzzy mode that contains 21 of 63 values and occurs near the central portion of the value distribution.

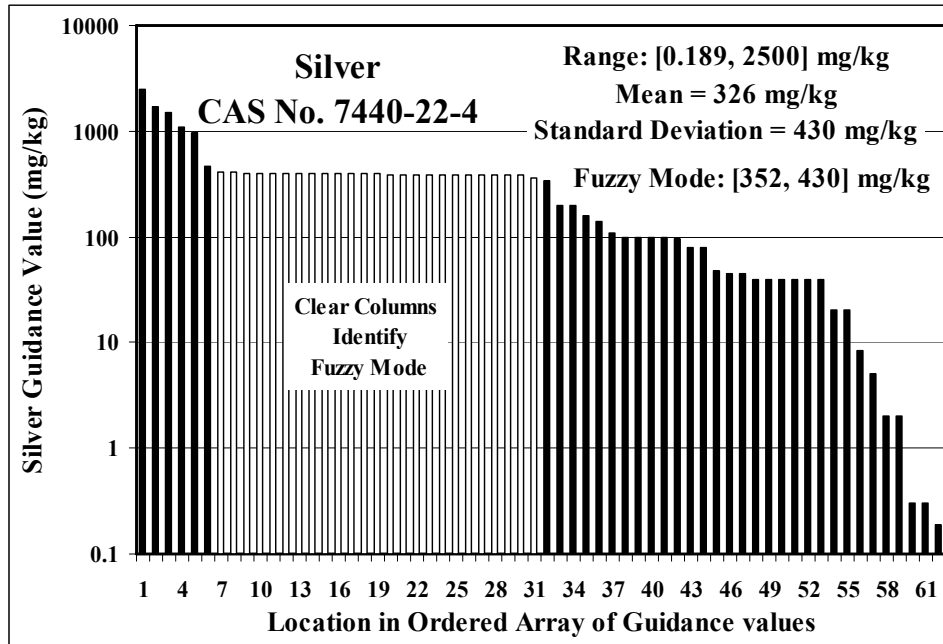


Figure 18. LOCD of Residential Surface Soil Regulatory Guidance Values for Silver

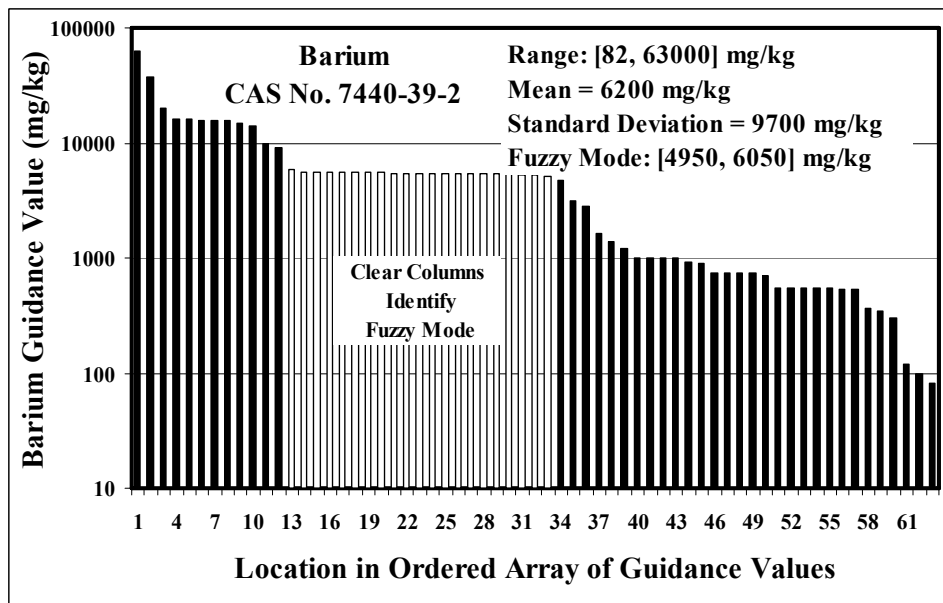


Figure 19. LOCD of Residential Surface Soil Regulatory Guidance Values for Barium

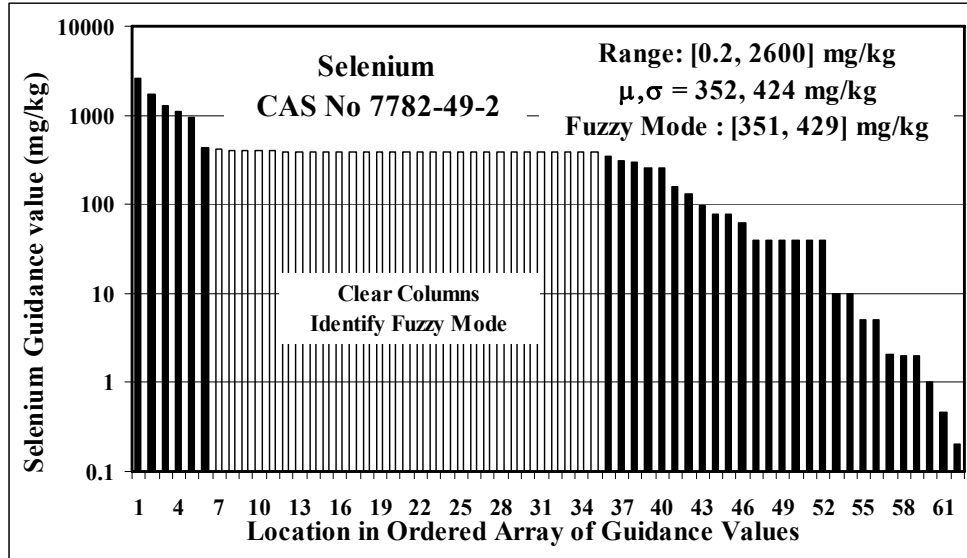


Figure 20. LOCD of Residential Surface Soil Regulatory Guidance Values for Selenium

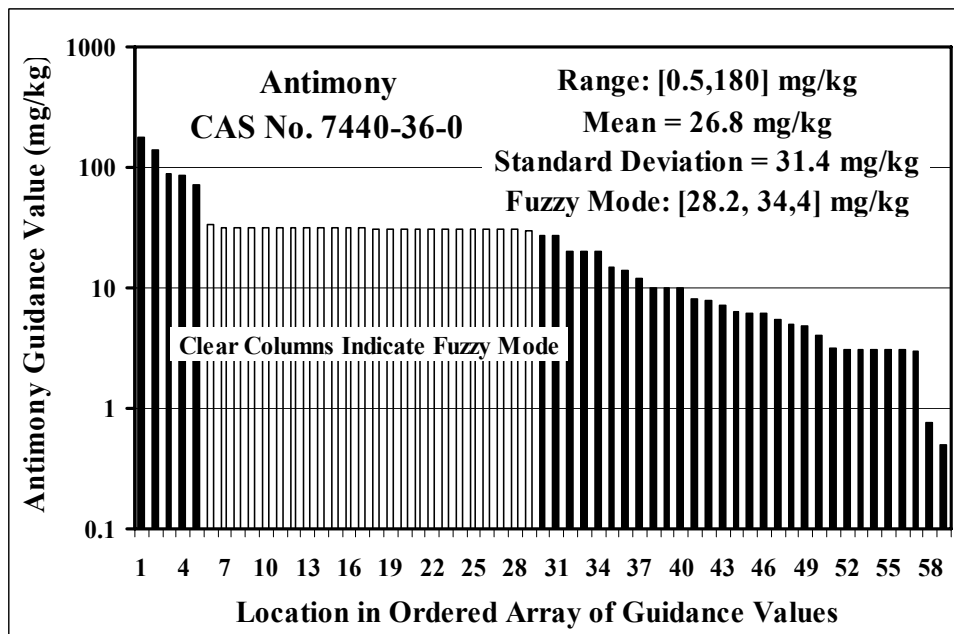


Figure 21. LOCD of Residential Surface Soil Regulatory Guidance Values for Antimony

2.8 Infeasible Guidance

The vast majority of the guidance values in S³GVD (99.2%) are feasible. Some of them are quite high, and there is a great deal of variability for each regulated pollutant, but the values are physically possible. However, there are 144 guidance values that are not feasible because they

have numerical values $\geq 1,000,000$ mg/kg. It is not possible for a mass burden to exceed this value, and it is not likely that anything approaching this value could be observed. Table 9 provides examples of nonfeasible guidance values for both residential and commercial/industrial site classifications.

There appear to be 3 explanations for nonfeasible guidance values. First, these may be errors such as typographical errors in number exponents. This appears to be the case for the 6.39E+33 phosphoric acid guidance value of MS. Others appear to be the result of automated value generation software. This appears to be the case for the 7.45 E+09 guidance value for 1,1-difluoro,1-chloroethane (and several others) of WI. Apparently the algorithm used resulted in unusual values for highly volatile contaminants. However, there is a large fraction of these infeasible values that appear to be intentional. Jennings et al. (2002) noted that, at the time, USEPA Region III was using an infeasible Cr (III) guidance value of 3,100,000 mg/kg and that discussions with their staff confirmed that this was the value intended. The number originated emerged from a rat feeding study estimate of toxicity to which a safety factor of 1000 was applied. The value has since been revised, but has lingered on in state guidance that was based on EPA Region III guidance.

3. DISCUSSION

The overriding observations that can be made about the state-of-the-art in regulatory guidance for residential surface soil contamination is that the values in current use are extremely variable. For many of the most commonly regulated contaminants, the range of values is 5 or 6 orders of magnitude, and there is modest “common” agreement among the values more central to the distribution. There appear to be several reasons why some of these values would differ.

- i. Guidance values may be based on fundamentally different approaches. For example, values based on “background” are likely to be much lower than values based on human health risk analysis. This may explain some of the differences observed in the element or inorganic standards, but is more difficult to extend to organics. Most of the regulated organics should have a background of zero since they are not naturally-occurring.
- ii. Guidance values may be based on alternative risk assessment formulations, exposure scenarios and/or coefficient value sets. Any of these could yield modest variations in the values calculated for any one pollutant.
- iii. Guidance values may be based on different levels of acceptable risk. In most instances, the values are based on cancer risk (for known carcinogens ?) of 1E-06 or a hazard quotient (HQ) of 1.0 for non-carcinogenic pollutants. However, some jurisdictions use higher levels of risk for known carcinogens (e.g. 1E07) or lower levels (1E -05) suspected carcinogens. Some jurisdictions also use alternative HQ values of 0.5, 0.2 or 0.1. These differences could yield an order of magnitude difference in computed guidance values.

- iv. Guidance values are often “rationalized” after they are computed. States use varying numbers of significant figures for this, and the results can be numbers that vary in the second or third digit.
- v. Some guidance values are inherited from elsewhere in a state’s legislative or regulatory history. These values may be inconsistent with the methods used to generate most of the state’s other guidance values.

Table 9. Soil Contaminants with Infeasible Surface Soil Guidance Values (mg/kg)

CAS No.	Compound	Residential * or C/I Guidance Value in mg/kg (State)
107-21-1	Ethylene glycol	2,040,000 (VA,VT); 2,000,000 (TX); 1,000,000(WV); 7,000,000 (WA)
107-98-2	Propylene glycol monomethyl ether	1,400,000(TX); 1,000,000 (WV); 2,500,000 (WA)
108-05-4	Vinyl acetate	1,020,000 (VA,VT) ; 1,000,000 (WV); 3,500,000 (WA)
108-38-3	m-Xylene	1,000,000 (WV); 7,000,000 (WA)
108-94-1	Cyclohexanone	5,110,000 (VA,VT); 1,000,000 (WV); 18,000,000 (WA)
108-95-2	Phenol	1,000,000 (WV); 2,100,000 (WA)
110-91-8	Morpholine	140,000,000 (TX)*; 1,000,000,000 (TX)
111-46-6	Diethylene glycol	2,000,000(TX); 7,000,000 (WA)
111-90-0	Diethylene glycol, monoethyl ether	1,000,000 (WV); 7,000,000 (WA)
120-12-7	Anthracene	1,100,000 (WA)
123-33-1	Maleic hydrazide	1,000,000 (WV); 1,800,000 (WA)
131-11-3	Dimethyl phthalate	1,000,000 (WV,IN,VA); 1,000,000 (IN)*; 3,500,000 (WA)
141-78-6	Ethyl acetate	1,000,000 (WV); 3,200,000 (WA)
39148-24-8	Fosetyl-al	1,000,000 (WV); 11,000,000 (WA)
52125-53-8	Propylene glycol monoethyl ether	2,500,000 (WA); 1,000,000 (WV)
57-55-6	Propylene glycol	3100000 (TX)*; 1,560,000 (MS)*; 1,000,000 (AZ,WV)* 1,600,000 (WA)*; 20,000,000 (TX); 1,000,000 (WV); 70,000,000 (WA)
65-85-0	Benzoic acid	14,000,000(WA); 4,100,000 (TX); 4,090,000 (VA,VT); 1,000,000 (IN, WV)
76-13-1	1,1,2-Trichloro- 1,2,2-trifluoroethane	2,350,000(VA)*; 30,700,000 (VA); 2,350,000 (VT)* 30,700,000(VT); 1,000,000 (WV)*; 1,000,000 (WV); 2,400,000(WA)*; 110,000,000 (WA)
78-93-3	Methyl ethyl ketone	1,000,000 (WV); 2,100,000 (WA)
79-10-7	Acrylic acid	1,800,000 (WA); 1,000,000 (WV,TX)
79-20-9	Methyl acetate	1,020,000 (VA,VT); 1,000,000 (WV); 3,500,000 (WA)
80-62-6	Methyl methacrylate	4,900,000 (WA); 1,439,000 (VA,VT)
84-66-2	Diethyl phthalate	1,000,000 (WV); 2,800,000 (WA)
84-72-0	Ethylphthalyl ethyl glycolate	1,000,000 (WV); 11,000,000 (WA)
95-47-6	o-Xylene	1,000,000 (WV); 7,000,000 (WA)
95-70-5	Toluene-2,5-diamine	1,000,000 (WV); 2,100,000 (WA)
10102-44-0	Nitrogen dioxide	1,000,000 (WV)
7647-01-0	Hydrogen Chloride	2,980,000 (WI)*
7664-38-2	Phosphoric Acid	1,490,000 (WI)*

Table 9 continued

CAS No.	Compound	Residential * or C/I Guidance Value in mg/kg (State)
7664-41-7	Ammonia	14,900,000 (WI)*
16065-83-1	Chromium III	1,530,000 (VT, VA); 1,000,000 (IN, WV); 5,300,000 (WA)
7429-90-5	Aluminum	1,000,000 (TX, WV)
7439-95-4	Magnesium	1,000,000 (MI)*
7440-24-6	Strontium	2,100,000 (WA); 1,000,000 (WV)
7440-31-5	Tin	2,100,000 (WA); 1,000,000 (WV)
7440-32-6	Titanium	38,000,000 (TX)*; 240,000,000 (TX)
7440-66-6	Zinc	1,100,000 (WA)
7723-14-0	Phosphorus (Total)	1,000,000 (MI)*

It is easy to envision these considerations impacting a few numbers at the extremes of a guidance value number distribution. It is much more difficult to see how these differences can impact so many of the guidance values across the heart of the distribution. There are examples where literally no two states agree on the magnitude of a contaminant's guidance value.

The analysis presented here has concentrated on residential soil guidance values. S³GVD also contains commercial and industrial site guidance values. The total number of contaminants covered is less than those for residential (or generic, unrestricted) site classifications, and the number of values per CAS designations is lower (not all states provide guidance for alternative site designations), but values specifically designated for commercial or industrial sites may be found for 809 distinct CAS numbers. On average, these are a factor of 20 times higher than the corresponding residential value. This is expected since the values are generally calculated from less conservative exposure scenarios (e.g. fewer hours per day and days per year) and for adults with larger body mass. Beyond this, the guidance value distributions for each CAS number appear to be similar to those for residential guidance values. If anything, there is a bit more agreement among the commercial and industrial values because there are less per chemical and because they more often approach the feasibility upper bound.

4. CONCLUSIONS

There is a great deal of variability in the states' surface soil contamination guidance values currently being applied. This variability leads to several questions, including questions (see Question #4) about the adequacy of current risk assessment methodology.

4.1 Question #1 – Comparability ?

Variability is observed by comparing guidance values taken from many sources and developed by several alternative methods applied over several years. Is this appropriate? The answer is yes. Although guidance values are developed by different methods, using different strategies, exposure scenarios and coefficient data, they were all developed for the same purpose. They were developed to identify levels of soil contamination that are high enough to be of health

concern, or high enough to prompt additional ecosystem assessment. It is the results of the methods that are applied (the actual guidance value mass burdens) that are comparable. This is not like comparing apples to oranges. This is like comparing the cost of apples to the cost of oranges (or taste or color or...) which are valid comparison criteria used daily by shoppers across the nation.

4.2 Question #2 – Feasibility ?

Some regulatory jurisdictions have promulgated guidance values that are not physically possible. Is this appropriate? The answer is no. No regulatory guidance value greater than 1,000,000 mg/kg is physically possible and it is very difficult for mass burdens to approach this value. Organic liquids may exist in pure form which, given a density greater than water, might yield a concentration above 1,000,000 mg/l. However, for these to become a soil contaminant, they must be mixed with soil, and in soil their mass burden would be limited by the soils porosity (often <0.4). This is a question because at least 11 jurisdictions (AZ, GA, IN, MI, MS, TX, VA, VT, WA, WI, and WV) publish guidance values that exceed the 1,000,000 mg/kg.

When a contaminant's guidance value exceeds 1,000,000 mg/kg, it is not possible for a single component risk analysis to yield an unacceptable result. For example, when hazard quotient (HQ) analysis is applied to contaminant "i", the calculation must yield a value less than 1.0 since the measured mass burden (C_i) cannot exceed the guidance value (C_{Si}).

$$HQ_i = \frac{C_i}{C_{Si}} < (?)1.0 \quad (1)$$

Unfortunately, at many sites, humans and ecosystems experience multiple contaminants and risk analysis must consider cumulative impacts. In index (HI) analysis, this is done by summing HQ_i exposures across the set of contaminants likely to inflict similar organism or ecosystem damage.

$$HI = \sum_{i=1}^I \frac{C_i}{C_{Si}} < (?)1.0 \quad (2)$$

Guidance values in excess of 1,000,000 mg/kg make it nearly impossible for contaminants to impact cumulative risk assessments. Even in the presence of other contaminants, they cannot significantly contribute to the HI result. If this is not the desired effect, the values should be lowered. Many states cap guidance values at 100,000 mg/kg. If this is the desired impact, then the "contaminant" should be dropped from regulation. When there is no way for a chemical to exceed the allowable maximum value, there is no need for the guidance value and no need for chemical analysis to quantify the site mass burden. The chemical should join the huge number of unregulated chemicals.

4.3 Question # 3 - Appropriate Value Set Size ?

Some jurisdictions provide guidance on hundreds of contaminants. Others do not. Is there a “correct” number of chemicals that should be regulated? The answer is unclear. There is probably a set of soil contaminants that should be regulated and jurisdictions should provide guidance values for all of the contaminants of this set. The size of this set is debatable, but it should probably include the 200 of the most common pollutants (the average state currently contains guidance on 291 contaminants). Some jurisdictions go far beyond this. Although promulgation of hundreds of additional guidance values may appear to be admirable human health and/or environmental vigilance, this can also have less desirable implications. One must wonder about how often these less common contaminants are encountered and how often their guidance is applied. If they are rarely encountered, is it cost-effective to require their analysis? If analysis is not mandated, how does a jurisdiction know that its guidance is being followed?

4.4 Question #4 – Risk-Assessment Implications of Guidance Value Variability?

There is a high degree of variability in the guidance values applied to surface soil contamination. This is the soil that humans come into contact with most frequently, and it is children who experience the critical exposure. We are unable to explain why there is so much disagreement about regulatory guidance values, but would offer the following observations.

- (i) The differences between guidance values cannot be attributed to disagreements about acceptable risk levels, risk models, or coefficient values. The magnitudes of differences are far too great for this.
- (ii) The differences between guidance values imply questions about economic equity and environmental justice. How can it be acceptable to expose children to a concentration of 10,000 mg/kg in one jurisdiction if it is unacceptable to expose them to more than 1 mg/kg in an adjacent jurisdiction? How can it be equitable to require analysis for hundreds of compounds and remediation to low mass burden levels in one jurisdiction if the same compounds are unregulated elsewhere?
- (iii) The differences imply questions about the reliability of current risk assessment practices. Jurisdictions using the same levels of risk compute vastly different guidance values.

With this much uncertainty in the analysis process, it is difficult to see how risk-based guidance can be adequately protective of human health and the environment.

Jennings (2005) discussed one method of mitigating these problems. There are few examples of strong national leadership on acceptable levels of surface soil contamination, but there is one. In 2001, the U.S. EPA established “national standard” guidance of 400 mg/kg for Pb in residential surface soil (USEPA, 2001). There are limitations on the application of this value, but its existence has done a great deal to reduce the variability of Pb regulatory guidance. All of the residential soil Pb guidance values fall within 2 orders of magnitude and, with the exception of two low values (2 mg/kg in OR, 16.5 mg/kg in WV), are within one order of magnitude. At

least 35 jurisdictions share 400 mg/kg as their residential Pb value. This suggests that, if the USEPA would provide stronger leadership on the number of contaminants for which guidance should be provided, and on appropriate mass burdens for these contaminants, states would have more incentive and justification for tightening the bounds about regulatory guidance variability.

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