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Modeling Transport and Deposition of Level 1 Substances to the Great Lakes

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April 2005

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Modeling Transport and Deposition of Level 1 Substances to the Great Lakes

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1.0 SUMMARY

Mass balance modeling of 18 chemicals that are representative of Level I substances identified under the Great Lakes Binational Toxics Strategy and targeted for virtual elimination from the Great Lakes has been carried out using a suite of models. The goals of this work are to assess the potential of each substance for transport from local and distant sources and subsequent deposition to the surface of the Great Lakes, and to make estimates of the contribution to total atmospheric loading attributable to emissions at different locations in North America and globally. Models are applied to analyze the efficiency of long-range transport and deposition of Level I substances to the Great Lakes (the Great Lakes transfer efficiency, GLTE). The GLTE is the percentage of chemical released to air in a source region that is expected to be deposited from the atmosphere to the surface waters of the Great Lakes.

Modeling at the North American and global scale is carried out using two models based on the Berkeley-Trent (BETR) contaminant fate modeling framework: BETR North America and BETR Global. Model-based assessments of Great Lakes transfer efficiency are used to group the substances according to the spatial scale of emission likely to impact the Lakes: (1) Local or regional scale substances: Dieldrin, Aldrin and benzo[a]pyrene, (2) Continental scale: chlordane, 2,3,7,8-tetrachlordibenzodioxin, *p,p*-DDT, toxaphene, octachlorostyrene and mirex, (3) Hemispheric scale: PCBs, (4) Global scale: hexachlorobenzene and α-HCH.

Using available emissions estimates and the models, the contribution of emissions of Level I substances in different regions of North America and globally to the total atmospheric loading to the Lakes has been estimated. These estimates are subject to large uncertainties, most notably because of uncertainties in emission scenarios, degradation rates of the substances in environmental media. However, model uncertainties due to simplified descriptions of exchange processes between environmental media and environmental conditions also contribute to overall uncertainty in the assessment. Mass balance calculations are presented for seven PCB congeners and

toxaphene at the North American spatial scale and for the PCBs and α-HCH at the global scale. Comparison of cumulative historical emissions scenarios with estimated emissions in the year 2000 indicates that relative contributions from sources outside North America are increasing as sources are curtailed in the United States and Canada. In particular, Eastern Europe appears to be becoming a relatively more important source to the Lakes. However, under all emission scenarios considered, the majority of PCB deposition to the Lakes from the atmosphere is attributable to sources in North America.

The mass balance models presented in this report provide a quantitative framework for assembling the best available information about properties, sources, partitioning, degradation, transport, and the ultimate fate of persistent organic substances. The uncertainties associated with these assessments are believed to be dominated by uncertainties in emission estimates and environmental degradation rates for the Level I substances and further research should be focused on better characterization of emissions and studies of degradation reactions in various environmental media. Given these uncertainties in the overall mass balance calculations, further model-based studies should concentrate on assessing the influence of more refined descriptions of fate and transport processes within the existing model frameworks, and not on increasing the spatial and temporal resolution of the existing models. Once our understanding of the basic mechanisms resulting in deposition to the Lakes has improved sufficiently, research should focus on spatial and temporal scaling issues.

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2.0 INTRODUCTION

Under the Great Lakes Binational Toxics Strategy [1] the United States and Canada have agreed to take steps to virtually eliminate persistent toxic substances from the Great Lakes environment. A set of 12 chemicals or chemical groups (the "Level 1 substances") were selected for immediate action, and significant emission reductions within the Great Lakes Basin have been achieved for many of these substances. As local sources are identified and eliminated the contribution of contaminant loadings to the Great Lakes system from distant sources by atmospheric transport and deposition may become the controlling factor determining of reduction rates of contaminants in the Lakes.

This report describes the application of mass balance contaminant fate models to improve our current understanding of the relative contributions of local and distant sources of Level 1 substances to the Great Lakes. The Level I substances include polychlorinated biphenyls (PCBs), dioxins and furans, hexachlorobenzene (HCB), benzo(a)pyrene (B[a]P), octachlorostyrene (OCS), chlordane, aldrin/dieldrin, DDT, mirex, toxaphene, mercury, and alkyl lead. The models used in this study are based on the Berkeley-Trent (BETR) contaminant fate modeling framework [2], and have been developed by researchers at the Lawrence Berkeley National Laboratory, Berkeley, California and Trent University, Peterborough, Ontario, Canada.

The models are most appropriate for describing long-term partitioning, fate, and transport of organic chemicals; therefore alkyl lead and mercury were not modeled in this study. The ten organic substances listed as Level I substances were modeled as well as α-hexachlorocyclohexane, a "Level II substance" for which there is an available global-scale emissions inventory. The models are applied to characterize the combined atmospheric transport and deposition efficiency of these substances and, where possible, to estimate the contribution of sources in different regions of North America and the world to atmospheric loadings to the Great Lakes.

The general goal of this research is to systematically assess the long-range transport potential of the Level I substances with a particular focus on transport and deposition to the Great Lakes. The assessment strategy is made up of four stages, as shown in Table 2.1.

Table 2.1. Four-stage assessment strategy for assessing long-range transport potential and depositional efficiency to the Great Lakes for Level I substances.

Stage 1	Compilation of physico-chemical properties and degradation rates in environmental media
Stage 2	Modeling of long-range transport potential and transport efficiency to the Great Lakes over continental and global scales for generic emissions scenarios
Stage 3	Compilation of emissions estimates and observed environmental concentrations
Stage 4	Assessment of regional contributions to atmospheric loading to the Great Lakes over continental and global scales

The assessment strategy was designed to sequentially build up information about the long-range transport potential for the Level I substances, from general information about physico-chemical properties (Stage 1) to generic indicators of long-range transport potential and transport and depositional efficiency to the Great Lakes (Stage 2) and finally provide comprehensive estimates of the contribution of emissions in different locations to atmospheric deposition rates to the Lakes (Stage 4).

At the outset of this project we anticipated that completing all four stages of the assessment strategy would be possible for only a subset of the Level I substances. We expected the availability of emission estimates required for Stage 3 and Stage 4 to be a limiting factor. From a survey of available literature we have assembled emissions information for seven PCB congeners, and α-HCH on a global scale, and for the PCB congeners and toxaphene on a continental scale. For the other Level I substances we have completed Stages 1 and 2, and these model results can be combined with emission

information as it comes available to estimate regional contributions to atmospheric loadings to the Lakes. This can be achieved without re-running the models since the equations describing transport and deposition are linear. Therefore the model results for the generic emission scenario can be scaled by the proportion of total emissions in each region to deduce the fraction of loading attributable to emissions in each region when data become available.

This report is organized into seven sections and two appendices.

Section 1 is a condensed summary of the study results and recommendations for future research.

This is Section 2, an introduction to the project and a guide to the information presented in the project report.

Section 3 provides background information about the Berkeley-Trent North American Contaminant Fate Model (BETR North America) and the Berkeley-Trent Global Contaminant Fate Model (BETR Global).

Section 4 presents results from Stage 1 and 2 of the assessment process for all of the Level I substances, including physico-chemical properties and degradation half-lives, generic modeling of transport potential and transport and deposition efficiency, and results of Great Lakes Transfer Efficiency calculations on North American and global scales.

Section 5 summarizes emissions inventories at the North American scale for seven PCB congeners and toxaphene, and at the global scale for the PCBs and α-HCH. Modeled concentrations of PCBs in air obtained from the BETR Global model are compared with data from eleven long-term monitoring stations in the Northern Hemisphere, including the International Atmospheric Deposition Network (IADN), which is located in the Great Lakes Basin.

Section 6 combines information from the generic modeling and emissions estimates to calculate the fraction of total loading from the atmosphere that is attributable to sources in different regions of North America and the world.

Section 7 presents overall conclusions from the study, and suggests avenues for future research to further improve our ability to identify sources of atmospherically derived persistent pollutants in the Lakes, and to more accurately quantify the relative contributions of these sources to total loadings.

3.0 MODELING TOOLS

This section provides background information about the Berkeley-Trent North American Contaminant Fate Model (BETR North America) and the Berkeley-Trent Global Contaminant Fate Model (BETR Global).

3.1 The BETR North America Model

A detailed description of the BETR model framework and environmental parameterization for North America is provided by MacLeod et al. [(2)] and Woodfine et al. [(3)]. The BETR model describes contaminant partitioning and fate in the environment using mass balance equations based on the fugacity concept. General background on the application of fugacity-based models to environmental problems can be found in the text by Mackay [(4)], and a review of the application of models of this type in fate and exposure assessments is provided by McKone and MacLeod [(5)].

The BETR North America model describes the North American environment as 24 ecological regions, as illustrated in Figure 3.1.1. Within each region, contaminant fate is described using a 7-compartment fugacity model including a vertically segmented atmosphere, vegetation, soil, freshwater, freshwater sediments, and coastal ocean/sea water. Contaminants can be transported between adjacent regions of the model in the atmosphere and in flowing rivers and by near-shore ocean currents.

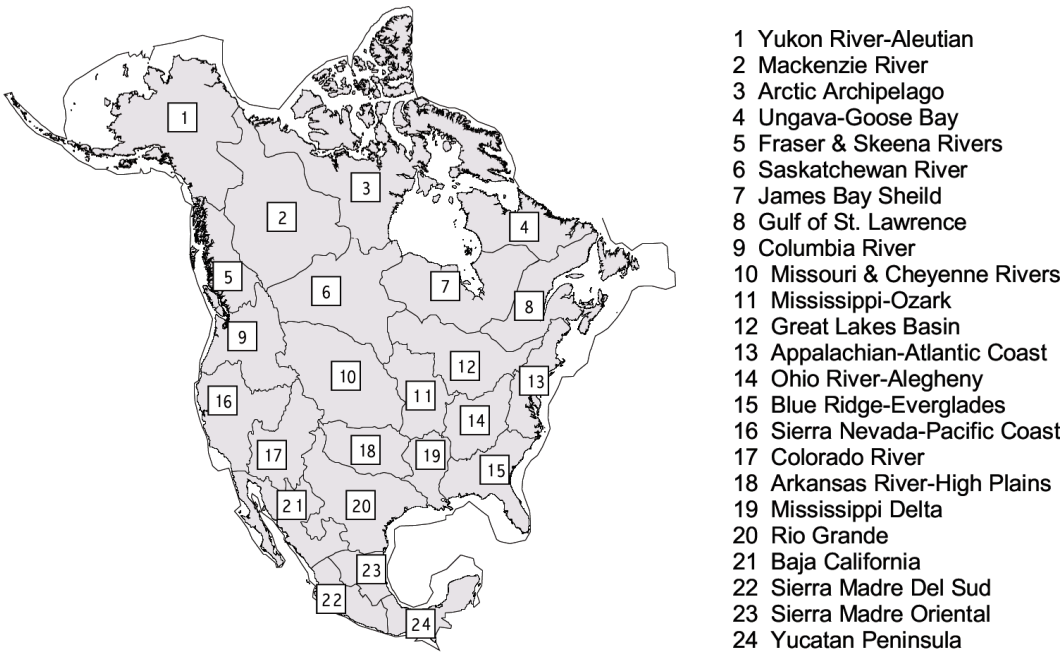

Figure 3.1.1. Regional segmentation of the BETR North America model.

Each of the BETR North America regions is parameterized to represent local environmental conditions, including hydrology, meteorology, and physical attributes. This requires the specification of more than 70 individual input parameters for each region. Geographic Information System (GIS) software has been used in combination with geo-referenced data sets from a variety sources to efficiently and accurately parameterize the North American environment in the model.

In the BETR North America model, the environment within each region is described as a connected system of seven discrete, homogeneous compartments. Figure 3.1.2 illustrates the seven compartment regional environment of the BETR model framework.

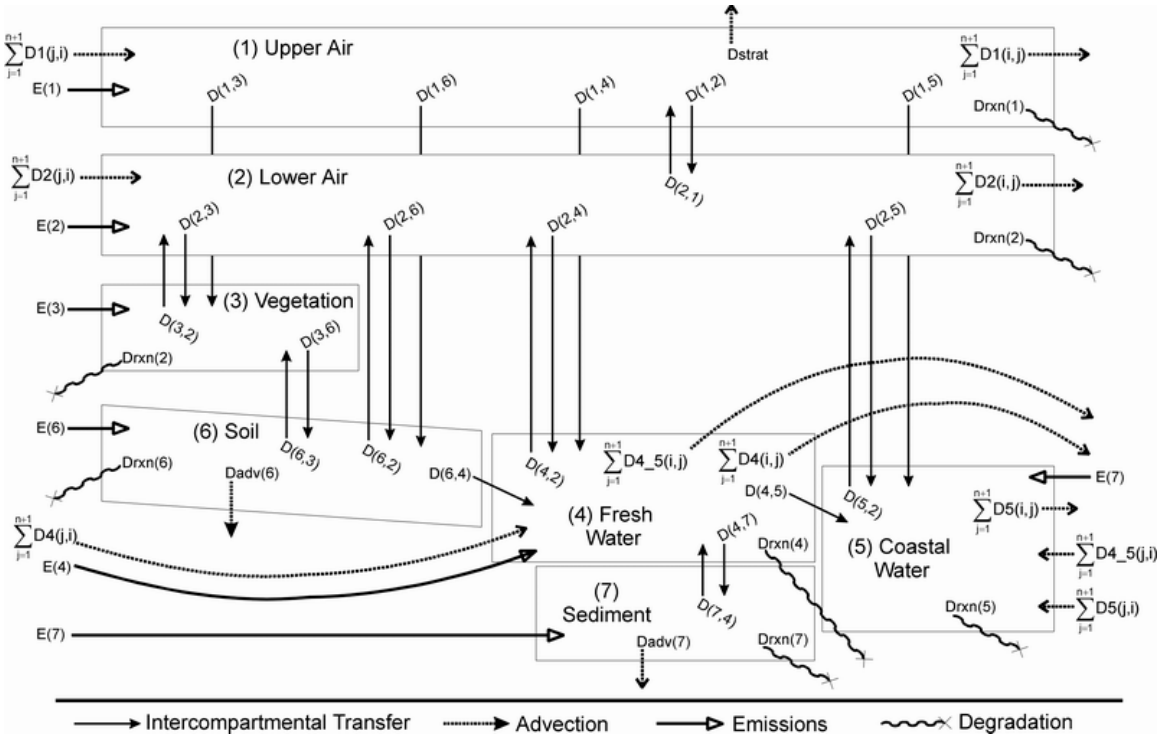

Figure 3.1.2. Contaminant fate and transport processes considered in each region of the BETR North America model. E values represent primary emissions to each compartment and D values indicate fate and transport processes available to the substance in each compartment.

Individual regional environments are connected in the BETR framework by inter-regional flows of air in the upper and lower atmosphere, and of fresh and coastal water. These inter-regional linkages are illustrated in Figure 3.1.2 and are specified in the model as five matrices of volumetric flow rates that describe movement of air or water in both directions across all regional boundaries. In total, the North American model requires compilation of five volumetric flow rate matrices: two for the atmosphere (upper and lower), one for freshwater exchange, one for freshwater flowing into coastal waters of an adjacent region and one for the exchange of coastal water. To satisfy the conditions of long-term steady state in each region the volumetric inflow rate of air, freshwater, and coastal water are balanced by an equal outflow rate.

Seven equations describe contaminant fate in each region, and therefore a total of 168 mass balance equations make up the 24-region linked model for North America. This system of seven equations and the seven unknown fugacities have been solved analytically using linear algebra, and by matrix algebra using a Gauss elimination algorithm. The BETR North America model can also be applied to describe the time course of contaminant concentrations in the linked set of regions by expressing the mass balance equations as a set of seven differential equations.

3.2 The BETR Global Model

The BETR-Global model is based on the same Berkeley-Trent contaminant fate modeling framework as the BETR North America Model, and many of the equations used to describe contaminant fate in BETR-Global are identical to those in BETR North America. However, the BETR Global model incorporates several refinements to the general structure to allow more flexibility and to describe the global environment in more detail and with higher temporal resolution. Previous applications of the BETR model framework use a single set of parameters to describe the long-term average transfer rates of air and water between the regions within the model domain. As a result, temporal resolution has been limited to describing trends in contaminant concentrations that take place over several years. The BETR Global model uses a monthly time scale to specify atmospheric conditions and other selected parameters, and a 15° by 15° grid coverage of the globe, resulting in 288 multimedia regions (Figure 3.2.1). Compared to previous multimedia models based on the BETR framework this approach significantly increases both spatial and temporal resolution.

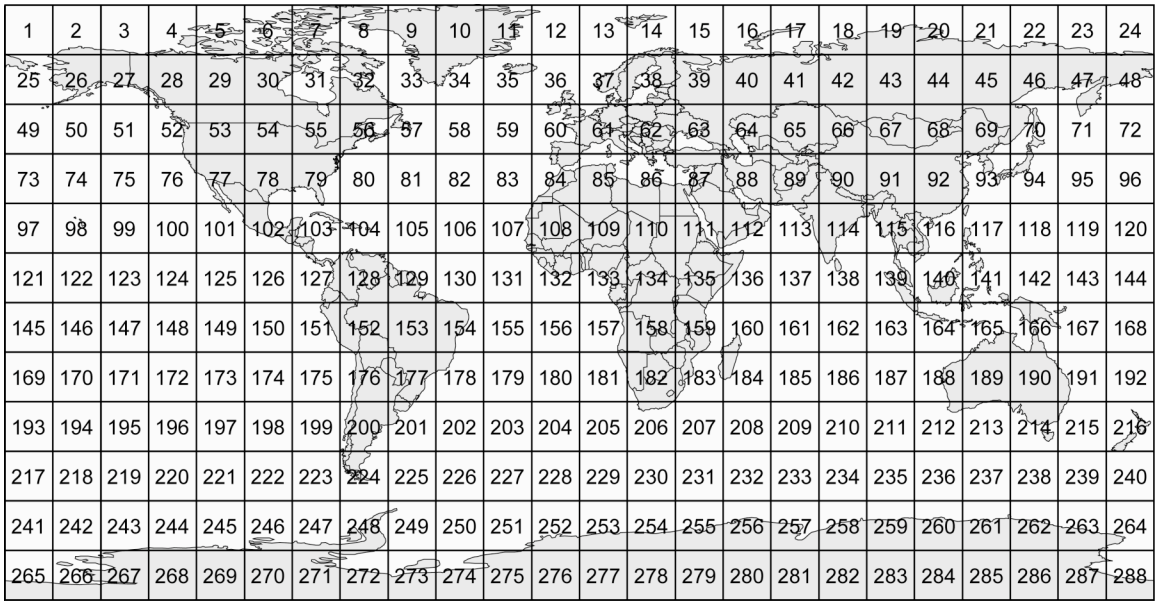

Figure 3.2.1. Regional segmentation of the BETR Global model showing numerical naming scheme for individual regions.

A complete description of the BETR Global model and its development can be found in MacLeod et al. [(6)].

3.3 Metrics of Long-range Transport Potential

Potential for long-range transport in the environment is recognized as an important indicator of environmental hazard for chemical substances. The Long Range Transport Potential (LRTP) can be characterized using model calculations; however several alternative models and modeling approaches are being used for this purpose. As a result, several different metrics for LRTP have been suggested in the literature. A key distinction is between (1) “transport-oriented” metrics that describe the potential for transport in air and/or water with simultaneous exchange with the surface media, and (2) “target-oriented” metrics, describing the percentage of emitted substance that migrates to surface media in selected target regions as a consequence of transport in air and/or water and subsequent deposition [(7)]. Great Lakes Transfer Efficiency is a “target-oriented”

LRTP metric. We have also examined LRTP of the Level I substances using the "transport-oriented" metric CTD.

3.3.1 Characteristic Travel Distance (CTD)

The Characteristic Travel Distance (CTD, (km)) is a transport-oriented long-range transport potential metric defined as the distance from a point source at which the concentration has decreased to $1/e$ ($\approx 37\%$) of the initial value [8]:

$$c(\mathrm{CTD}) = c_0 / e$$

Beyer et al. [9] showed that in a single region steady-state model the CTD in the mobile media air or water could be approximated as the product of the overall persistence (P_{OV}, hours), the fraction of chemical partitioning to the mobile medium (ϕ, dimensionless) and an assumed velocity of the mobile media (ν, km h^{-1}).

$$\mathrm{CTD} = P_{OV}\, \phi\, \nu.$$

CTD can therefore be calculated from the results provided by any multimedia model which estimates P_{OV} and ϕ.

For the present purposes, we conduct CTD calculations using ChemSCORER [10], which is based on the generic Level III model developed by Mackay [4]. While it is possible to calculate CTD from the output of the BETR model, we have instead applied ChemSCORER since it provides an independent second model for comparison. CTDs calculated by a generic Level III model and by BETR were observed to be highly correlated in initial investigations using a set of hypothetical chemical property combinations. The ChemSCORER software also provides an informative generic hazard profile for each substance, including comparative scores for Persistence (P_{OV}),

Bioaccumulation potential (B), and LRTP. Results from ChemSCORER for the Level I substances are included in Appendix A.

3.3.2 Great Lakes Transfer Efficiency (GLTE)

Great Lakes Transfer Efficiency is a target oriented long-range transport potential metric using the fresh water in the Great Lakes Basin as the target ecosystem [11]. It is defined as the ratio of the deposition mass flux from air to water in the Great Lakes Basin to the emission mass flux in a source region (Figure 3.3.2.1). GLTE can be calculated for simple emission scenarios (i.e., emissions individually to air, water, or soil in a single source region) or for combined emission to several media in several regions.

$$\textbf{GLTE} = \frac{\text{Rate of atmospheric deposition to the Great Lakes (kg/y)}}{\text{Emission rate to the atmosphere in the source region (kg/y)}} \times 100\%$$

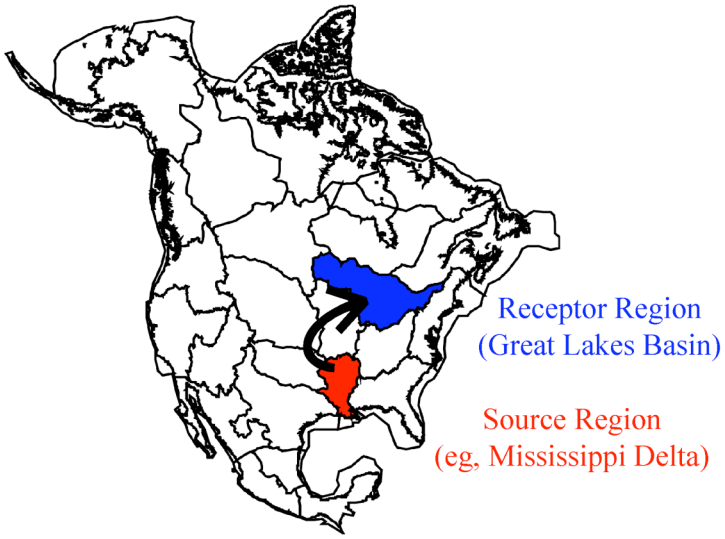

Figure 3.3.2.1. Conceptual illustration of the Great Lakes Transfer Efficiency calculated for transport from the Mississippi River Delta Region using BETR North America.

Conceptually, the Great Lakes transfer efficiency represents the percentage of chemical released to air in a source region that is expected to be deposited from the atmosphere to

the surface waters of the Great Lakes. The GLTE is a convenient LRTP metric for the BETR North America model since the regional segmentation is partially based on watershed boundaries. Thus there is a model region that explicitly represents the Great Lakes Basin watershed, and it is a simple matter to calculate the depositional flux to water in this region.

In the BETR Global model the Great Lakes straddle the boundary between two model regions. Therefore GLTE calculations are made by combining the mass flux to freshwater in these two regions in the numerator. Because it is not based on watershed boundaries, GLTE calculated by the BETR Global model includes deposition to surface water outside of the Great Lakes Basin. Based only on freshwater areas in the two model's target regions, GLTE calculated using the BETR Global model is expected to be a factor of 2.4 higher than that calculated using BETR North America.

4.0 MODELING RESULTS

In this section, we provide results from Stage 1 and 2 of the assessment process for all of the Level I substances, including physico-chemical properties and degradation half-lives, generic modeling of transport potential and transport and deposition efficiency, and results of Great Lakes Transfer Efficiency calculations on North American and global scales.

4.1 Physicochemical Properties of Level I Substances

Chemical properties required as inputs for the multimedia models include molecular mass, equilibrium partition coefficients between air, water and octanol, and estimates of degradation half lives in air, water, soil, and sediments. The BETR North America and BETR Global models describe contaminant fate in realistic environmental systems with different conditions, for example, temperature, soil, water, etcetera. Enthalpies of phase change that describe the temperature dependence of the partition coefficients between air, water, and octanol are therefore also required as inputs to the models. In addition, the BETR Global model applies generic corrections to estimated media-specific degradation half-lives to account for reduced degradability in colder environments. These correction factors are the same for all chemicals considered in this study, and they result in roughly doubling the degradation rate constants in all media for a temperature increase of 10° above the reference temperature of $25^{o}C$. In Stage 1 of the assessment procedure for the Level I substances we conducted a literature search to select appropriate values for these properties for use in the modeling exercises.

Accurate measurement of partitioning properties is challenging, particularly for semi-volatile organic chemicals that may have properties at or near the limits of analytical techniques. Pontolillo and Eganhouse [(12)], who recently reviewed data for DDT and DDE on aqueous solubility and octanol-water partition coefficients, report high variability in reported values, and reporting errors. These findings raised questions about

available data quality for these chemical properties. They recommended improvement of measurement and reporting techniques in order to increase data reliability of reported physicochemical properties of hydrophobic organic compounds. An important contribution in this regard was made by Cole and Mackay [13] who suggested partitioning data be evaluated for consistency using thermodynamic relationships linking the solubilities in air, water, and octanol and the three corresponding partition coefficients—air/water, octanol/water, and octanol/air. This "three solubility" approach can be extended to interpret data on the temperature dependence of partitioning properties since the relationships between the three solubilities and the three partition coefficients are valid at any temperature. The temperature dependence of solubilities and partition coefficients can be expressed in terms of energies of phase transition (ΔU), and the ΔU values must conform to similar constraints as the partition coefficients [14].

Table 4.1.1 presents values for partitioning properties of the Level I substances gathered from our literature search and used in the modeling described in this report. Whenever possible we have used data that have been harmonized to conform to thermodynamic constraints using the three solubility adjustment procedure recommended by Beyer et al. [14]. This ensures that no incompatible data for individual property measurements of a given substance are used in the assessment.

Also listed in Table 4.1.1 are estimated degradation half-lives for the Level I substances in environmental media. These half-life estimates encompass all possible transformation reactions that might alter the chemical structure of the substance, including reaction with hydroxyl radicals in the gas phase, hydrolysis, photolysis and biodegradation, for example by microbes. Unfortunately, these data are highly uncertain and quality assurance procedures akin to the three solubility approach that was applied to the partitioning properties are not available. Uncertainties associated with these estimated degradation half lives are estimated to be approximately an order of magnitude, and contribute significantly to the overall uncertainty in the model assessments. Uncertainties in the overall assessment process are discussed in detail in Section 7.0.

Table 4.1.1. Physico-chemical properties and estimated degradation half-lives of the Level I substances.

Name	Molecular Weight (g/mol)	Log Kow	Log Kaw	Estimated Degradation half-lives (hours)				ΔUaw (J/mol)	ΔUow (J/mol)	References
				Air	*Water*	*Soil*	*Sediment*			
PCB 28	257.54	5.66	-2.19	550	17000	55000	55000	52300	-26300	[1],[2]
PCB 52	291.99	5.91	-2.31	1700	55000	55000	55000	54100	-27300	[1],[2]
PCB 101	326.43	6.33	-2.40	1700	55000	55000	55000	59700	-23800	[1],[2]
PCB 118	236.43	6.69	-2.67	1700	55000	55000	55000	60500	-28500	[1],[2]
PCB 138	360.88	7.21	-2.44	5500	55000	55000	55000	61300	-25000	[1],[2]
PCB 153	360.88	6.87	-2.57	5500	55000	55000	55000	62800	-31100	[1],[2]
PCB 180	395.32	7.16	-3.04	5500	55000	55000	55000	63600	-29100	[1],[2]
Dieldrin	380.90	5.88	-1.93	22.3	15200	16700	13200	55000	-20000	[3],[4],[5]
Aldrin	364.90	4.94	-3.38	2.86	2670	3830	26700	55000	-20000	[3],[4],[5]
hexachlorobenzene (HCB)	284.79	5.59	-1.58	22600	34100	34100	341000	50490	-24700	[4],[6]
Total chlordanes	409.80	6.20	-2.65	55	17000	17000	55000	55000	-20000	[2],[3],[5]
2,3,7,8-TCDD	321.98	6.83	-3.17	97	2580	23000	23000	74440	-18220	[7],[8]
α-hexachlorocyclohexane	290.85	3.98	-3.39	1420	3360	3360	1690	51350	-10510	[7],[9]
p,*p*'-DDT	354.50	6.39	-3.34	170	550	17000	55000	55000	-20000	[3],[5]
Toxaphene	413.80	5.50	-3.75	170	55000	55000	55000	61432	24500	[10]
octachlorostyrene	379.71	7.46	-1.23	227	3600	3600	14400	55000	-20000	[5],[11]
benzo[a]pyrene	252.30	5.94	-5.21	1.52	56	5490	28100	36890	-25400	[4],[7]
Mirex	545.59	7.46	-1.79	170	170	55000	55000	55000	-20000	[2],[5],[12]

[1] Partitioning properties and enthalpies of phase transition from Li, N, F. Wania, Y.D. Lei and G.L. Daly. 2003. A comprehensive and critical compilation, evaluation and selection of physical-chemical property data for selected polychlorinated biphenyls. Journal of Physical Chemical Reference Data, 32 (4), 1545 - 1590.

[2] Degradation half-lives from Mackay, D., W.Y. shiu and K.C. Ma. 2000. Illustrated handbook of physical-chemical properties and environmental fate. Chapman & Hall/CRCnetBase, Boca Raton, FL.

[3] Partitioning properties from Shen, L. and F. Wania. 2004. Compilation, evaluation and selection of physical-chemical property data for organochlorinated pesticides. Journal of Physical Chemistry Reference Data (In Press).

[4] Degradation half-lives from McKone, T. E. 1993. CalTOX, a multimedia total exposure model for hazardous waste sites. Part 1: Executive summary. UCRL-CR-111456PTI, prepared for the Department of Toxic Substances Control, California Environmental Protection Agency. Livermore, CA: Lawrence Livermore National Laboratory.

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[7] Partitioning properties and enthalpies of phase transition from Beyer, A., F. Wania, T. Gouin, D. Mackay and M. Matthies. 2002. Selecting internally consistent physicochemical properties of organic compounds. Environmental Toxicology and Chemistry. 21(5), 941-953.

[8] Degradation half-lives are the recommended values of M. Scheringer, ETH Zurich (Personal Communication, 2004) used in the OECD multi-media model comparison exercise.

[9] Degradation half-lives from Toose, L., D.G. Woodfine, M. MacLeod, D. Mackay and J. Gouin. 2004. Environmental Pollution 128, 223-240.

[10] Properties selected by MacLeod, M., D.G. Woodfine, J.R. Brimacombe, L. Toose and D. Mackay. 2002. A dynamic mass budget for toxaphene in North America. Environmental Toxiclology and Chemistry 21(8), 1628-1637.

[11] Partitioning properties and degradation half-lives estimated using the EPIWIN quantitative structure-activity relationship program: http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

[12] Log Kow recommended value from Mackay, D., W.Y. Shiu and K.C. Ma. 2000. Illustrated handbook of physical-chemical properties and environmental fate. Chapman & Hall/CRCnetBase, Boca Raton, FL. Log Kaw from Yin, C.Q. and J.P. Hassett. 1986. Gas-Partitioning Approach For Laboratory and Field Studies of Mirex Fugacity in Water. Environmental Science and Technology, 20(12), 1213-1217.

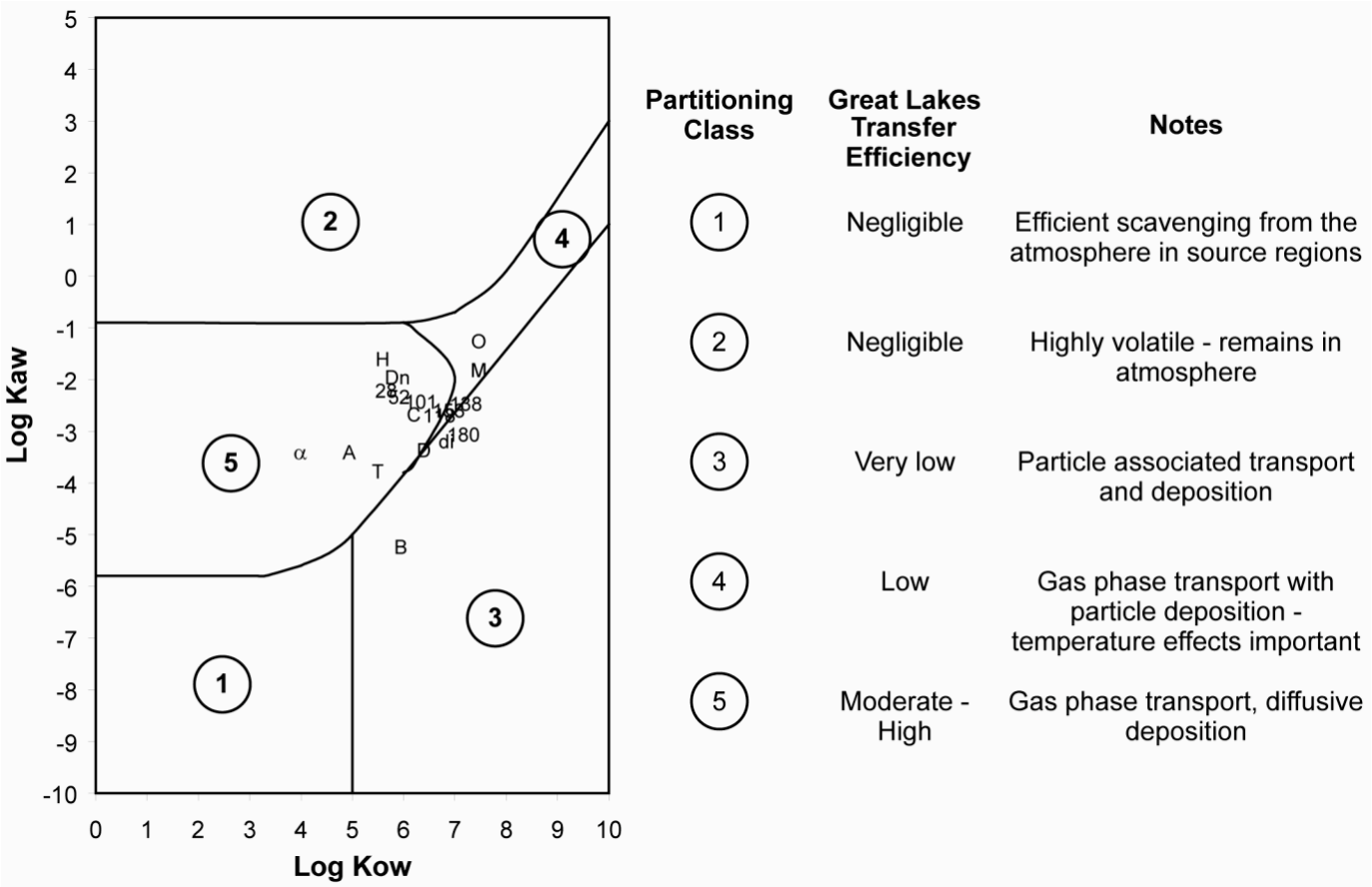

Figure 4.1.1. Screening assessment of potential for transport and deposition to the Great Lakes based on partitioning properties. Partitioning of the Level I substances are indicated by the following symbols: 28 – PCB 28, 52 – PCB 52, 101 – PCB 101, 138 – PCB 138, 153 – PCB 153, 180 – PCB 180, Dn – Dieldrin, A – Aldrin, H – HCB, C – total Chlordanes, di – 2,3,7,8-TCDD, α – α-HCH, D – *p,p*-DDT, T – toxaphene, O – octachlorostyrene, B – benzo[a]pyrene, M – Mirex.

An initial screening of the Level I substances for potential for long-range transport and deposition to the Great Lakes is possible at this stage using the graphical method derived from results from the BETR North America model [11]. Figure 4.1.1 shows the position of each of the Level I substances in the K_{OW}/K_{AW} partitioning space with the five regions of dominant fate and transport processes identified by MacLeod and Mackay. This preliminary analysis illustrates that the majority of the Level I substances have partitioning properties that make transport and deposition to the Lakes possible, provided the substances are sufficiently persistent in the atmosphere.

4.2 Generic Modeling of Persistence and Long-range Transport Potential of Level I Substances

Generic modeling of P_{OV} and LRTP is possible using the data gathered on physicochemical properties and degradation half lives. Generic assessments are useful for building an understanding of how the environmental hazards posed by substances varies with their inherent physicochemical properties. Assessments of this type are useful and informative and they do not require estimates of actual emission rates or emission patterns. They can be used to rank or score chemicals based on intrinsic environmental hazard. Generic assessments also provide a valuable reference point and information about the likely behavior of substances. These generic assessments can be compared against results of more detailed site-specific and emission scenario-specific modeling.

Table 4.2.1 provides model results from ChemSCORER for overall persistence and characteristic travel distance of each of the Level I substances, and Great Lakes Transfer Efficiencies calculated from BETR North America and BETR Global. The GLTE values presented here are for emissions to air in Region 16 (Sierra Nevada Pacific Coast) in the BETR North America model, and for emissions to air in Eastern China (Region 92) in the BETR Global model. These emission scenarios were selected as representative of continental and global-scale transport, respectively, to the Great Lakes target region.

Table 4.2.1. Generic modeling results for overall persistence (P_{OV}) and long-range transport potential of the Level I substances. (CTD – characteristic travel distance, BETR NA – BETR North America model, GLTE – Great Lakes transfer efficiency).

Name	Pov (days) for emissions to:			Maximum	CTD (km) in:		Maximum	BETR NA	BETR Global
	Air	*Water*	*Soil*	Pov (days)	*Air*	*Water*	CTD (km)	GLTE (%)	GLTE (%)
PCB 28	616	1551	3254	3254	9337	3360	9337	1.24	0.11
PCB 52	1935	2680	3293	3293	15122	3637	15122	1.55	0.19
PCB 101	2573	3148	3304	3304	8093	2802	8093	0.96	0.18
PCB 118	3041	3288	3306	3306	2932	2461	2932	0.37	0.17
PCB 138	3258	3305	3307	3307	1876	2122	2122	0.27	0.18
PCB 153	3236	3303	3307	3307	2715	2288	2715	0.33	0.19
PCB 180	3284	3307	3307	3307	891	2184	2184	0.16	0.15
Dieldrin	341	790	1006	1006	302	1427	1427	0.0023	0.00013
Aldrin	1	1147	231	1147	59	1323	1323	0.0000022	0.00000000005
hexachlorobenzene (HCB)	3335	4490	85423	85423	176980	4741	176980	1.54	0.55
Total chlordanes	207	2617	1027	2617	993	3916	3916	0.063	0.010
2,3,7,8-TCDD	7431	3064	9462	9462	1927	2310	2310	0.12	0.079
α-hexachlorocyclohexane	225	272	196	272	13821	13879	13879	1.86	0.58
p,*p*'-DDT	775	2822	1027	2822	1472	3320	3320	0.12	0.063
Toxaphene	1688	3141	3302	3302	1735	10296	10296	0.076	0.029
octachlorostyrene	91	805	217	805	3486	1060	3486	0.23	0.049
benzo[a]pyrene	17	187	330	330	30	260	260	0.015	0.000011
Mirex	1375	985	3288	3288	1900	616	1900	0.11	0.040

Pov and CTD calculated from Level III ChemSCORER Beta1.01 (http://www.trentu.ca/cemc/models/ChemScor.html).

BETR North America GLTE for emissions to lower air in Region 16 (Sierra Nevada-Pacific Coast)

BETR Global GLTE for emissions to lower air in Region 92 (eastern China)

The Organization for Economic Cooperation and Development (OECD) has recently sponsored an expert group of model developers, who made recommendations for applying multimedia models to identify persistent organic pollutants (POPs) in screening assessments [7,15]. One of the recommendations of this working group was that plots of overall persistence versus long-range transport potential are a useful tool for interpreting model results and prioritizing chemicals. In such a plot, potential POP-like substances with high P_{OV} and high LRTP lie in the upper right portion of the plot. Figure 4.2.1 shows a plot of P_{OV} versus characteristic transport distance (CTD) in air calculated by ChemSCORER. Reference lines provided for travel distances are taken from Beyer et al [9] who suggested CTD cut-offs of 700 km and 2000 km between high, medium and low travel distances.

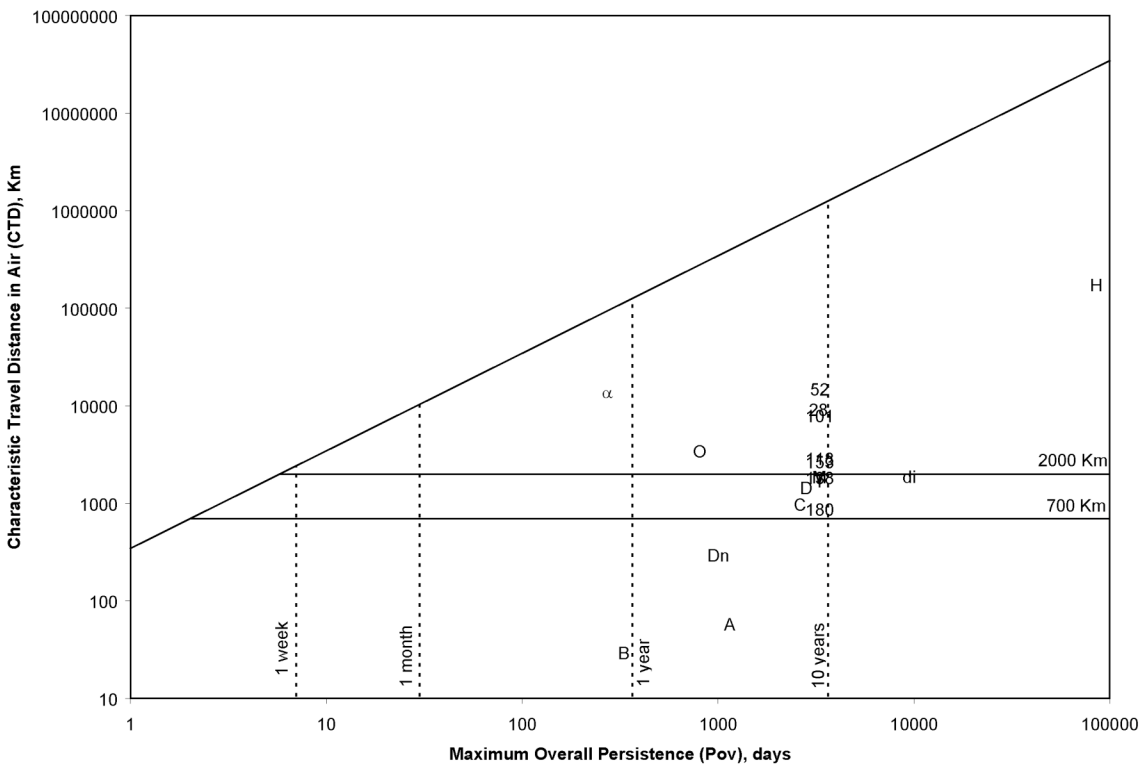

Figure 4.2.1. Hazard identification plot for the Level I substances using characteristic travel distance as the metric of long-range transport potential. The diagonal line represents CTD of volatile substances that partition entirely to air, and is the maximum limit of transport distance in air for a given overall persistence. Substances that are

conventional persistent organic pollutants (POPs) combine high long-range travel potential with high overall persistence. 28 – PCB 28, 52 – PCB 52, 101 – PCB 101, 118 – PCB 118, 138 – PCB 138, 153 – PCB 153, 180 – PCB 180, Dn – Dieldrin, A – Aldrin, H – HCB, C – total Chlordanes, di – 2,3,7,8-TCDD, α – α-HCH, D – *p,p*-DDT, T – toxaphene, O – octachlorostyrene, B – benzo[a]pyrene, M – Mirex.

Figure 4.2.1 confirms that the majority of the Level I substances are expected to behave like conventional POPs in the environment, i.e., they have high persistence and potential for long-range transport. Exceptions are Dieldrin, Aldrin and Benzo(a)pyrene, which are persistent, but exhibit relatively low LRTP compared to other Level I substances. It is notable that α-HCH has remarkably high LRTP, especially considering its relatively low P_{OV}. This is attributable to its resistance to degradation in air and partitioning properties that favor distribution to all available environmental media.

Great Lakes-specific P_{OV} vs. LRTP plots of this type from BETR North America and BETR Global are shown in Figures 4.2.2 and 4.2.3. These results are broadly consistent with those from ChemSCORER using CTD as the metric of LRTP. On the continental scale, low, and middle-range chlorination level PCBs (28, 52 and 101) are more efficiently transported and deposited to the Great Lakes than higher chlorination level congeners (138, 153 and 180). However, on the Global scale the GLTE of the lighter congeners is comparable to that of the higher chlorinated congeners. This shift in the relative LRTP of the PCB congeners may be due to the higher proportion of water in the global model, which enhances the diffusive deposition rates for lighter congeners more than heavier congeners. Hexachlorobenzene and α-HCH exhibit the highest GLTE over both continental and global scales.

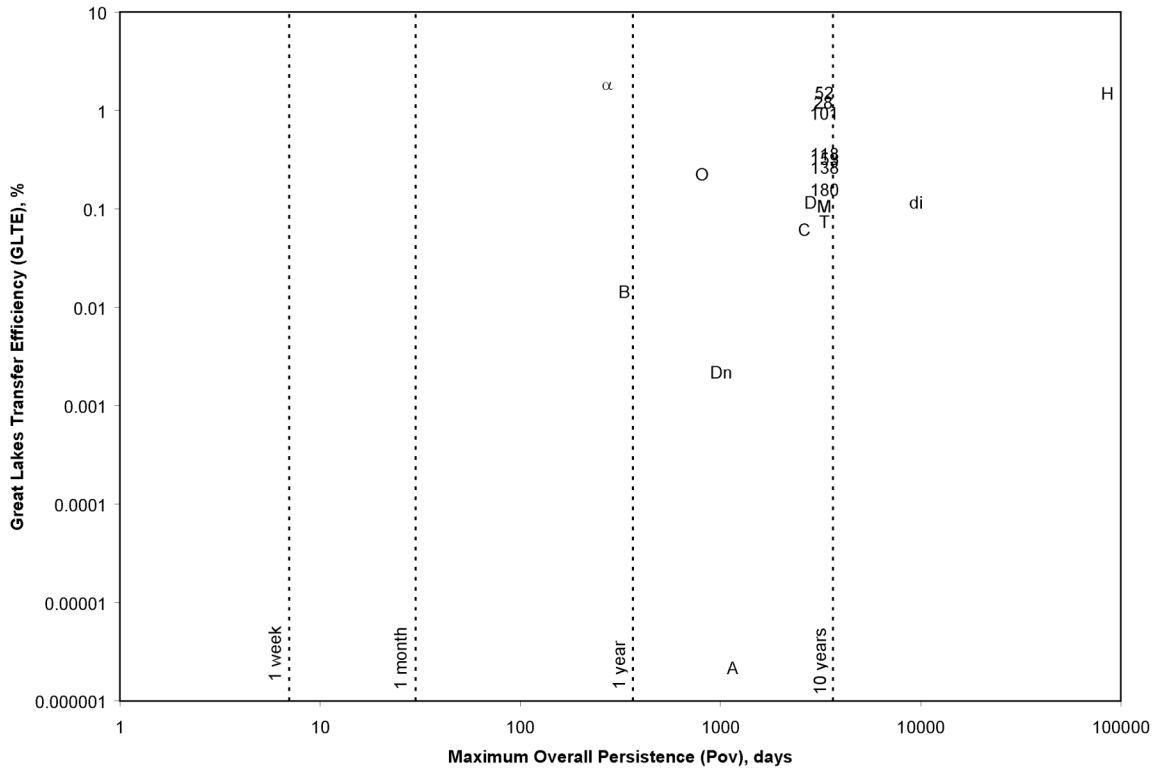

Figure 4.2.2. Hazard identification plot for the Level I substances using Great Lakes transfer efficiency calculated by BETR North America as the metric of long-range transport potential, assuming emissions to air in Region 16 (Sierra Nevada Pacific Coast). 28 – PCB 28, 52 – PCB 52, 101 – PCB 101, 118 – PCB 118, 138 – PCB 138, 153 – PCB 153, 180 – PCB 180, Dn – Dieldrin, A – Aldrin, H – HCB, C – total Chlordanes, di – 2,3,7,8-TCDD, α – α-HCH, D – *p,p*-DDT, T – toxaphene, O – octachlorostyrene, B – benzo[a]pyrene, M – Mirex.

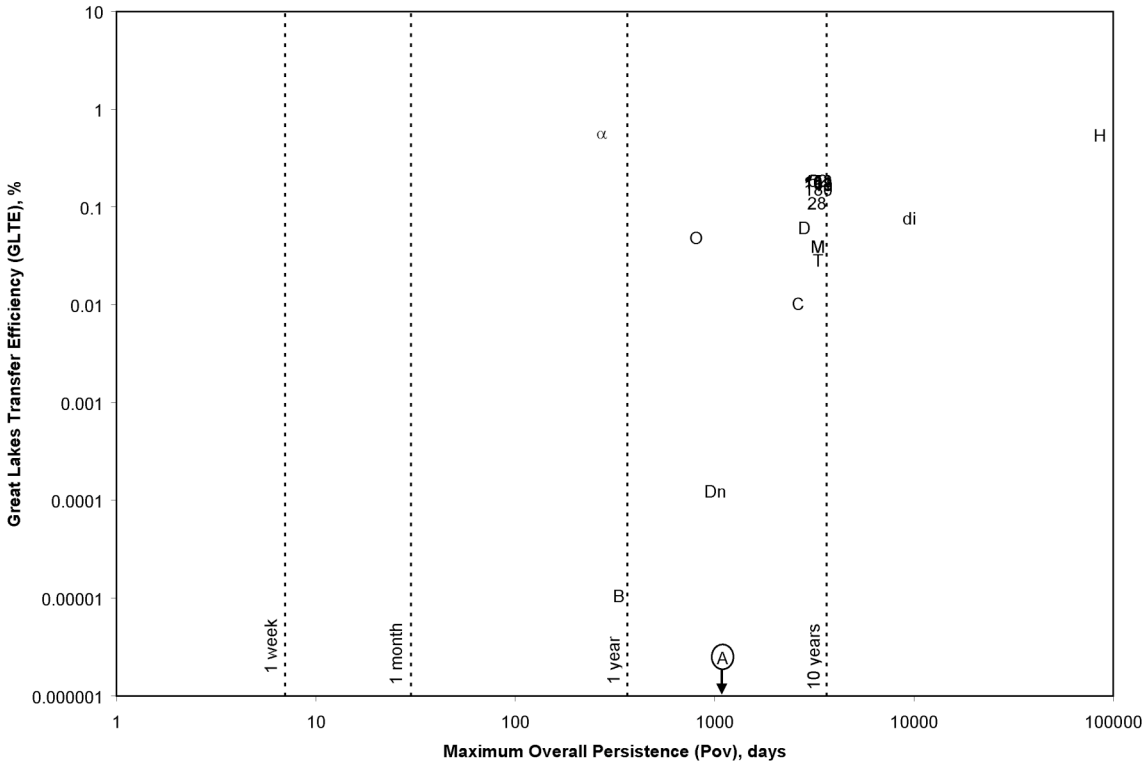

Figure 4.2.3. Hazard identification plot for the Level I substances using Great Lakes transfer efficiency calculated by BETR Global as the metric of long-range transport potential, assuming emissions to air in Region 92 (East China Coast). 28 – PCB 28, 52 – PCB 52, 101 – PCB 101, 118 – PCB 118, 138 – PCB 138, 153 – PCB 153, 180 – PCB 180, Dn – Dieldrin, A – Aldrin, H – HCB, C – total Chlordanes, di – 2,3,7,8-TCDD, α – α-HCH, D – *p,p*-DDT, T – toxaphene, O – octachlorostyrene, B – benzo[a]pyrene, M – Mirex.

4.3 Great Lakes Transfer Efficiency of Level I Substances from within North America

For each of the individual chemicals selected to represent the Level I substances, Figures 4.3.1 – 4.3.18 present Great Lakes transfer efficiency for emissions to air in each region of the BETR North America Model. Color shading using a semi-logarithmic scale relative to the maximum calculated GLTE is provided to aid visual interpretation of the figures.

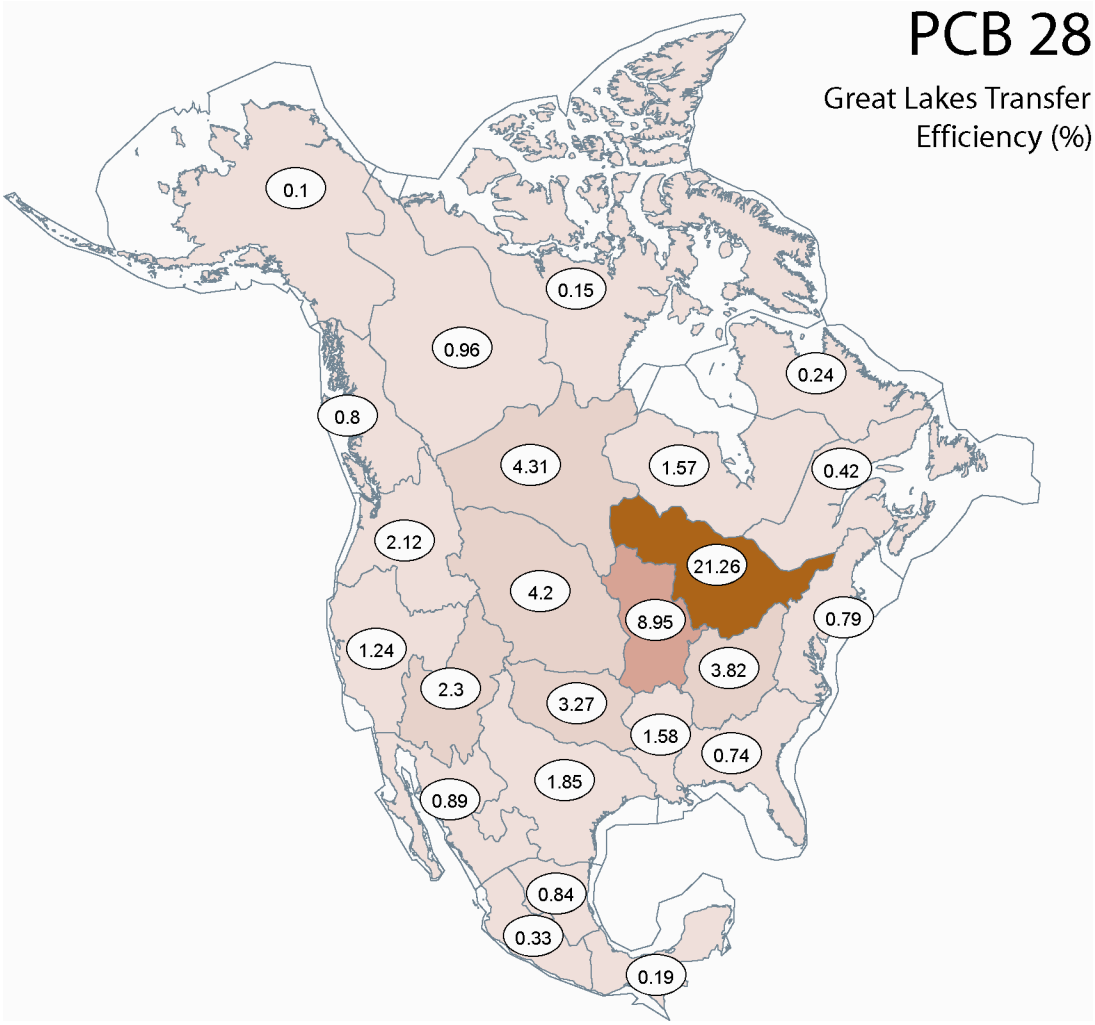

Figure 4.3.1. Great Lakes Transfer Efficiency of PCB 28 for emissions to air in each of the 24 regions of the BETR North America model.

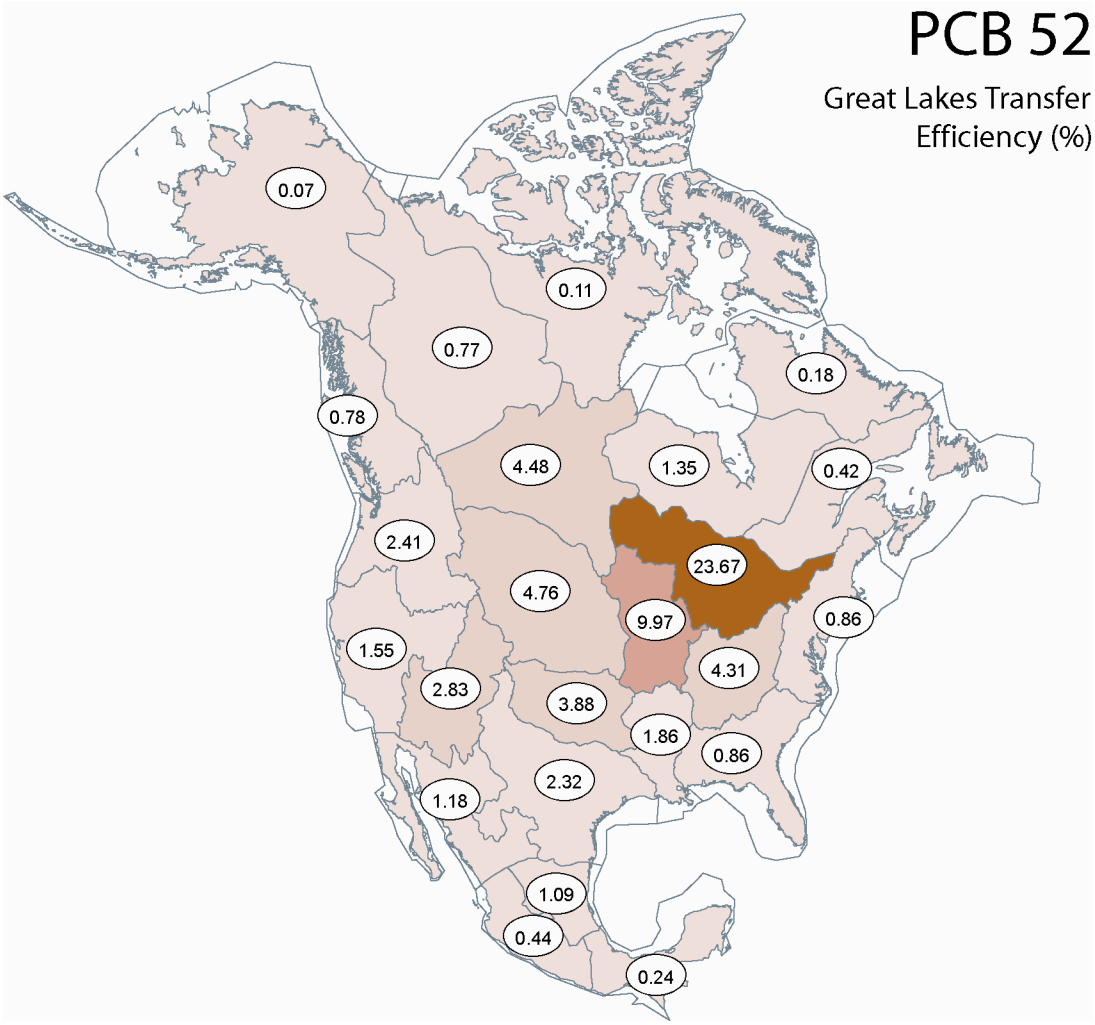

Figure 4.3.2. Great Lakes Transfer Efficiency of PCB 52 for emissions to air in each of the 24 regions of the BETR North America model.

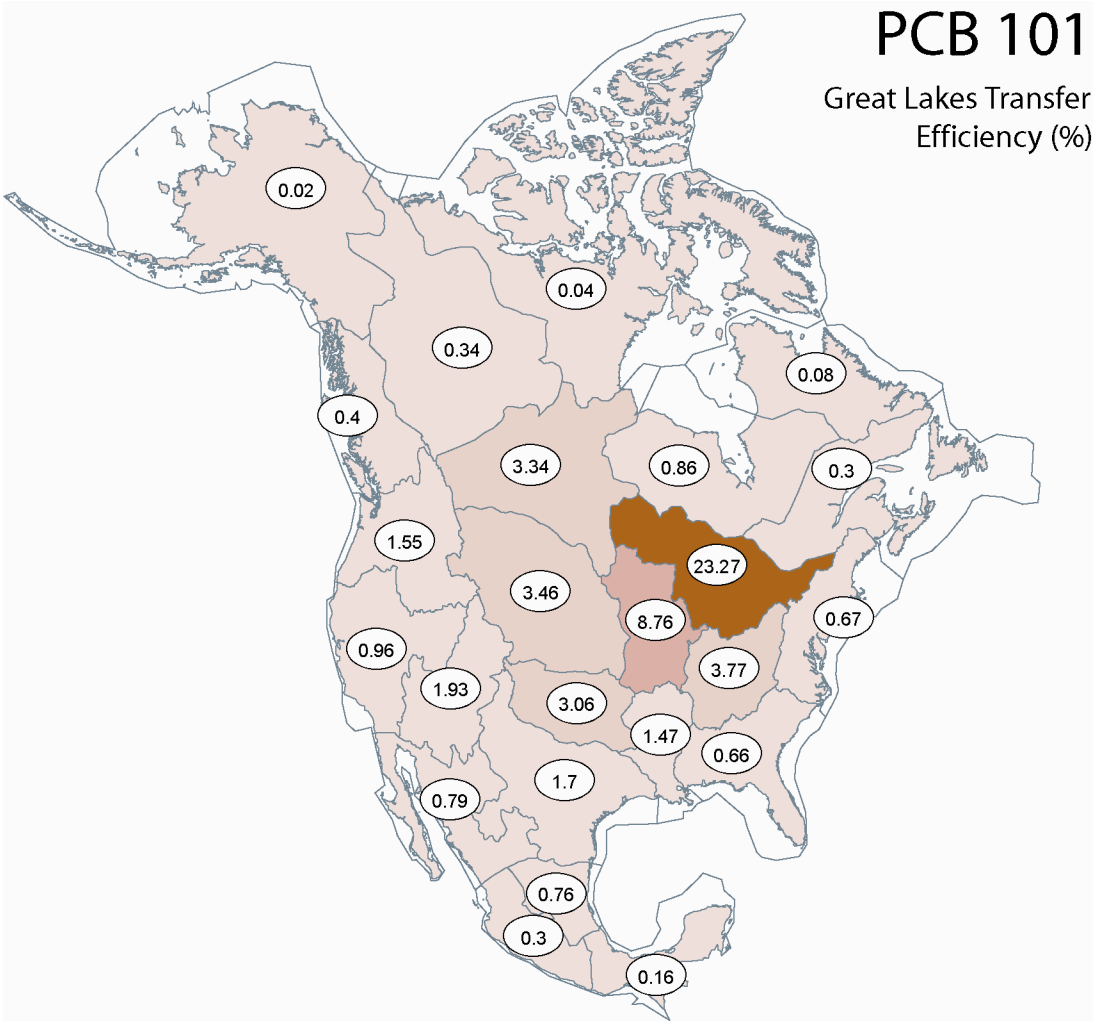

Figure 4.3.3. Great Lakes Transfer Efficiency of PCB 101 for emissions to air in each of the 24 regions of the BETR North America model.

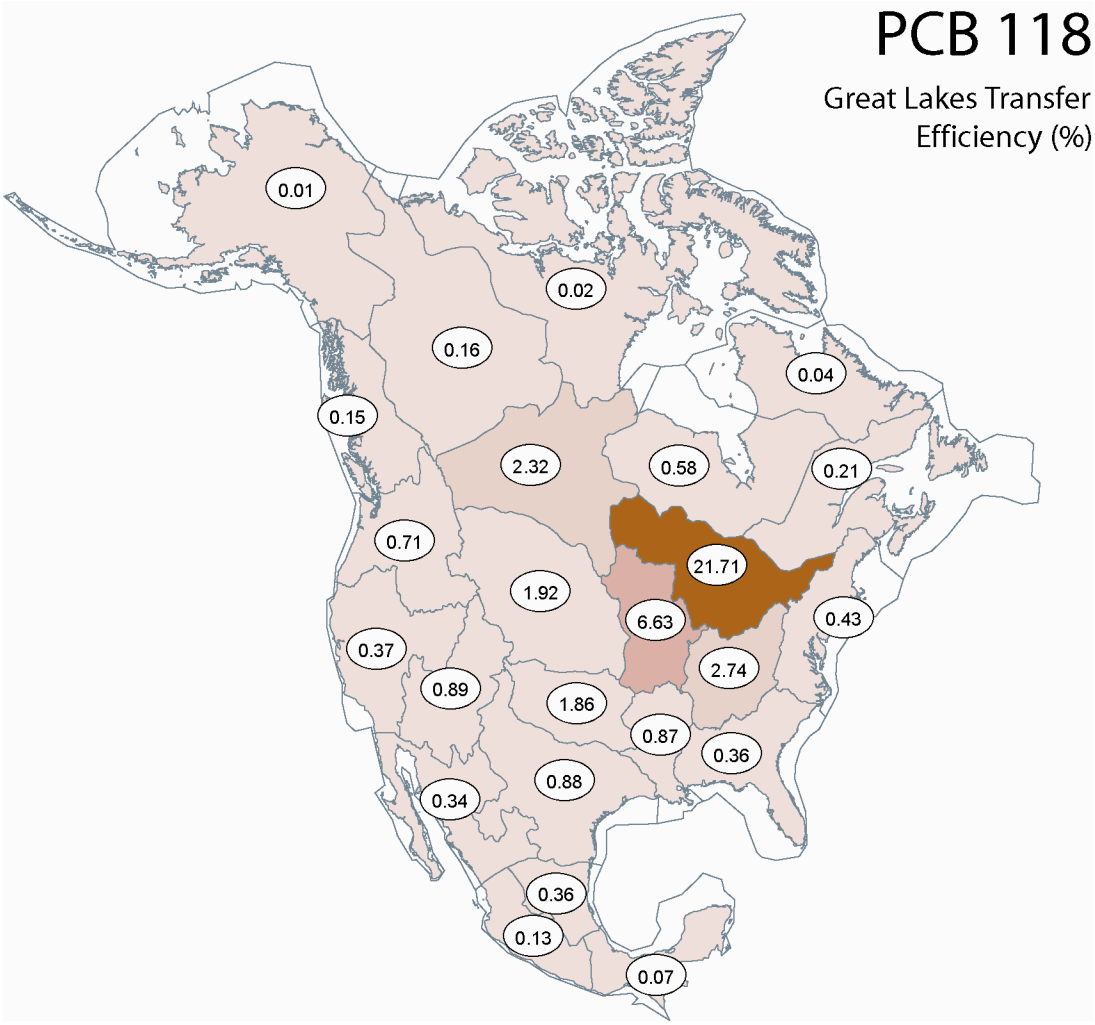

Figure 4.3.4. Great Lakes Transfer Efficiency of PCB 118 for emissions to air in each of the 24 regions of the BETR North America model.

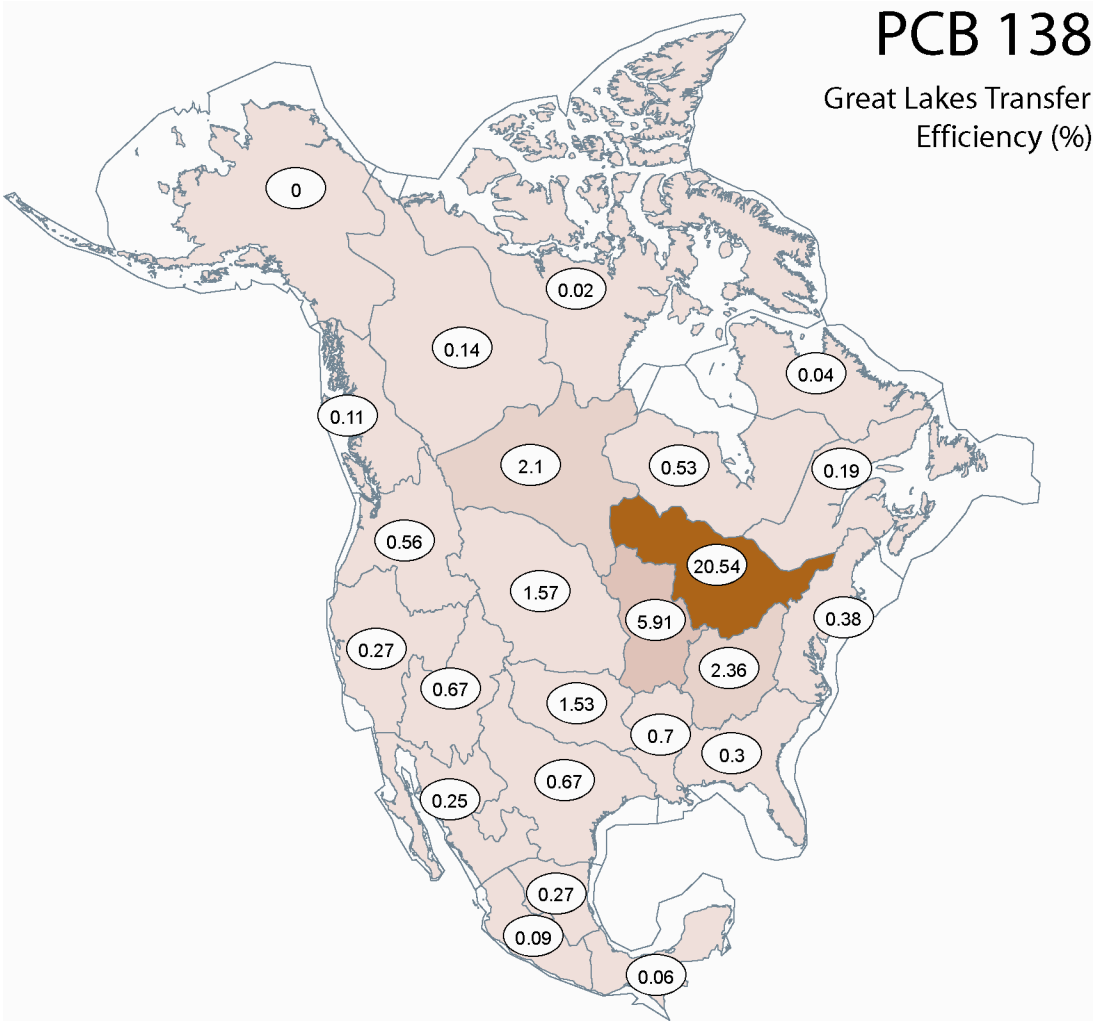

Figure 4.3.5. Great Lakes Transfer Efficiency of PCB 138 for emissions to air in each of the 24 regions of the BETR North America model.

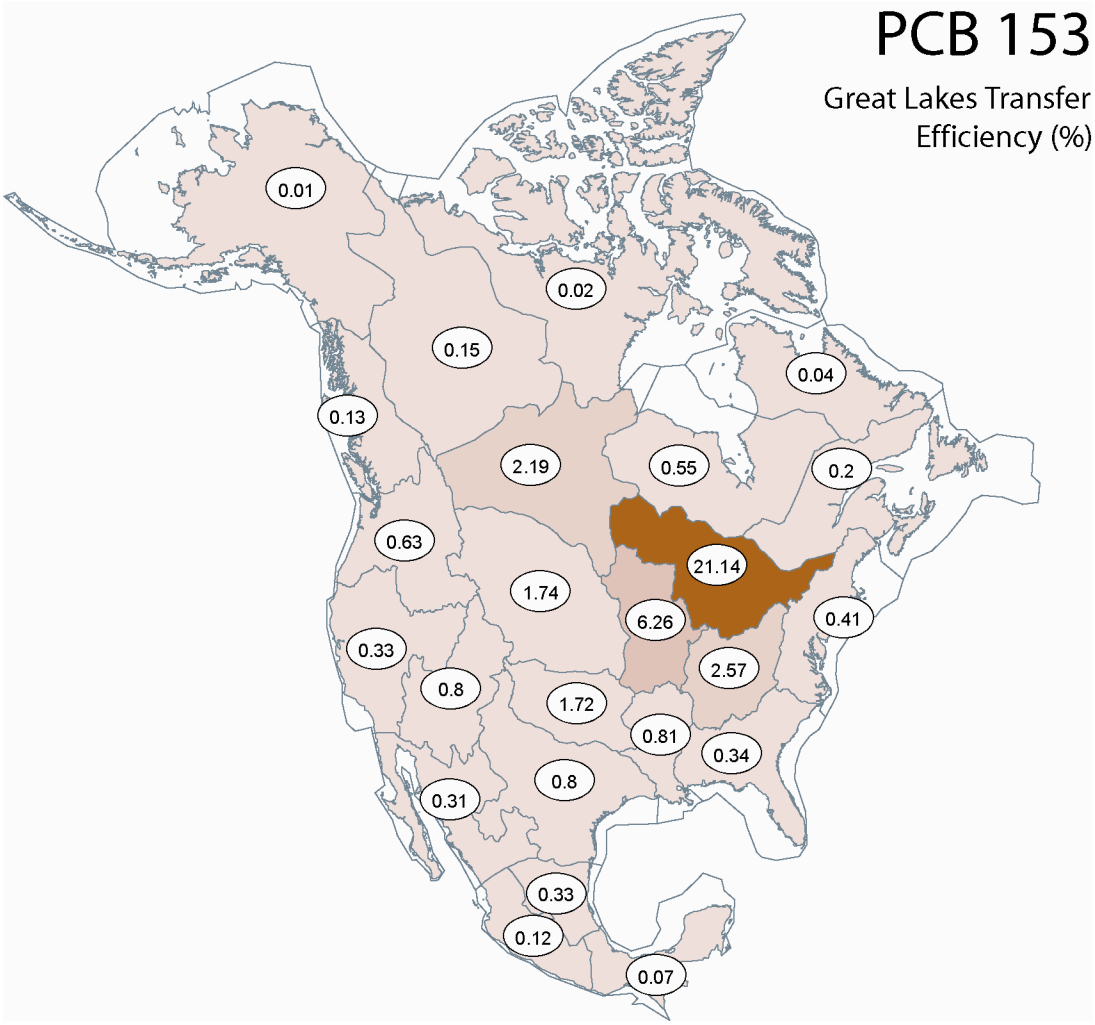

Figure 4.3.6. Great Lakes Transfer Efficiency of PCB 153 for emissions to air in each of the 24 regions of the BETR North America model.

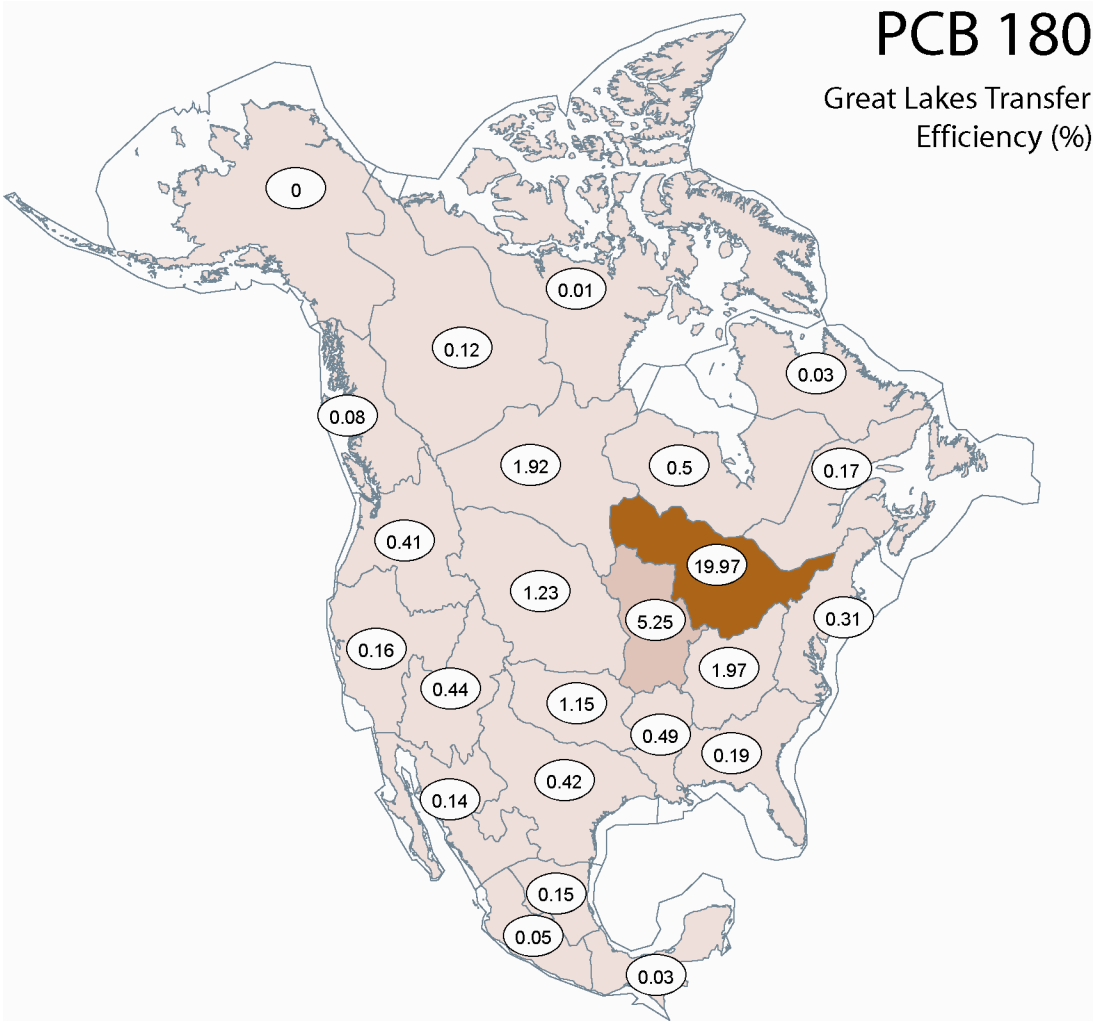

Figure 4.3.7. Great Lakes Transfer Efficiency of PCB 180 for emissions to air in each of the 24 regions of the BETR North America model.

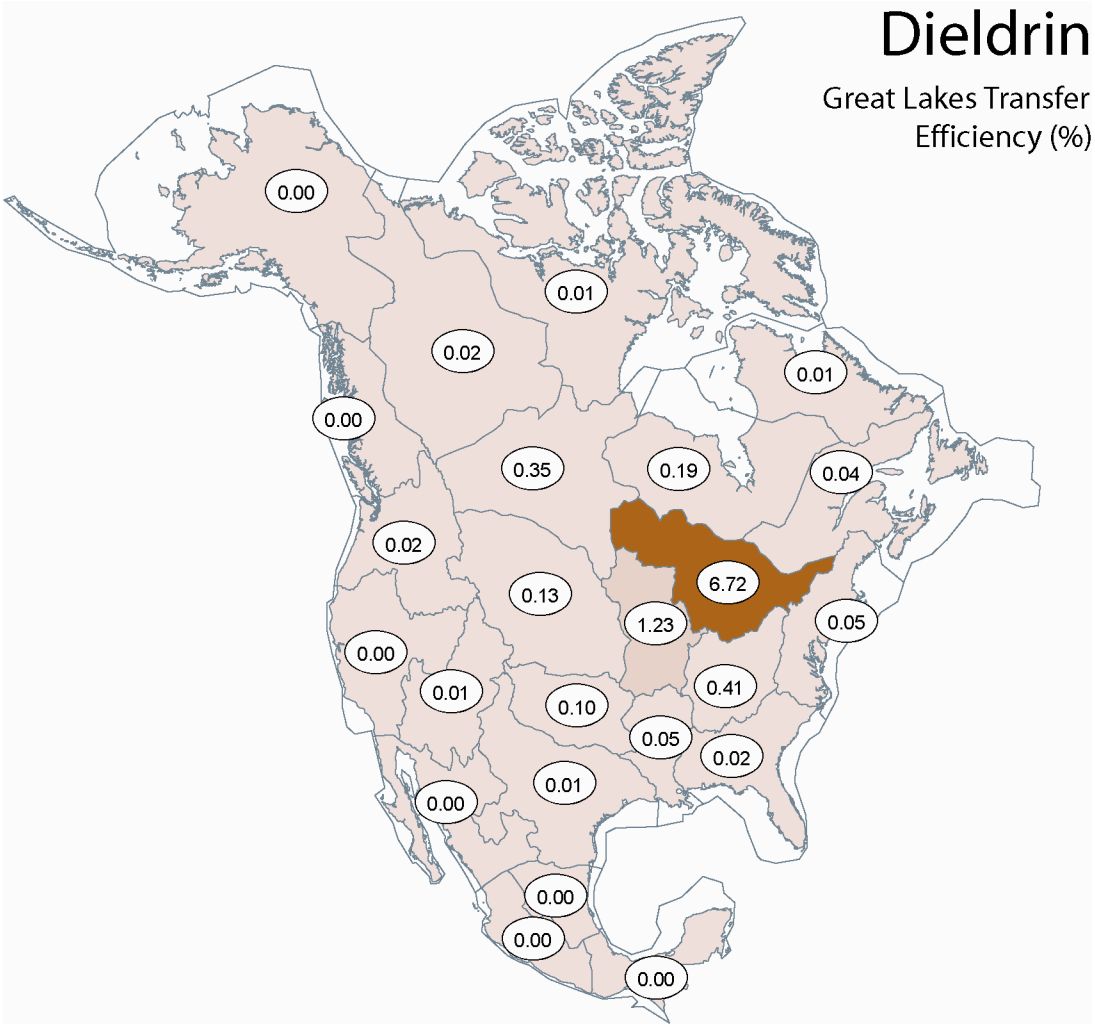

Figure 4.3.8. Great Lakes Transfer Efficiency of Dieldrin for emissions to air in each of the 24 regions of the BETR North America model.

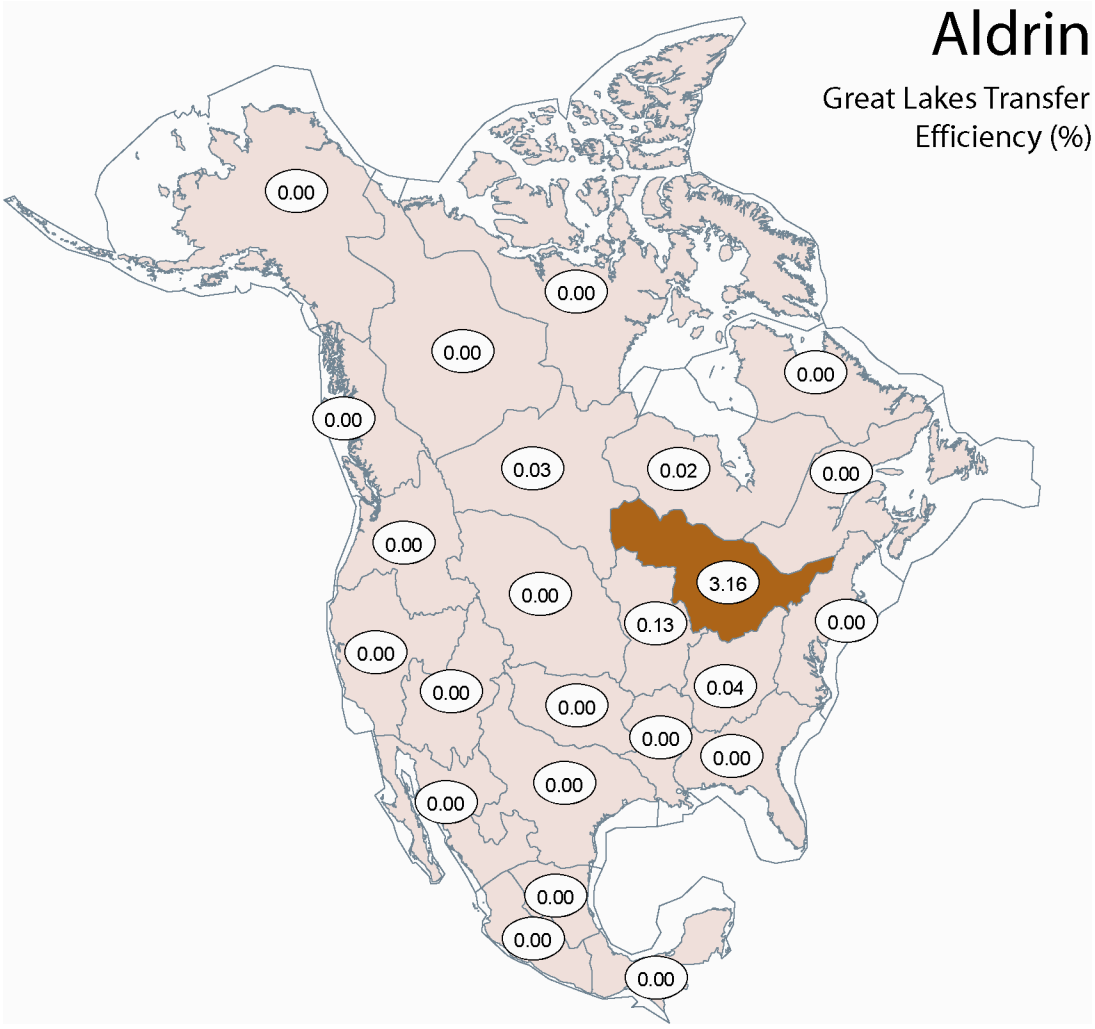

Figure 4.3.9. Great Lakes Transfer Efficiency of Aldrin for emissions to air in each of the 24 regions of the BETR North America model.

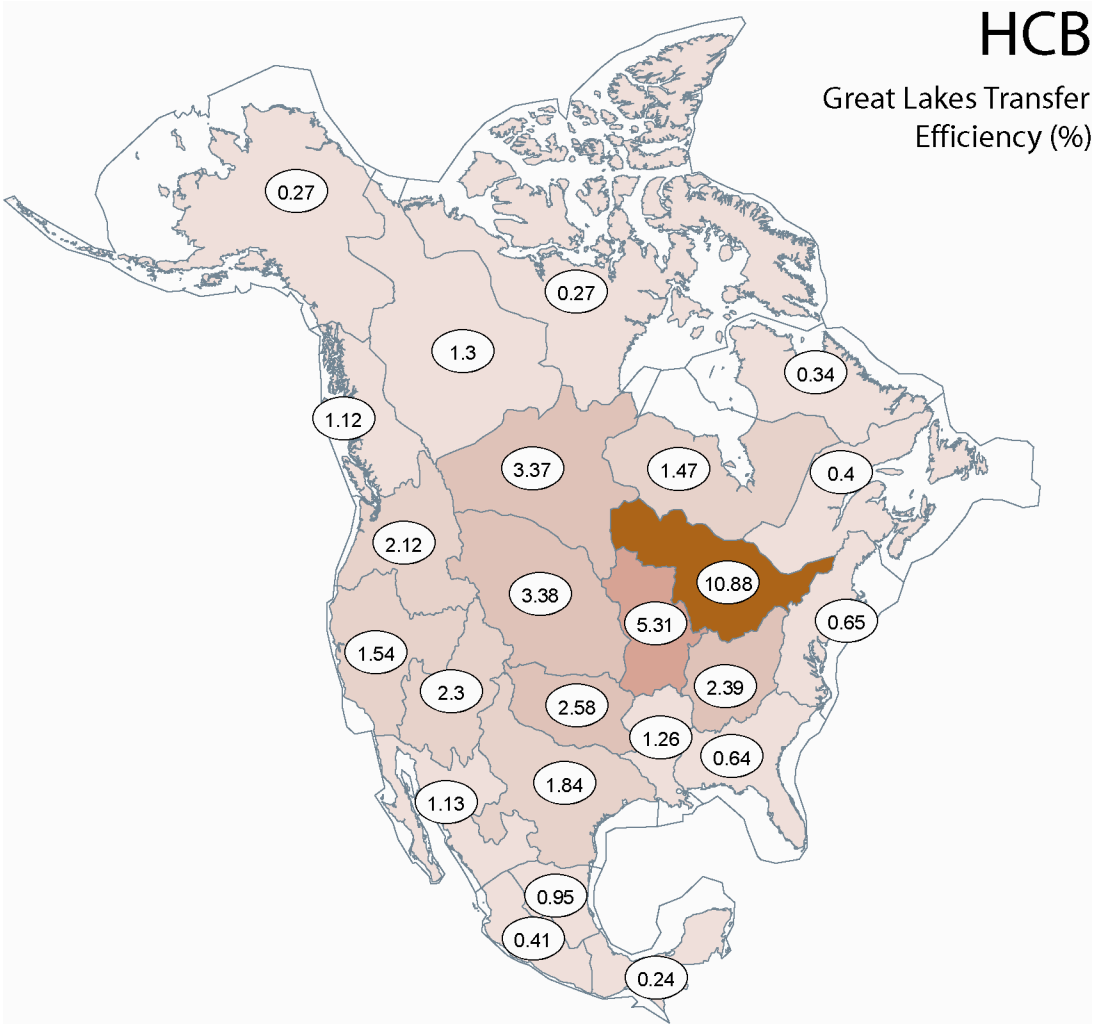

Figure 4.3.10. Great Lakes Transfer Efficiency of hexachlorobenzene (HCB) for emissions to air in each of the 24 regions of the BETR North America model.

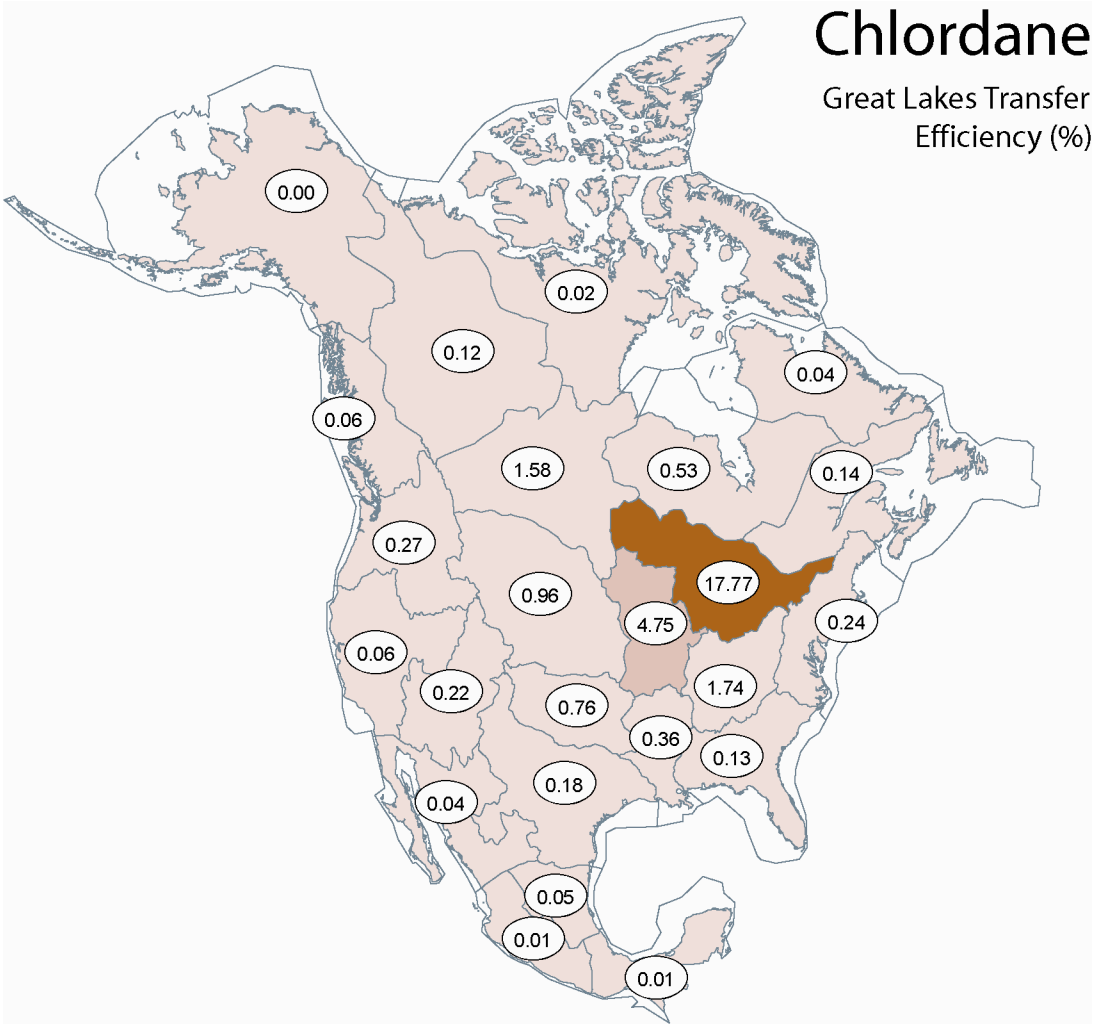

Figure 4.3.11. Great Lakes Transfer Efficiency of total chlordanes for emissions to air in each of the 24 regions of the BETR North America model.

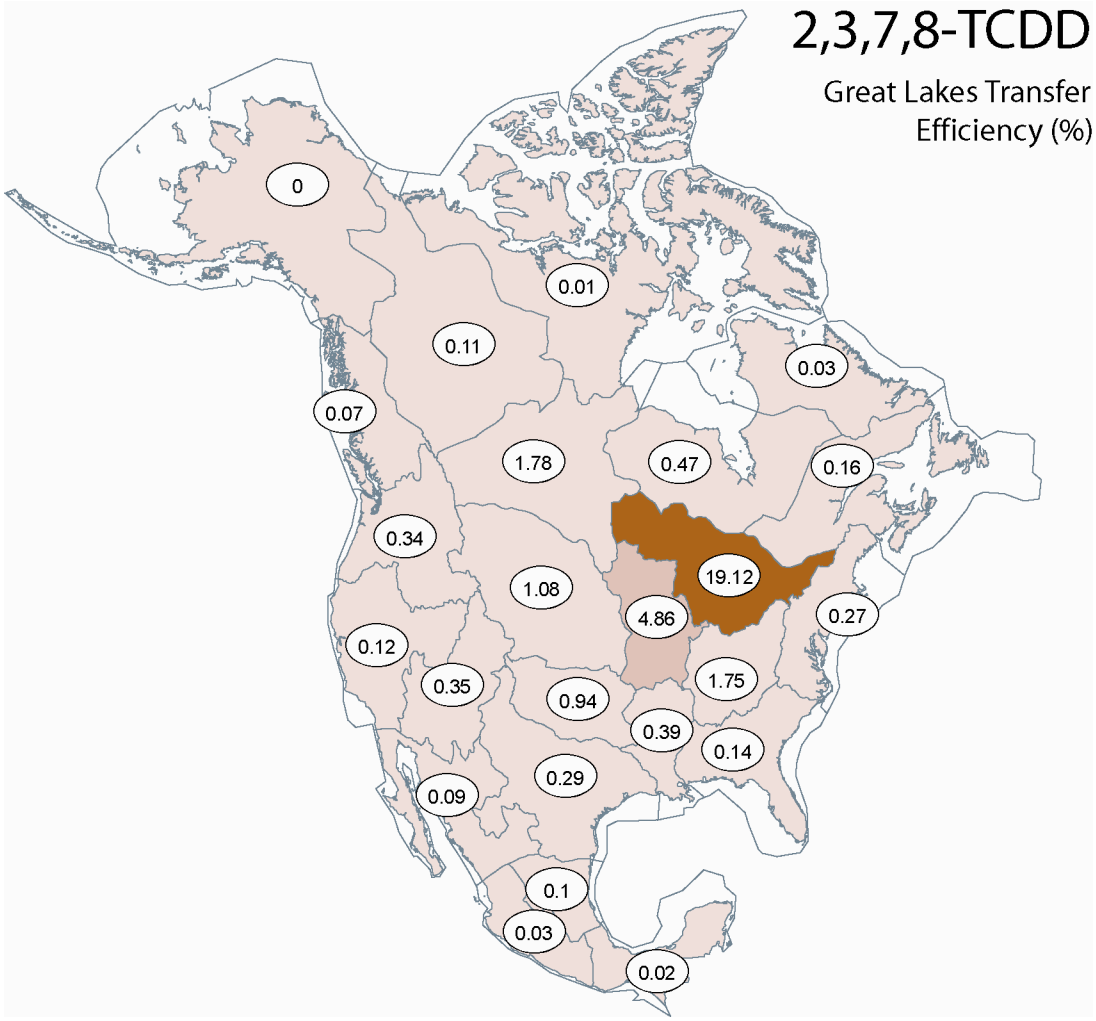

Figure 4.3.12. Great Lakes Transfer Efficiency of 2,3,7,8-tetrachlorodibenzodioxin for emissions to air in each of the 24 regions of the BETR North America model.

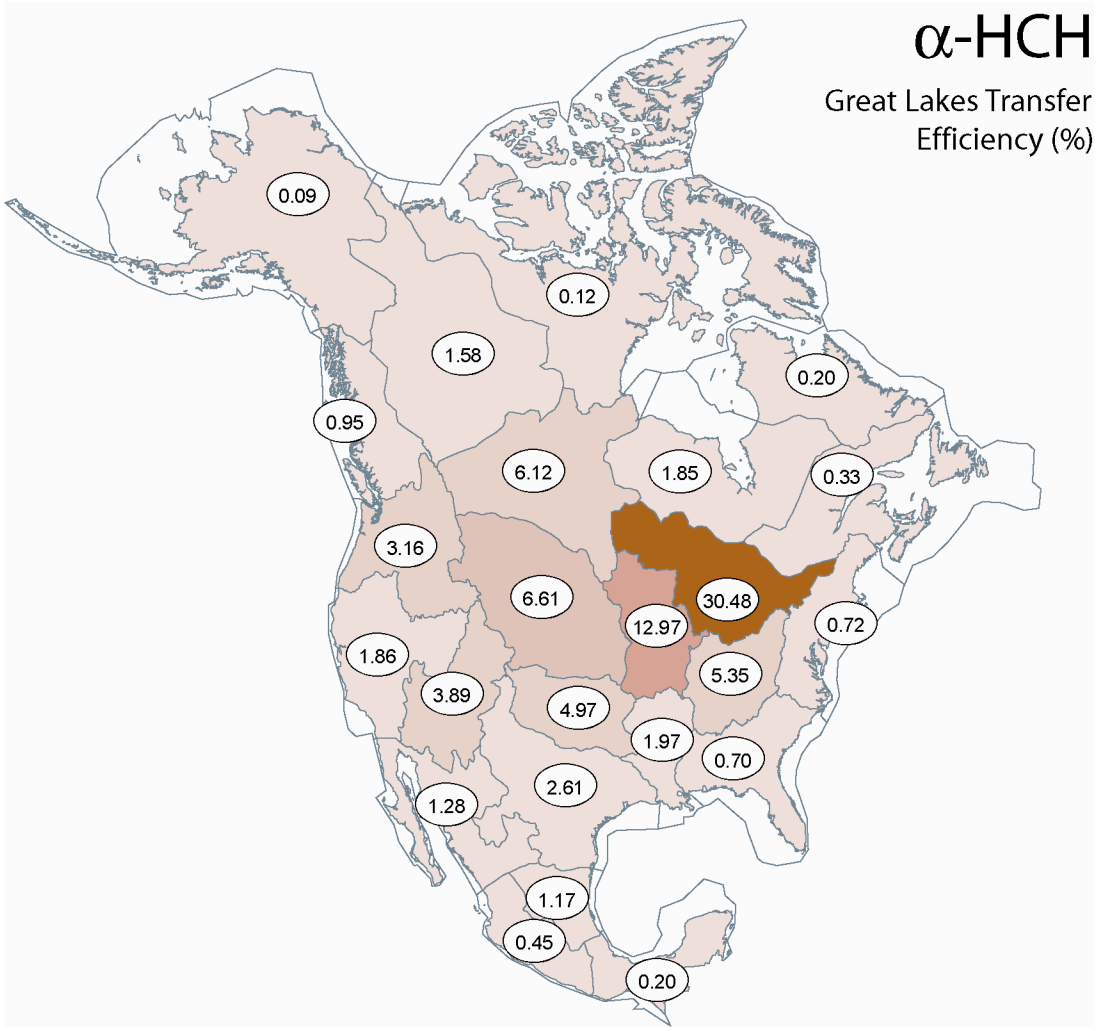

Figure 4.3.13. Great Lakes Transfer Efficiency of α-hexachlorocyclohexane (α-HCH) for emissions to air in each of the 24 regions of the BETR North America model.

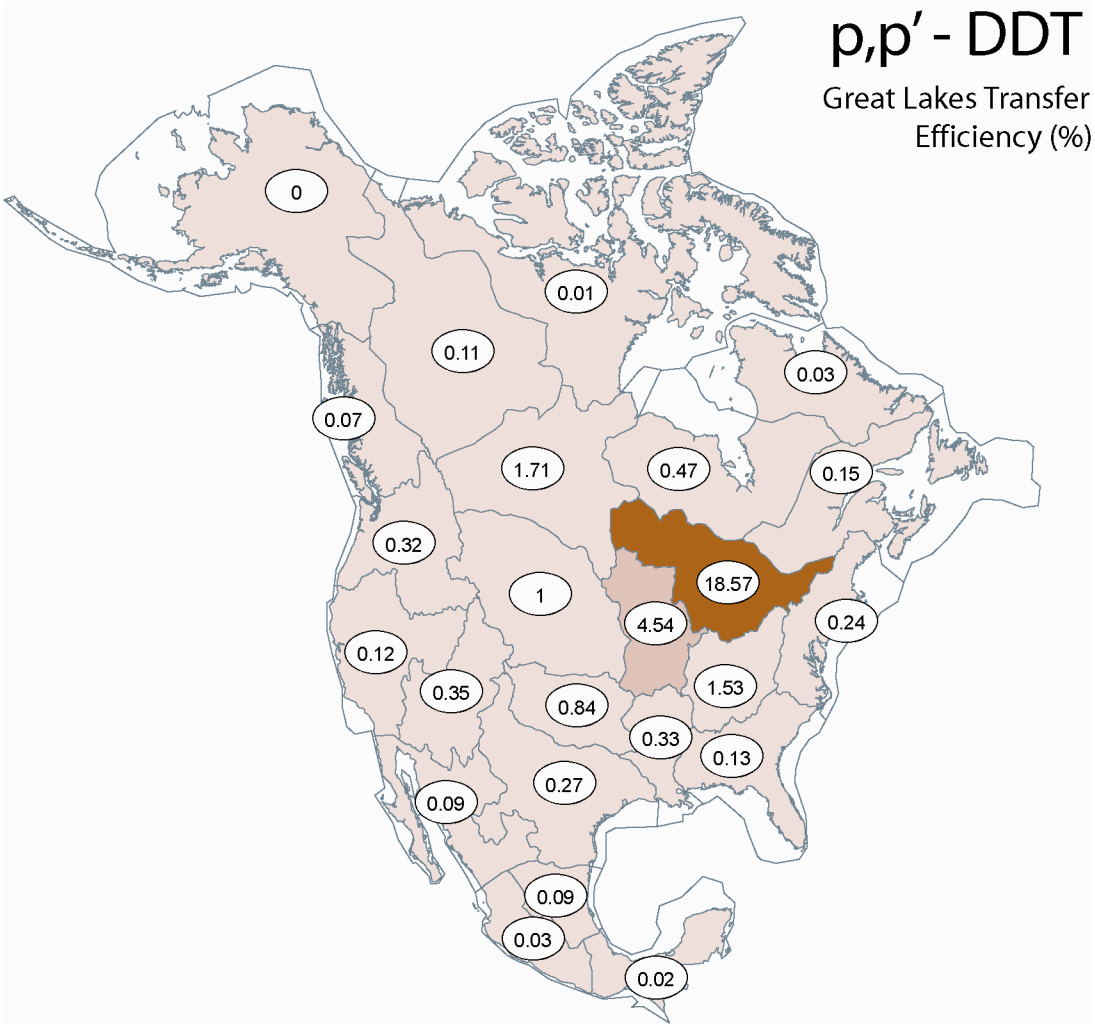

Figure 4.3.14. Great Lakes Transfer Efficiency of *p,p*'-DDT for emissions to air in each of the 24 regions of the BETR North America model.

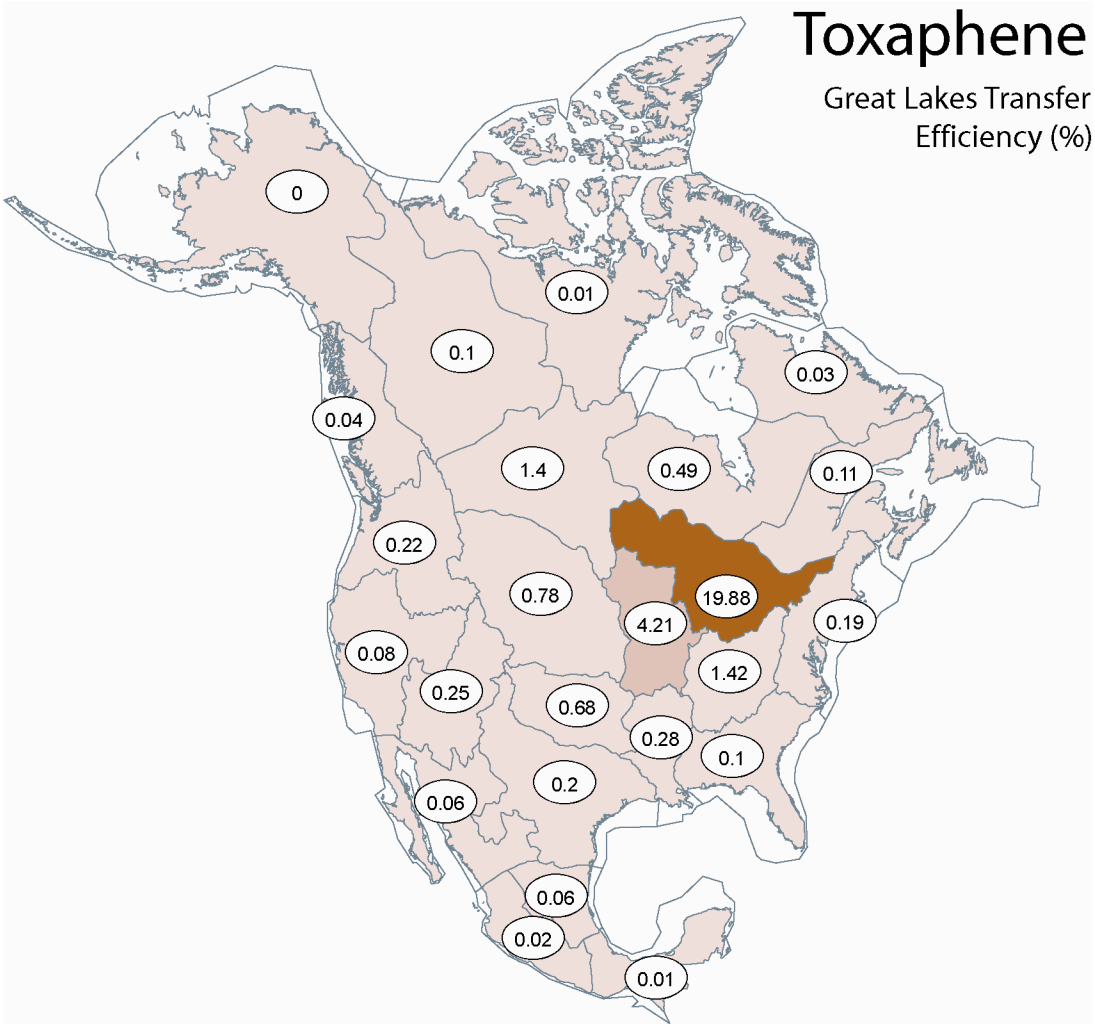

Figure 4.3.15. Great Lakes Transfer Efficiency of toxaphene for emissions to air in each of the 24 regions of the BETR North America model.

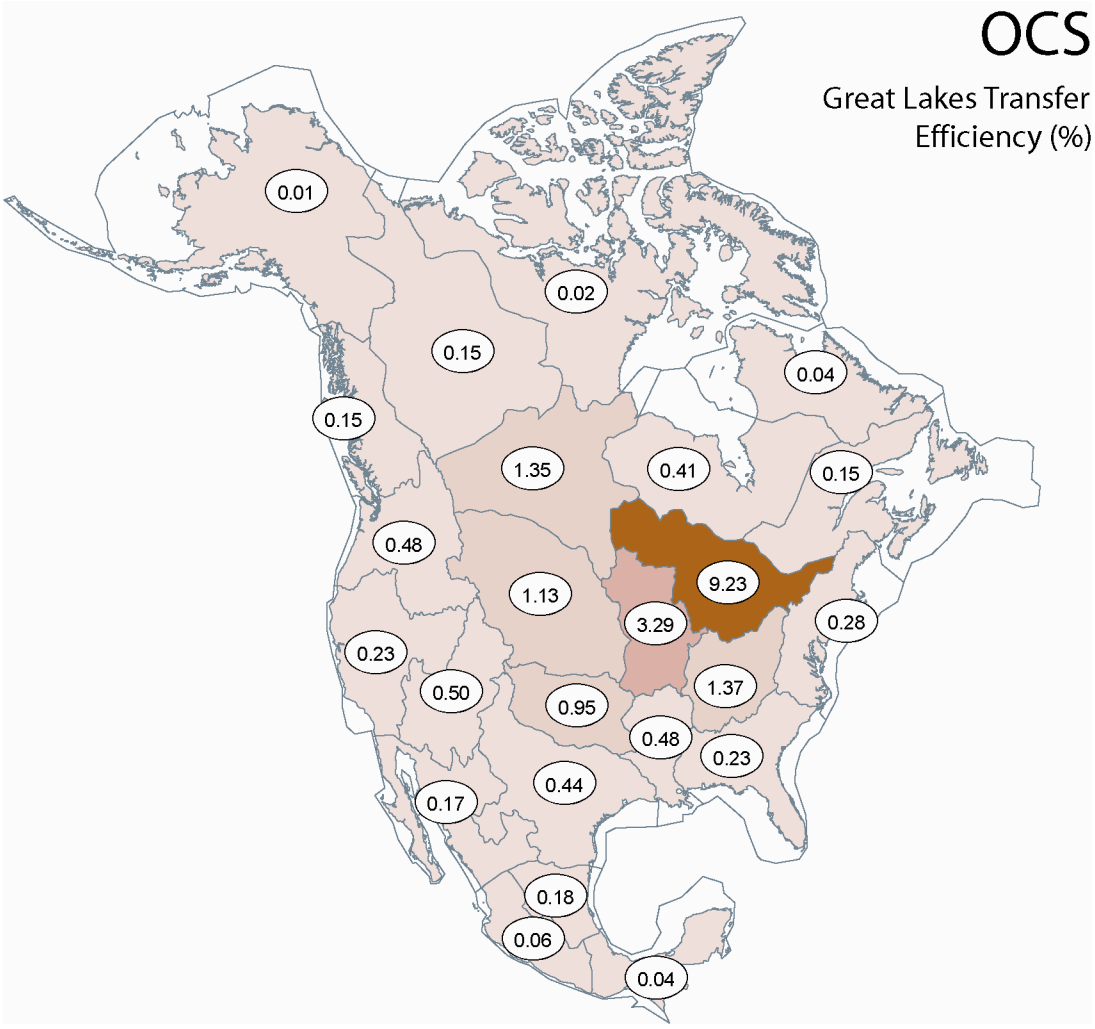

Figure 4.3.16. Great Lakes Transfer Efficiency of octachlorostyrene (OCS) for emissions to air in each of the 24 regions of the BETR North America model.

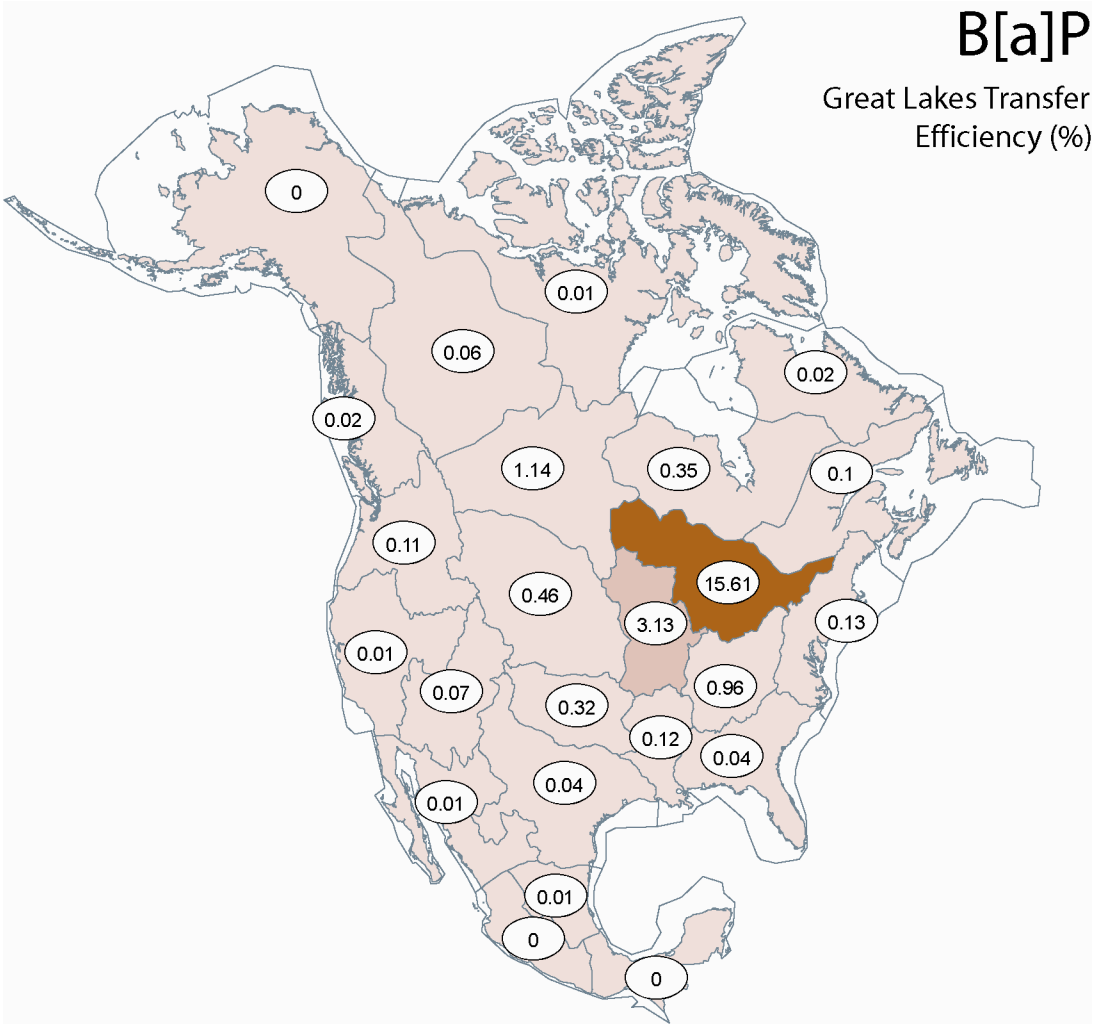

Figure 4.3.17. Great Lakes Transfer Efficiency of benzo[a]pyrene (B[a]P) for emissions to air in each of the 24 regions of the BETR North America model.

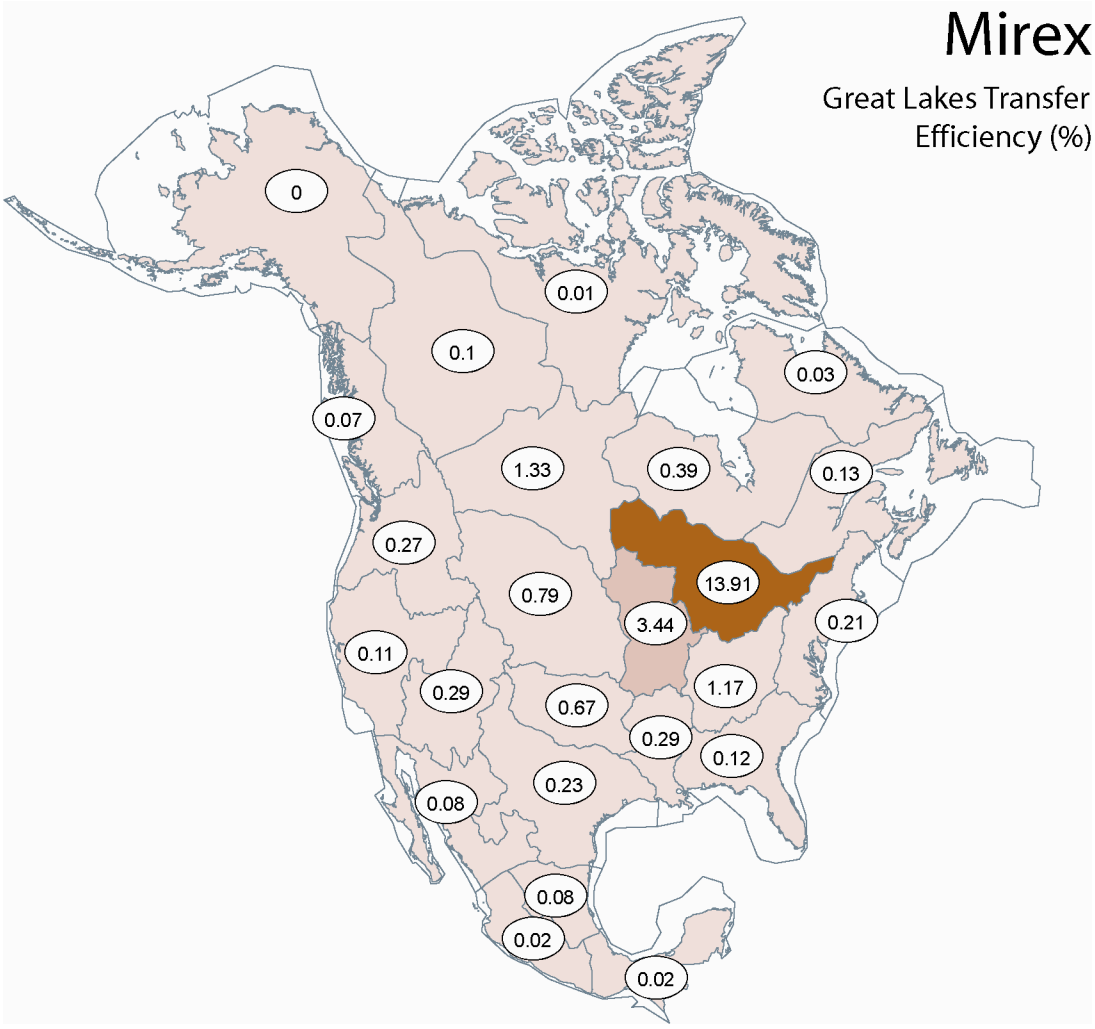

Figure 4.3.18. Great Lakes Transfer Efficiency of Mirex for emissions to air in each of the 24 regions of the BETR North America model.

The model results shown in Figures 4.3.1 – 4.3.18 build upon the generic model results illustrated by the hazard identification plots, in particular Figure 4.2.2. Great Lakes transfer efficiencies for Aldrin, Dieldrin and B[a]P decline relatively sharply with increasing distance of the source region from the Great Lakes basin. The less chlorinated PCBs are more efficiently transported and deposited over continental scales than the higher chlorinated congeners.

It is interesting to compare HCB and PCB 28. These two substances have similar GLTE from regions on the west coast of North America to the Great Lakes, but the transfer efficiency for PCB 28 emitted to air in the Great Lakes Basin region is approximately a factor of 2 higher than that for HCB. The decline in GLTE with distance for HCB is more gradual than for any other substance. These results suggest that HCB is transported over large distances, but is not particularly well suited to deposition into the Great Lakes system, when compared to PCB 28.

In contrast, α-HCH has the highest transfer efficiency for emissions in the Great Lakes Basin, as a consequence of its partitioning properties (see Figure 4.1.1). Although it is less persistent than many of the other Level I substances, it also demonstrates a relatively shallow decline in transfer efficiency with increasing distance from the target region.

4.4 Global Great Lakes Transfer Efficiency of Level I Substances

Figures 4.4.1 – 4.4.18 present Great Lakes transfer efficiency for each of the Level I substances for emissions to air in each region of the BETR Global Model. Color shading and scaling of GLTE is consistent for all figures to allow direct visual comparisons.

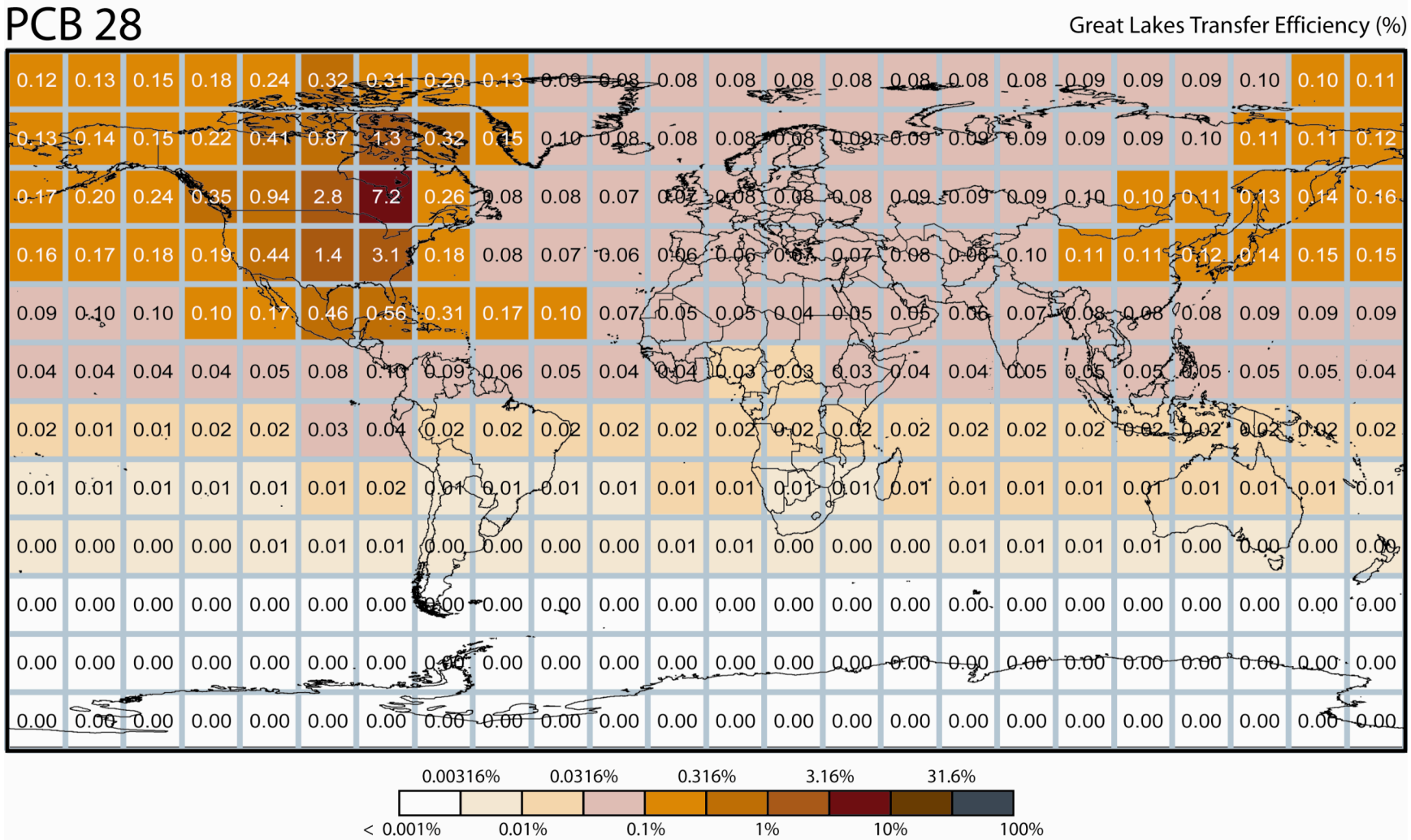

Figure 4.4.1. Great Lakes Transfer Efficiency of PCB 28 for emissions to air in each of the 288 regions of the BETR Global model.

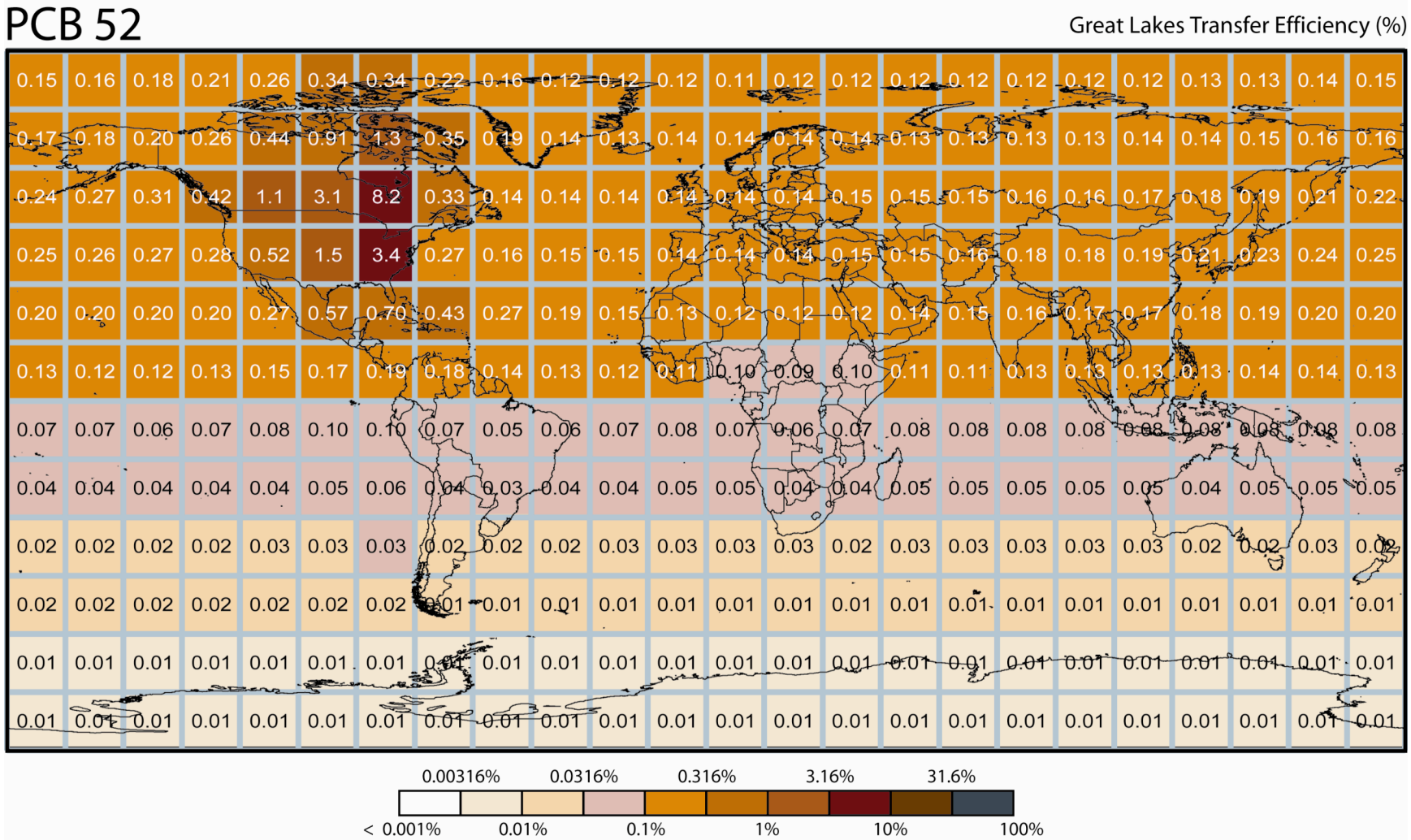

Figure 4.4.2. Great Lakes Transfer Efficiency of PCB 52 for emissions to air in each of the 288 regions of the BETR Global model.

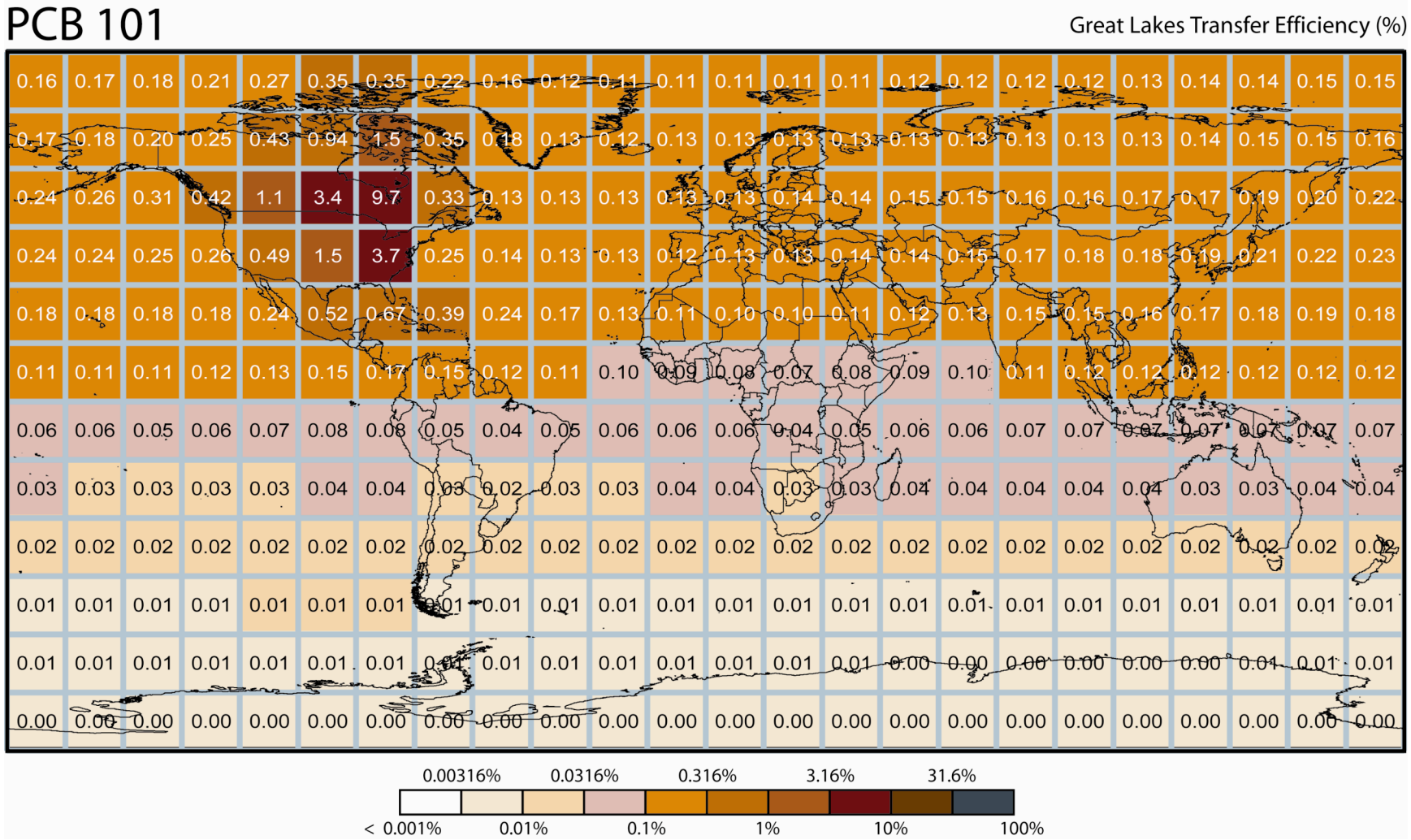

Figure 4.4.3. Great Lakes Transfer Efficiency of PCB 101 for emissions to air in each of the 288 regions of the BETR Global model.

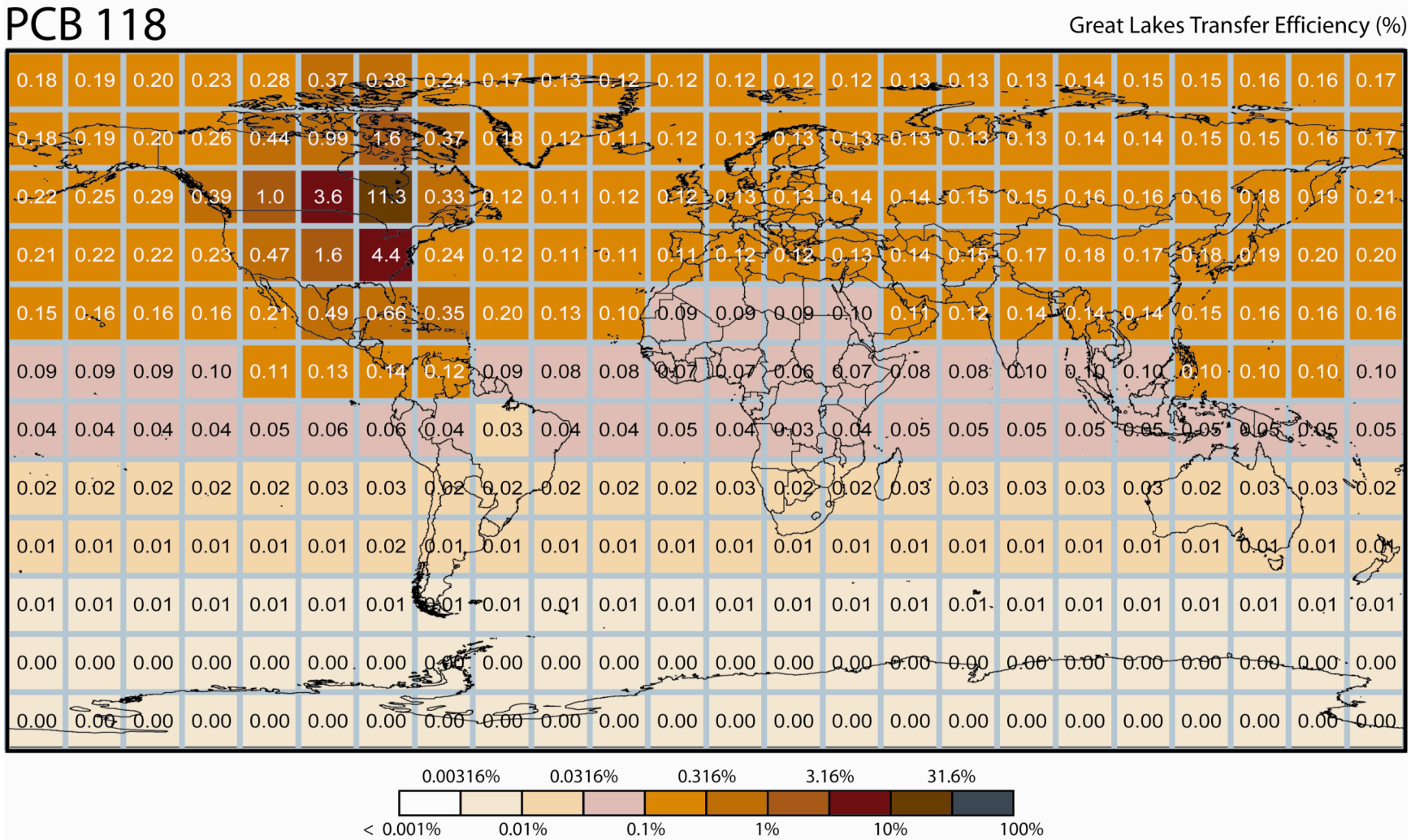

Figure 4.4.4. Great Lakes Transfer Efficiency of PCB 118 for emissions to air in each of the 288 regions of the BETR Global model.

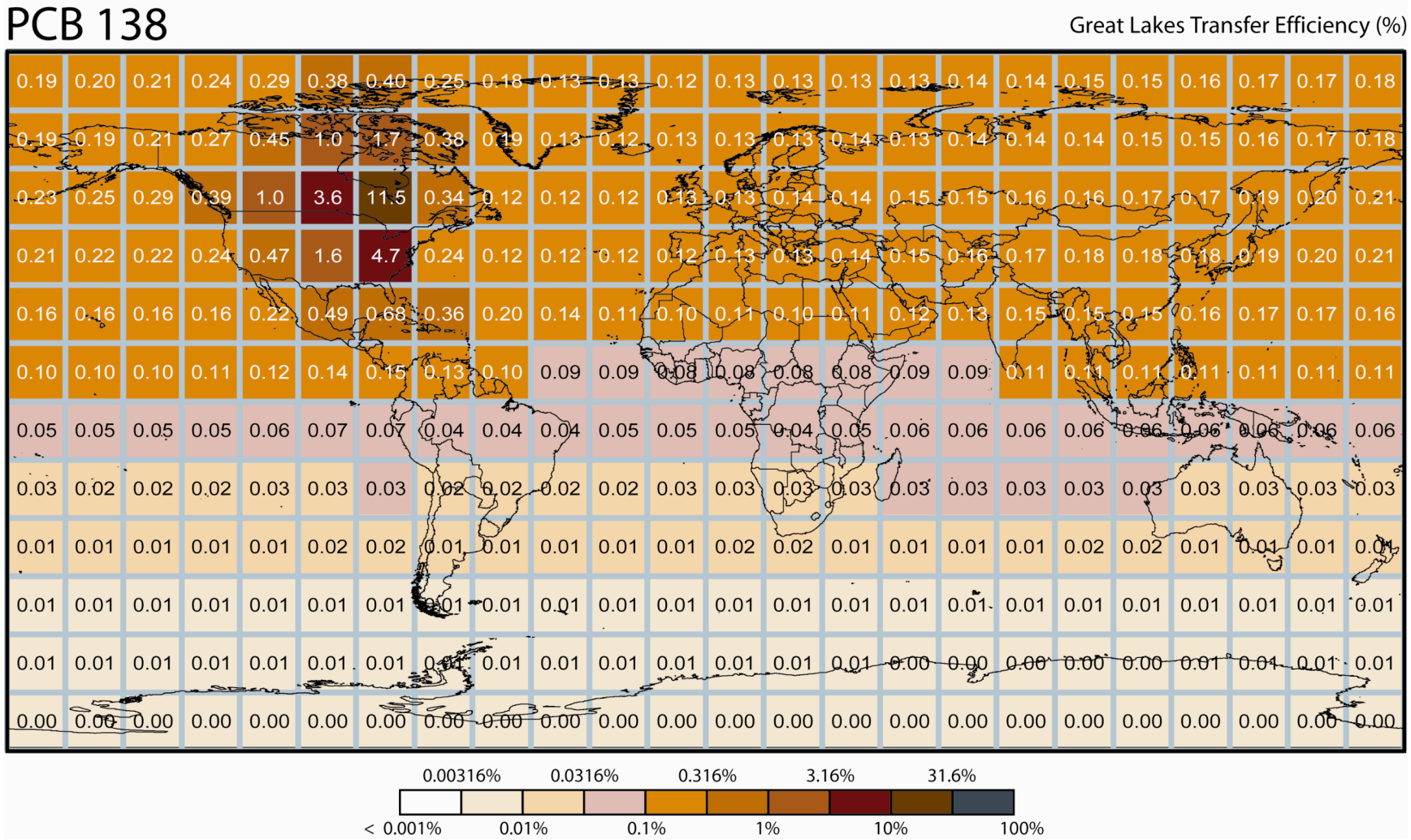

Figure 4.4.5. Great Lakes Transfer Efficiency of PCB 138 for emissions to air in each of the 288 regions of the BETR Global model.

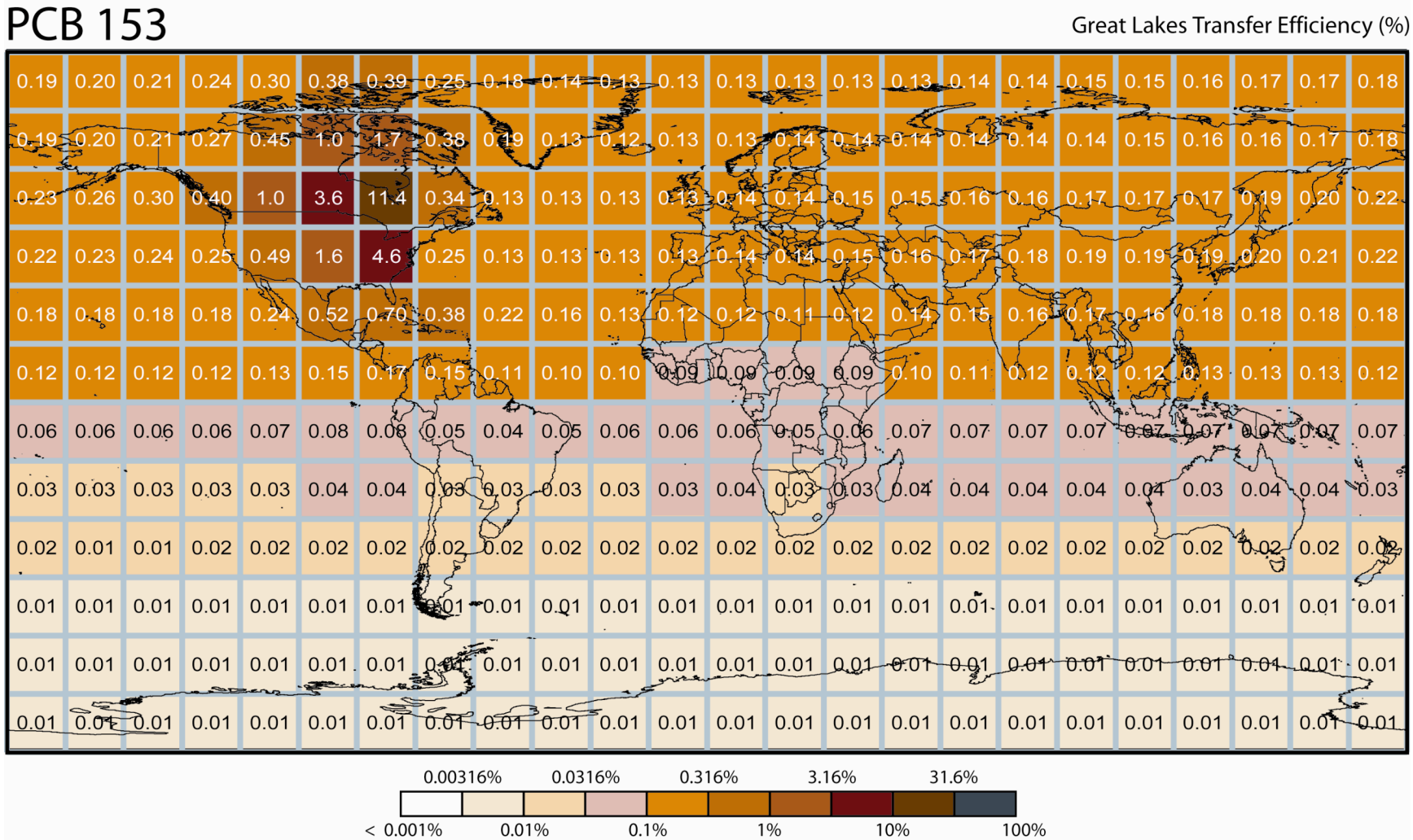

Figure 4.4.6. Great Lakes Transfer Efficiency of PCB 153 for emissions to air in each of the 288 regions of the BETR Global model.

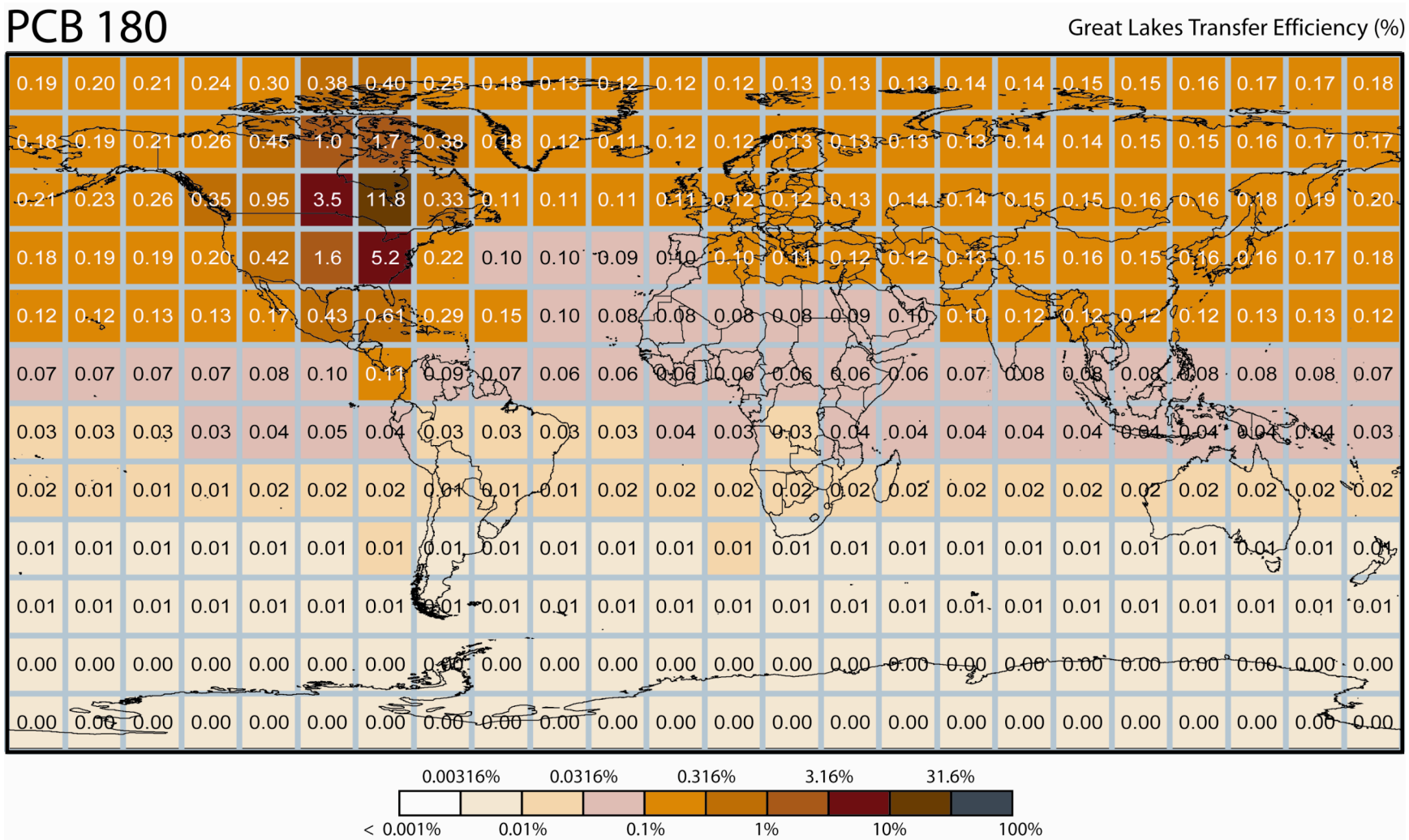

Figure 4.4.7. Great Lakes Transfer Efficiency of PCB 180 for emissions to air in each of the 288 regions of the BETR Global model.

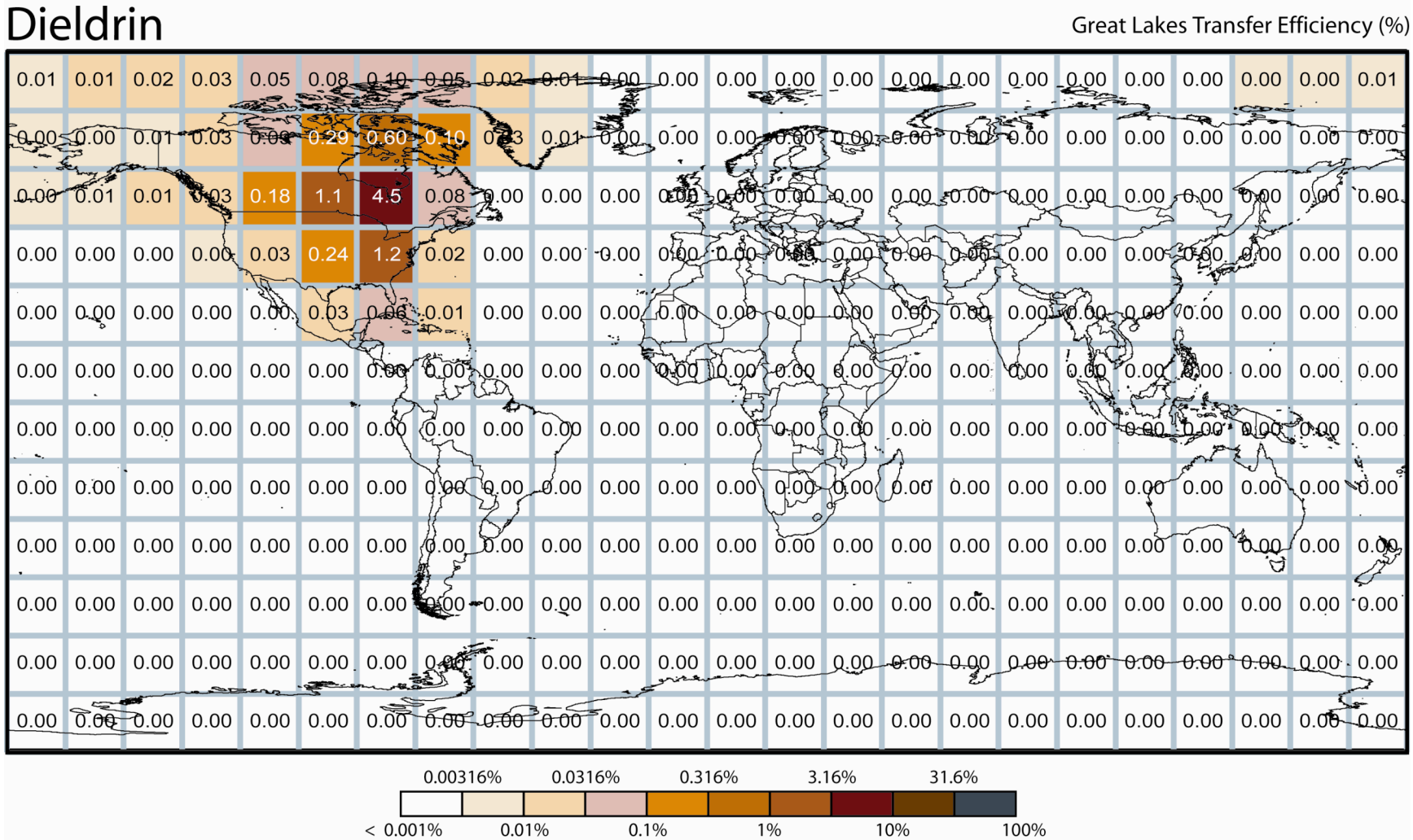

Figure 4.4.8. Great Lakes Transfer Efficiency of Dieldrin for emissions to air in each of the 288 regions of the BETR Global model.

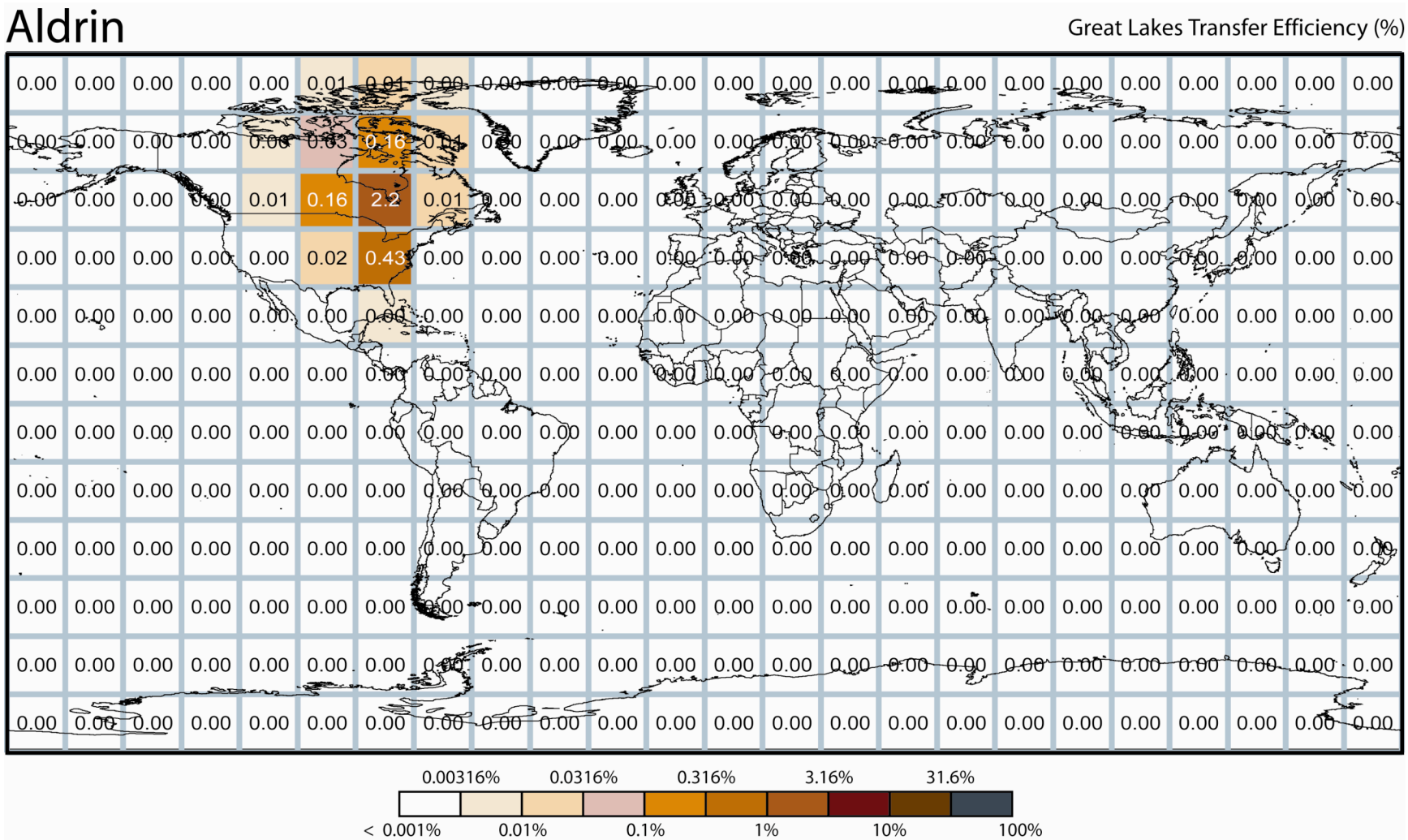

Figure 4.4.9. Great Lakes Transfer Efficiency of Aldrin for emissions to air in each of the 288 regions of the BETR Global model.

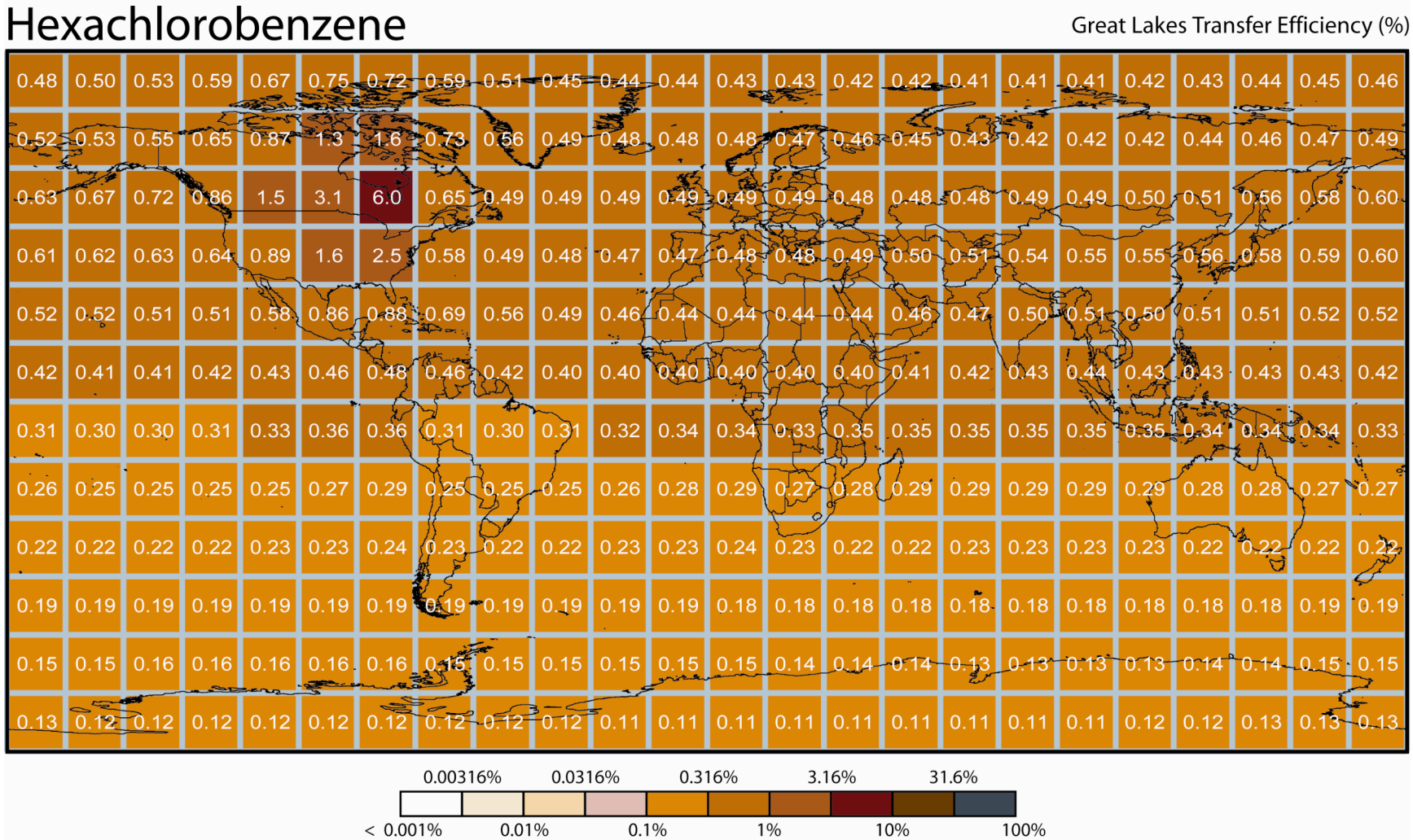

Figure 4.4.10. Great Lakes Transfer Efficiency of hexachlorobenzene for emissions to air in each of the 288 regions of the BETR Global model.

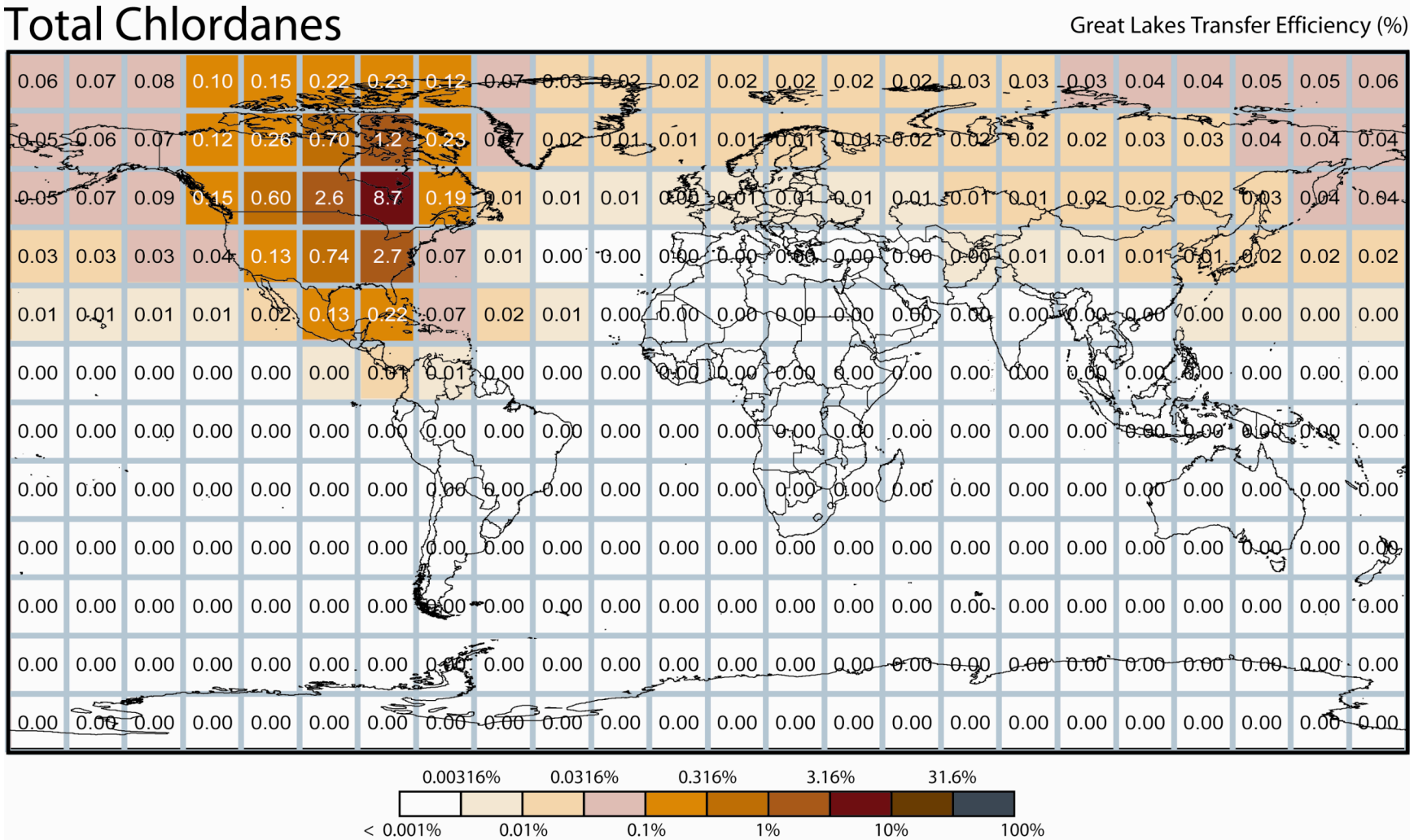

Figure 4.4.11. Great Lakes Transfer Efficiency of chlordane for emissions to air in each of the 288 regions of the BETR Global model.

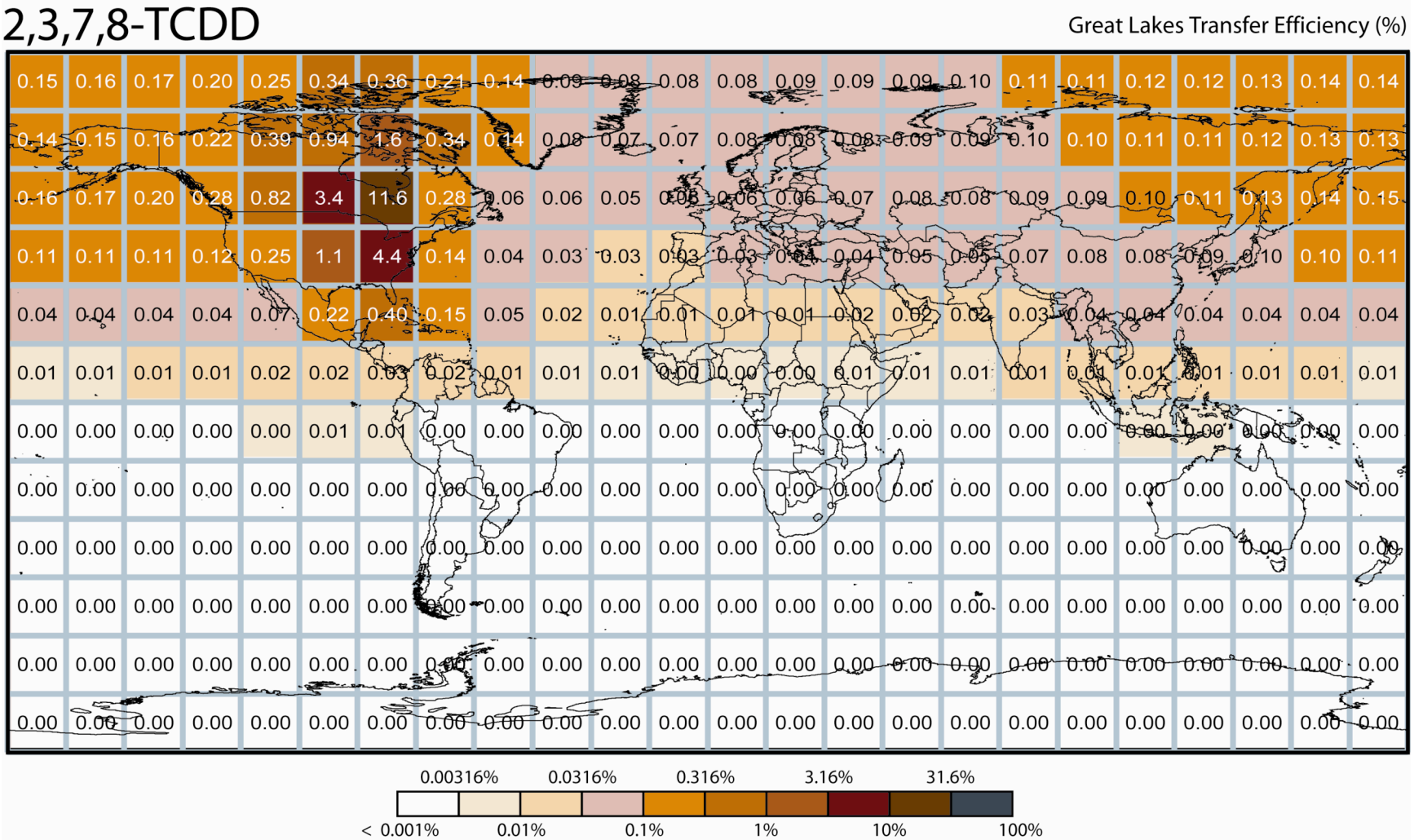

Figure 4.4.12. Great Lakes Transfer Efficiency of 2.3,7,8-tetrachlorodibenzodioxin for emissions to air in each of the 288 regions of the BETR Global model.

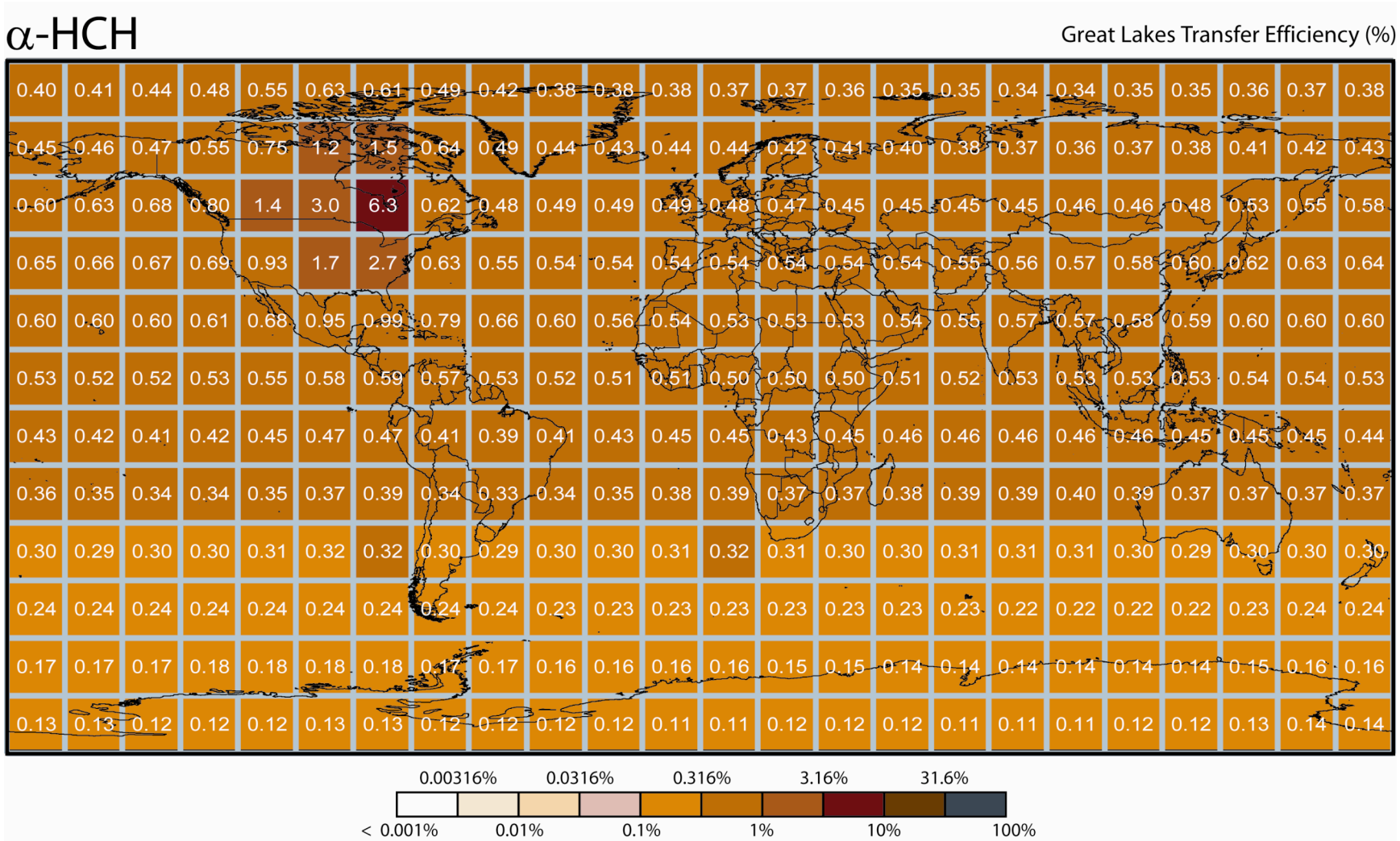

Figure 4.4.13. Great Lakes Transfer Efficiency of α-hexachlorocyclohexane for emissions to air in each of the 288 regions of the BETR Global model.

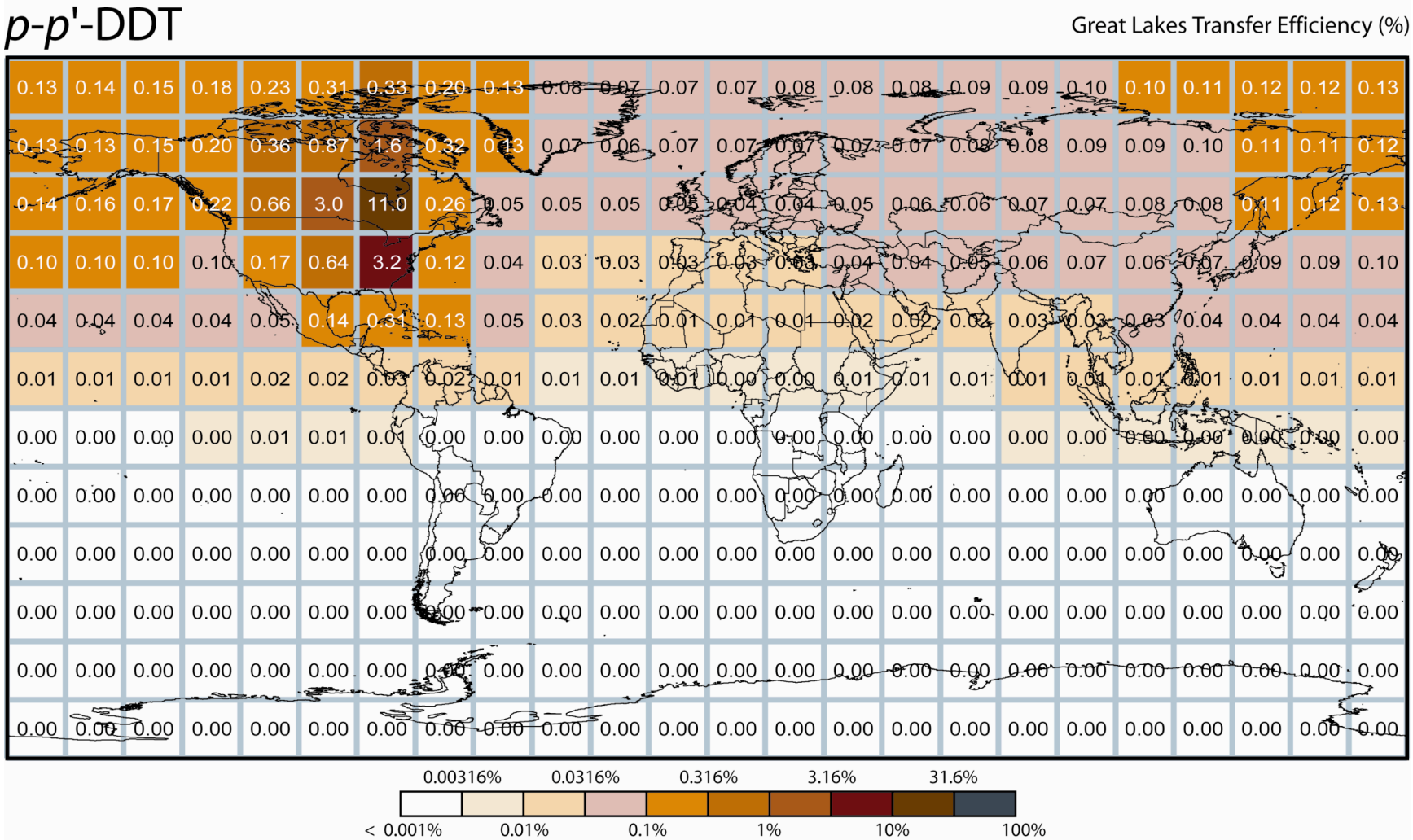

Figure 4.4.14. Great Lakes Transfer Efficiency of *p-p*'-DDT for emissions to air in each of the 288 regions of the BETR Global model.

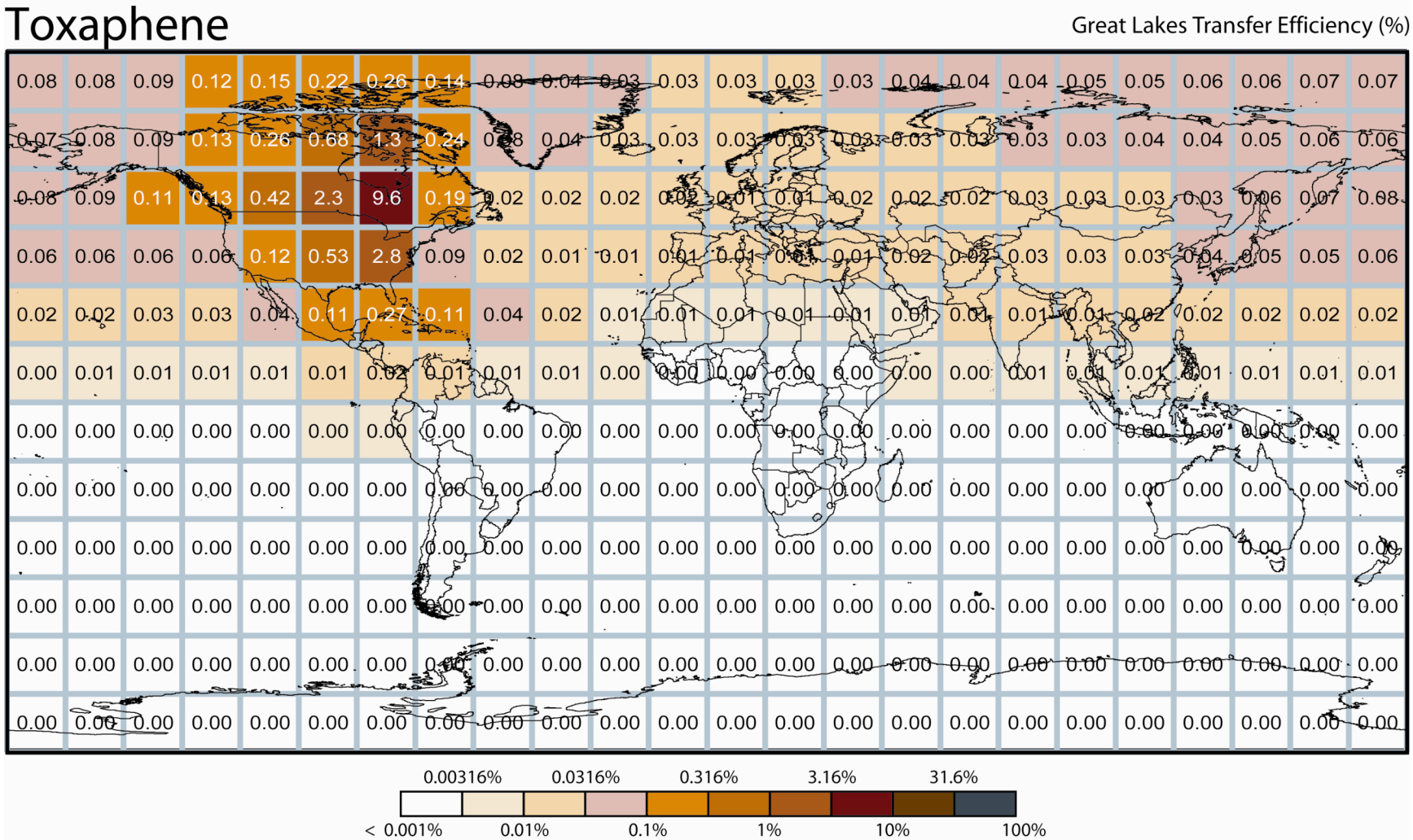

Figure 4.4.15. Great Lakes Transfer Efficiency of toxaphene for emissions to air in each of the 288 regions of the BETR Global model.

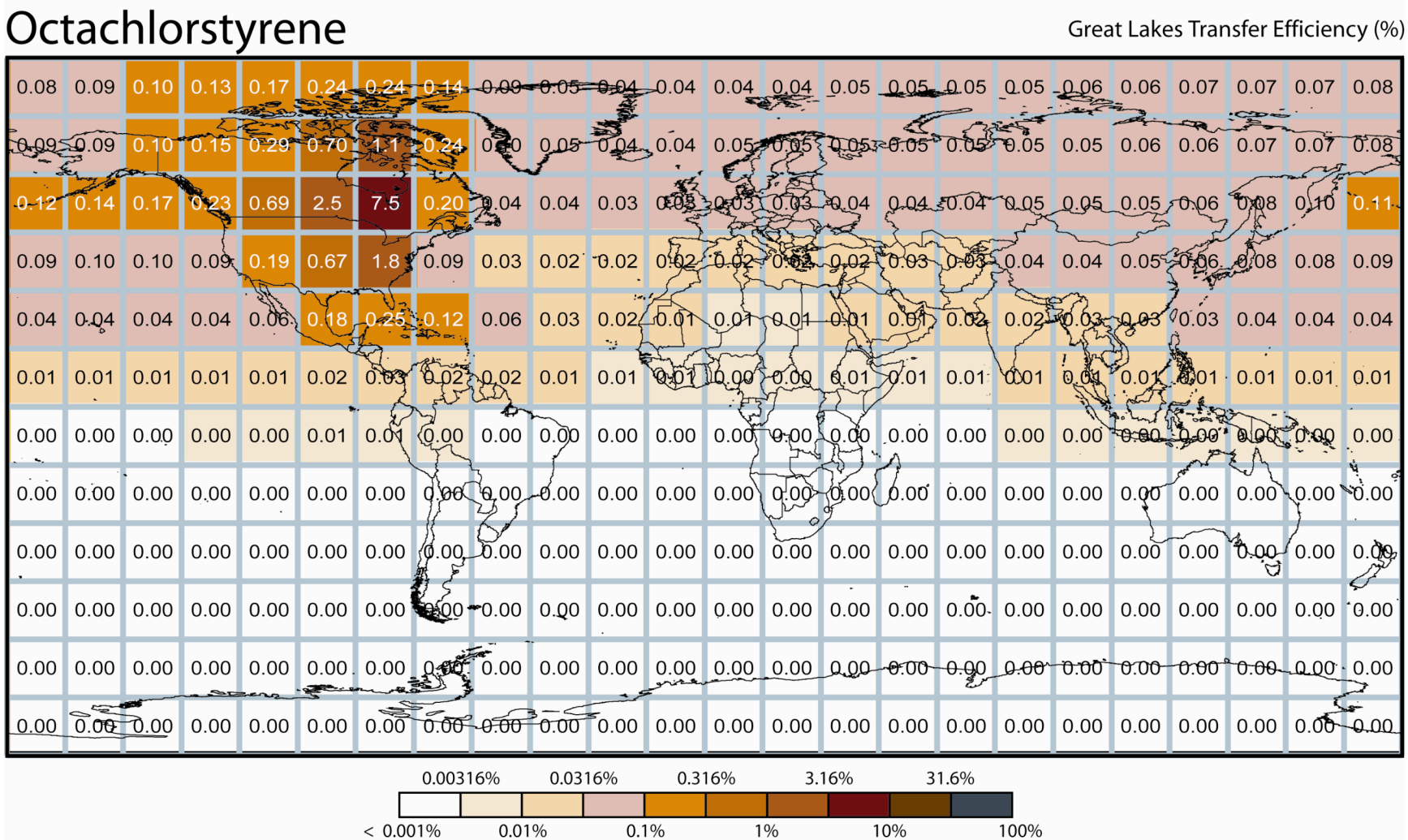

Figure 4.4.16. Great Lakes Transfer Efficiency of octachlorostyrene for emissions to air in each of the 288 regions of the BETR Global model.

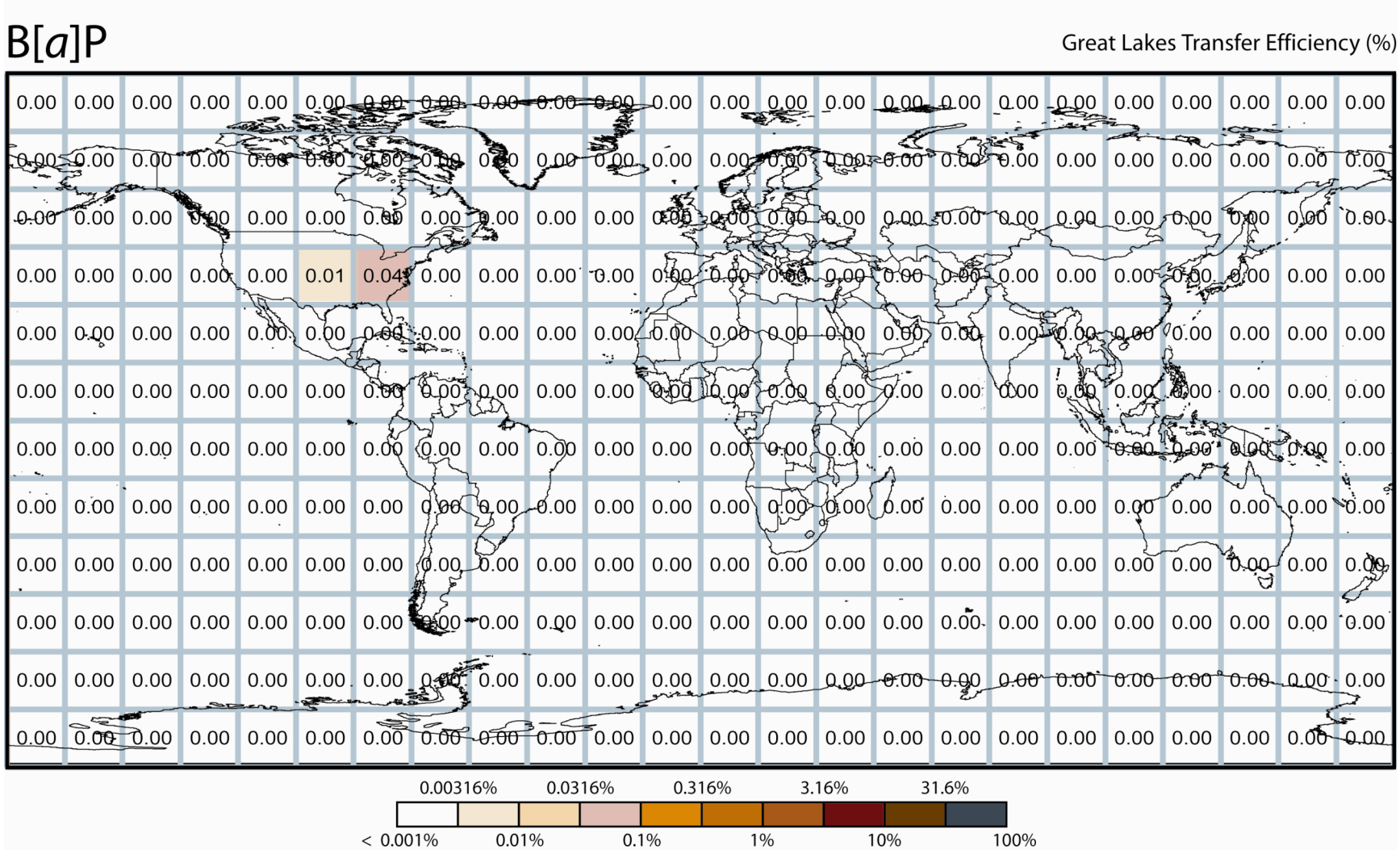

Figure 4.4.17. Great Lakes Transfer Efficiency of benzo[a]pyrene for emissions to air in each of the 288 regions of the BETR Global model.

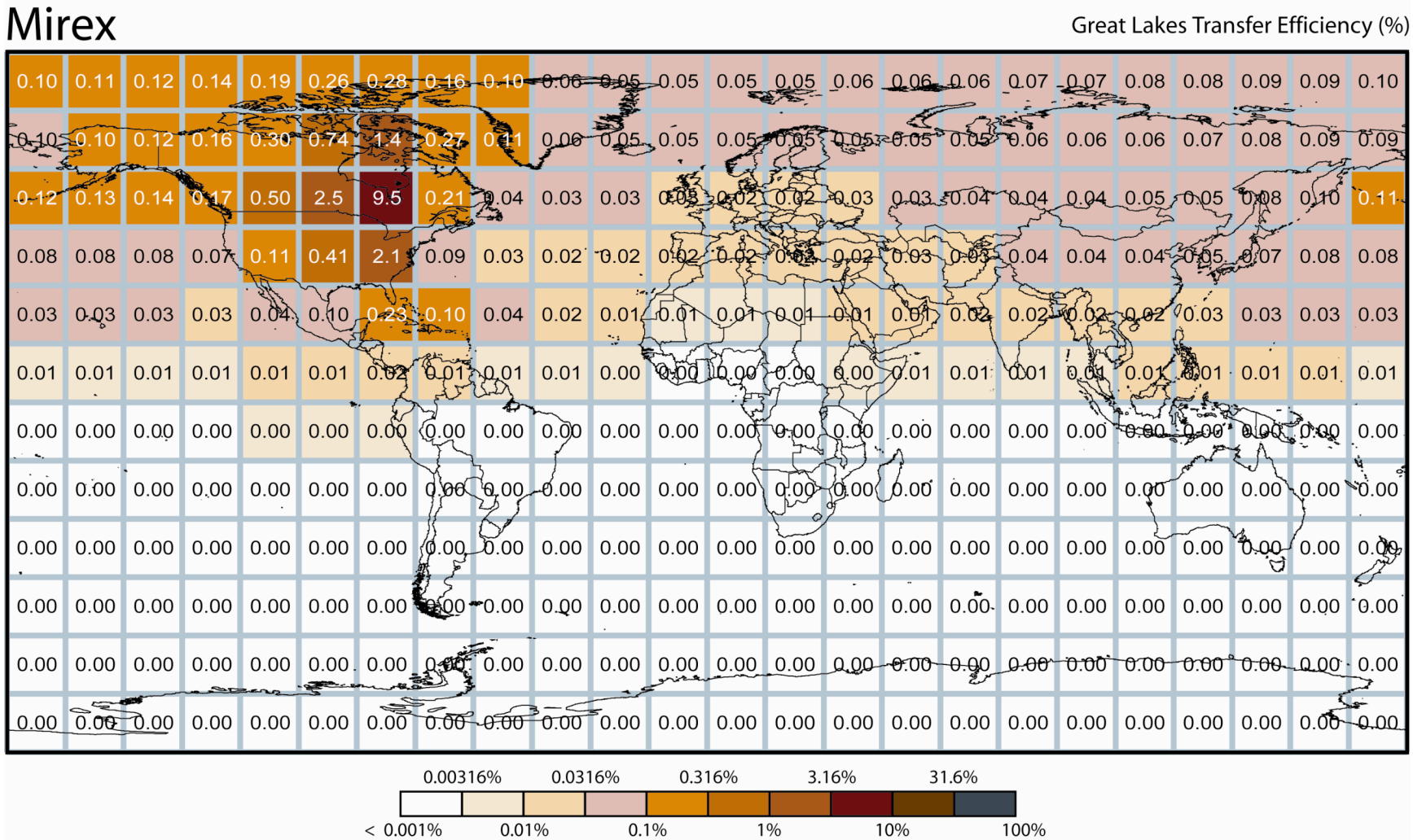

Figure 4.4.18. Great Lakes Transfer Efficiency of Mirex for emissions to air in each of the 288 regions of the BETR Global model.

As was the case for the results from the North American Model, the maps of GLTE from each region of the BETR Global model are best interpreted with reference to the generic results, which are provided in see Figure 4.2.3. Dieldrin, Aldrin, and B[a]P show very rapid declines in GLTE with distance from the target region. Atmospheric deposition of these three Level I substances is likely dominated by local and regional sources. Chlordane, 2,3,7,8-TCDD, DDT, toxaphene, OCS, and Mirex all have GLTE from within North America that are within a factor of about 30 of transfer efficiencies for releases in the target region itself, but lower efficiencies for emissions from outside North America. These substances can therefore be classified as having potential for continental scale transport and deposition to the Great Lakes. The seven PCB congeners show GLTE from locations in the Northern Hemisphere that are within approximately a factor of 30 of transfer efficiencies for local emissions, but transfer from the Southern Hemisphere is less efficient. HCB and α-HCH are transported and deposited to the Lakes from any emission location in the world with efficiencies that are within a factor of 30 to 60 of efficiencies for local releases. Thus, our model results indicate that these pollutants are subject to global-scale transport and redistribution.

5.0 EMISSION ESTIMATES

In this section, we summarize emissions inventories at the North American scale for seven PCB congeners and toxaphene, and at the global scale for our full set of PCBs and α-HCH. Modeled concentrations of PCBs in air obtained from the BETR Global model are compared with data from nine long-term monitoring stations in the Northern Hemisphere, including the International Atmospheric Deposition Network (IADN), which is located in the Great Lakes Basin.

5.1 North American Emissions of PCBs and Toxaphene

PCB emission estimates to air for Canada, the United States, and Mexico have been made by Breivik et al. [16,17] for individual congeners as part of their global emissions inventory. Breivik et al. [16,17] report large uncertainties in these estimates. In order to

convey these uncertainties they provide three emissions scenarios (*maximum*, *default*, and *minimum*) to reflect the range of possible emissions that are consistent with their analysis. The range of emissions estimates between the *minimum* and *maximum* scenarios spans more than two orders of magnitude.

In order to estimate emissions in each BETR region, we apportioned the country-specific emissions estimates made by Breivik et al. [16,17] into the regions of the BETR North America model based on geographically referenced global population distribution using data provided by Environment Canada [18]. Figures 5.1.1 – 5.1.7 show the proportion of total emissions in the *default* emission scenario allotted to each BETR North America region using this methodology.

Emissions estimates for toxaphene in North America appropriate for use in BETR North America have been made previously by MacLeod et al. [19] and are shown in Figure 5.1.8.

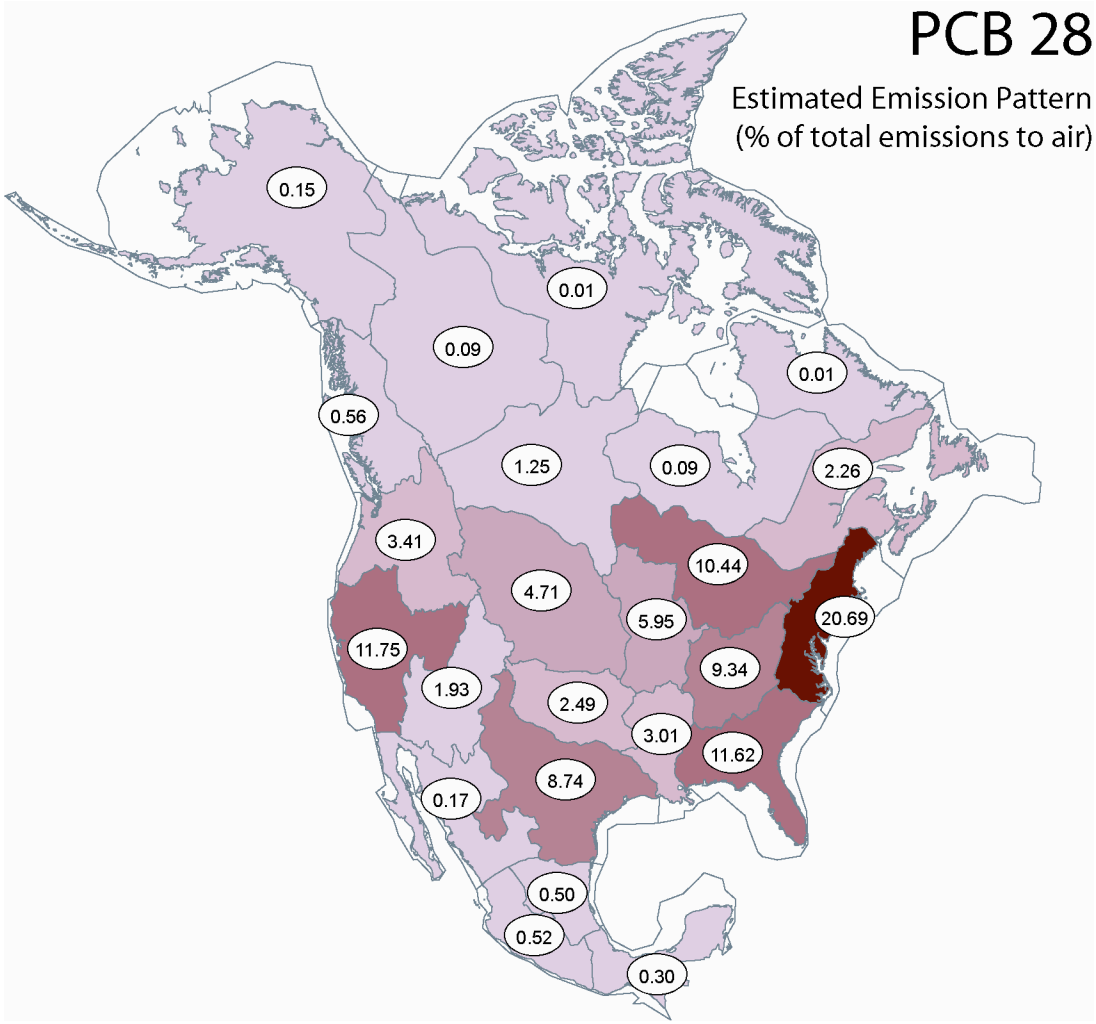

Figure 5.1.1. Estimated percentage of cumulative emissions of PCB 28 to air in North America occurring in each region of the BETR North America model.

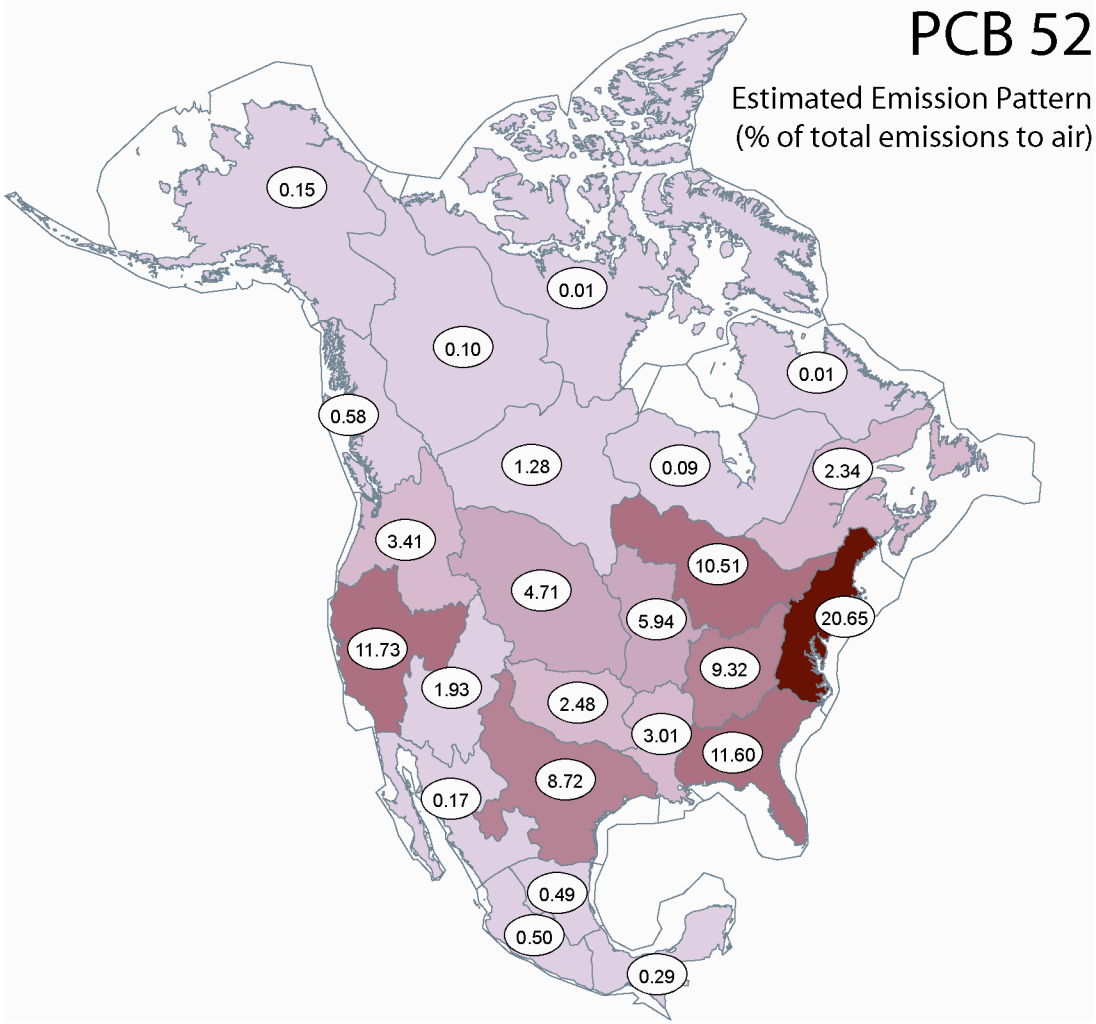

Figure 5.1.2. Estimated percentage of cumulative emissions of PCB 52 to air in North America occurring in each region of the BETR North America model.

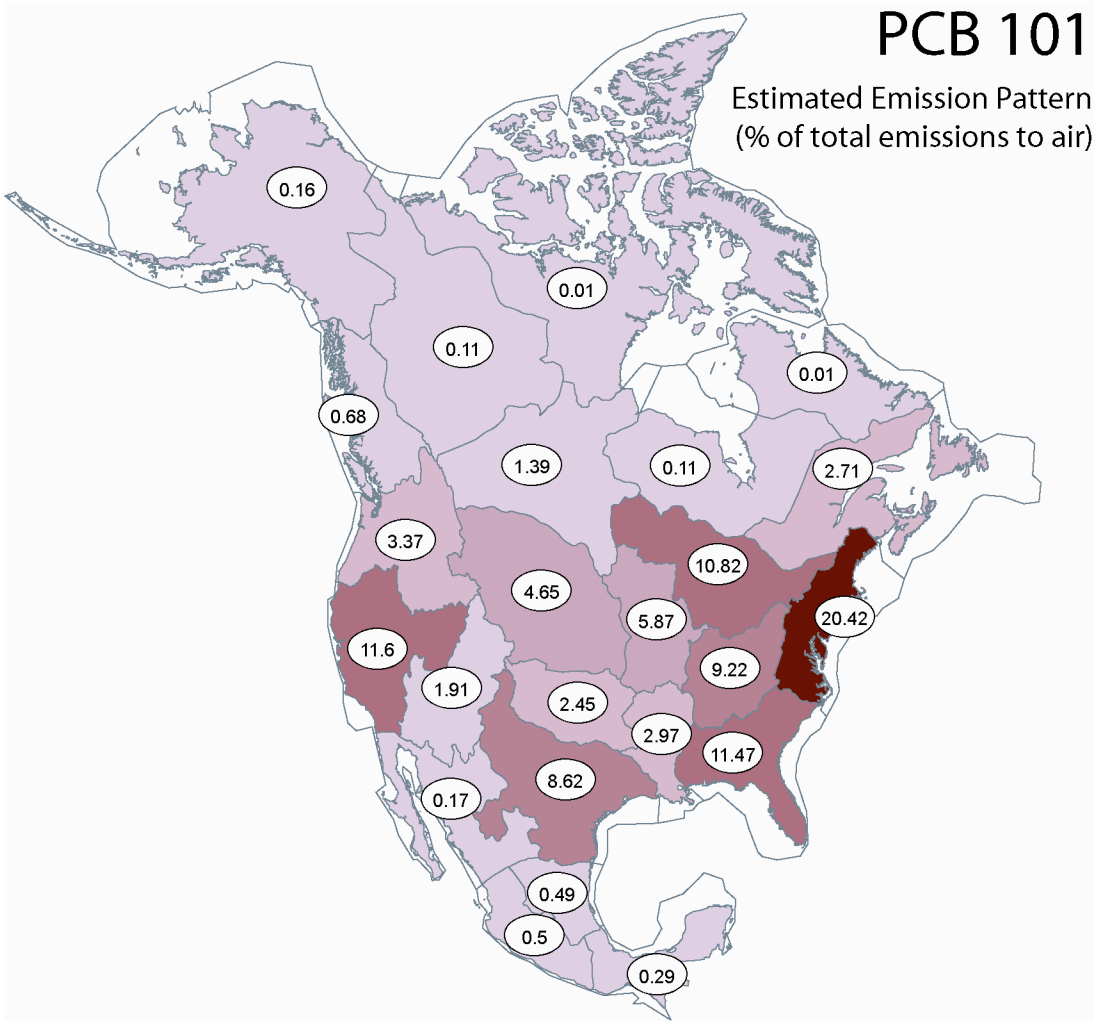

Figure 5.1.3. Estimated percentage of cumulative emissions of PCB 101 to air in North America occurring in each region of the BETR North America model.

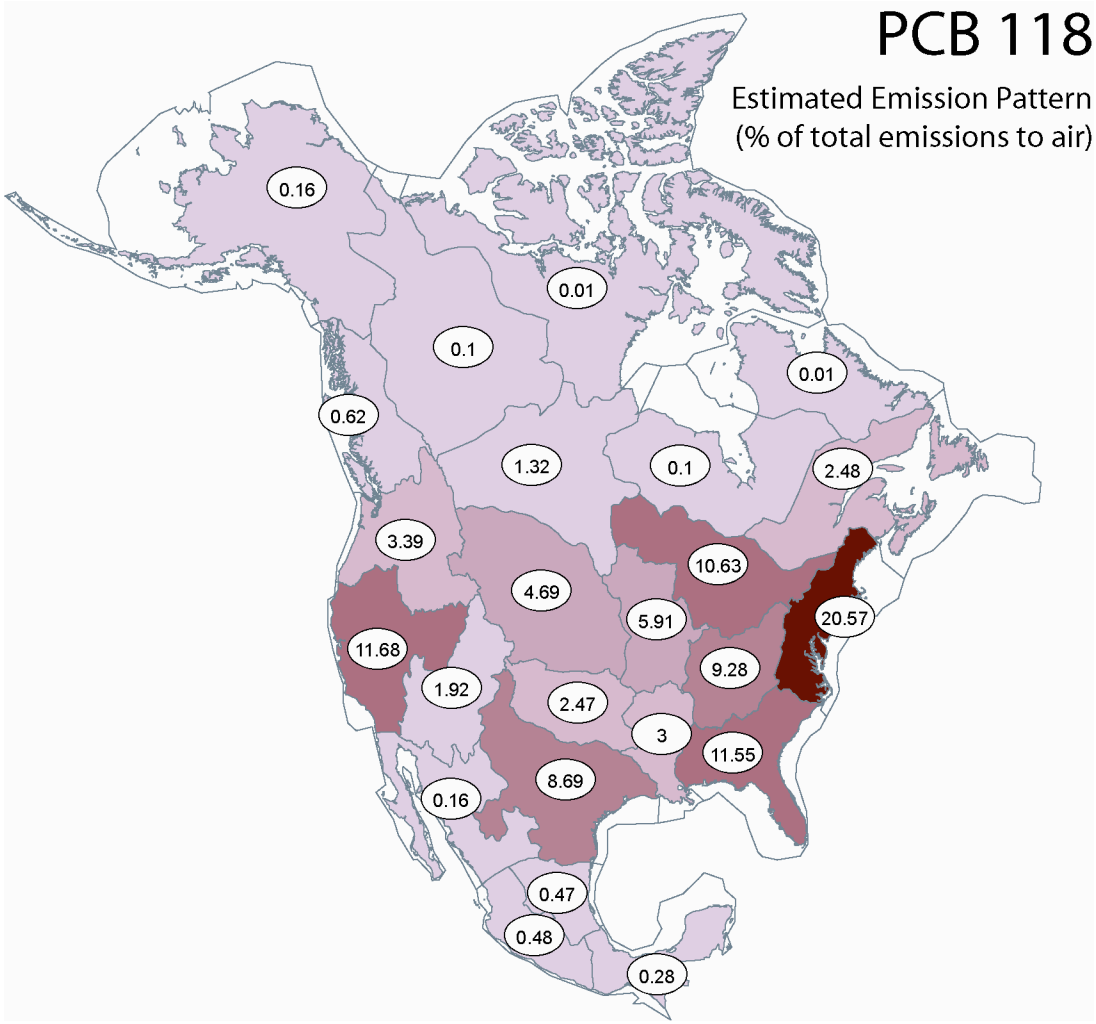

Figure 5.1.4. Estimated percentage of cumulative emissions of PCB 118 to air in North America occurring in each region of the BETR North America model.

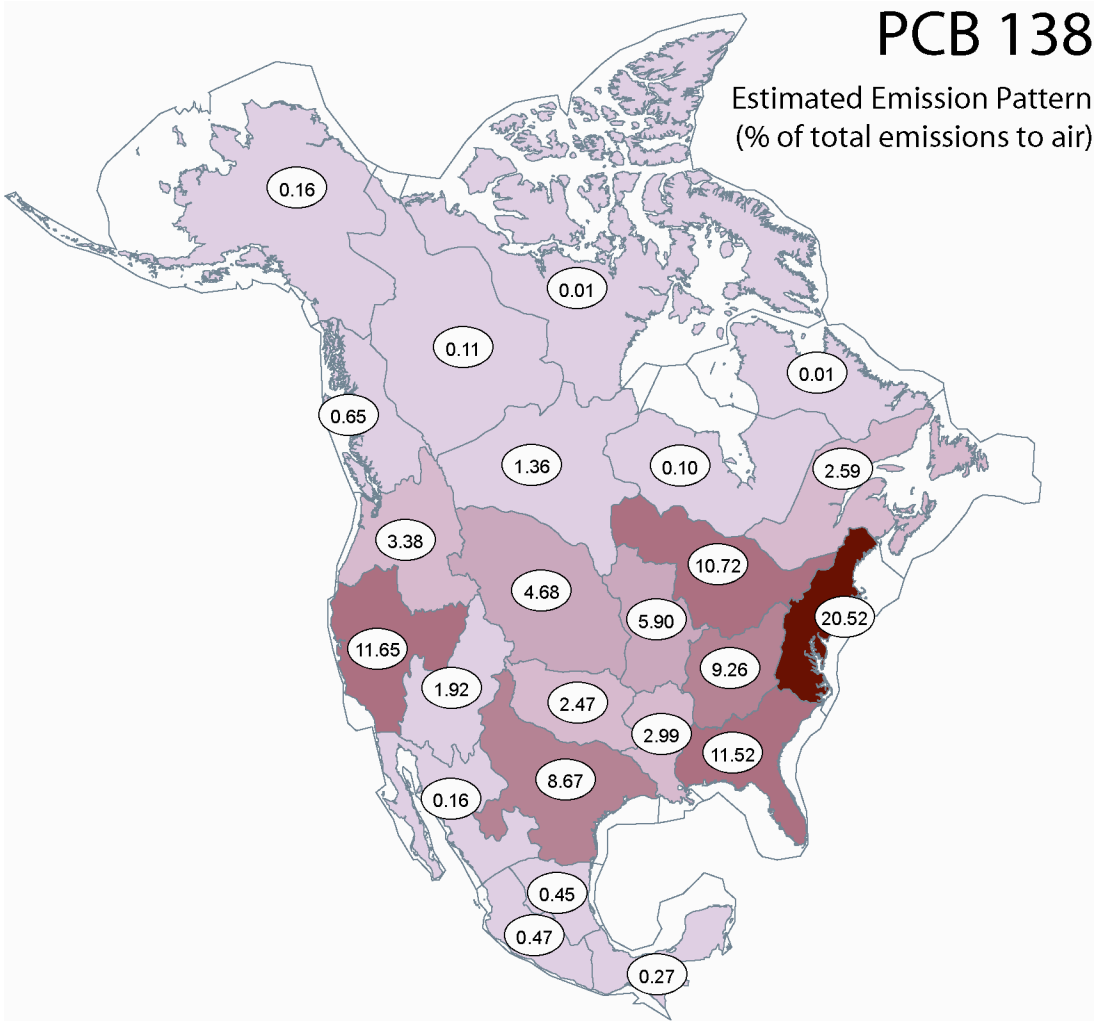

Figure 5.1.5. Estimated percentage of cumulative emissions of PCB 138 to air in North America occurring in each region of the BETR North America model.

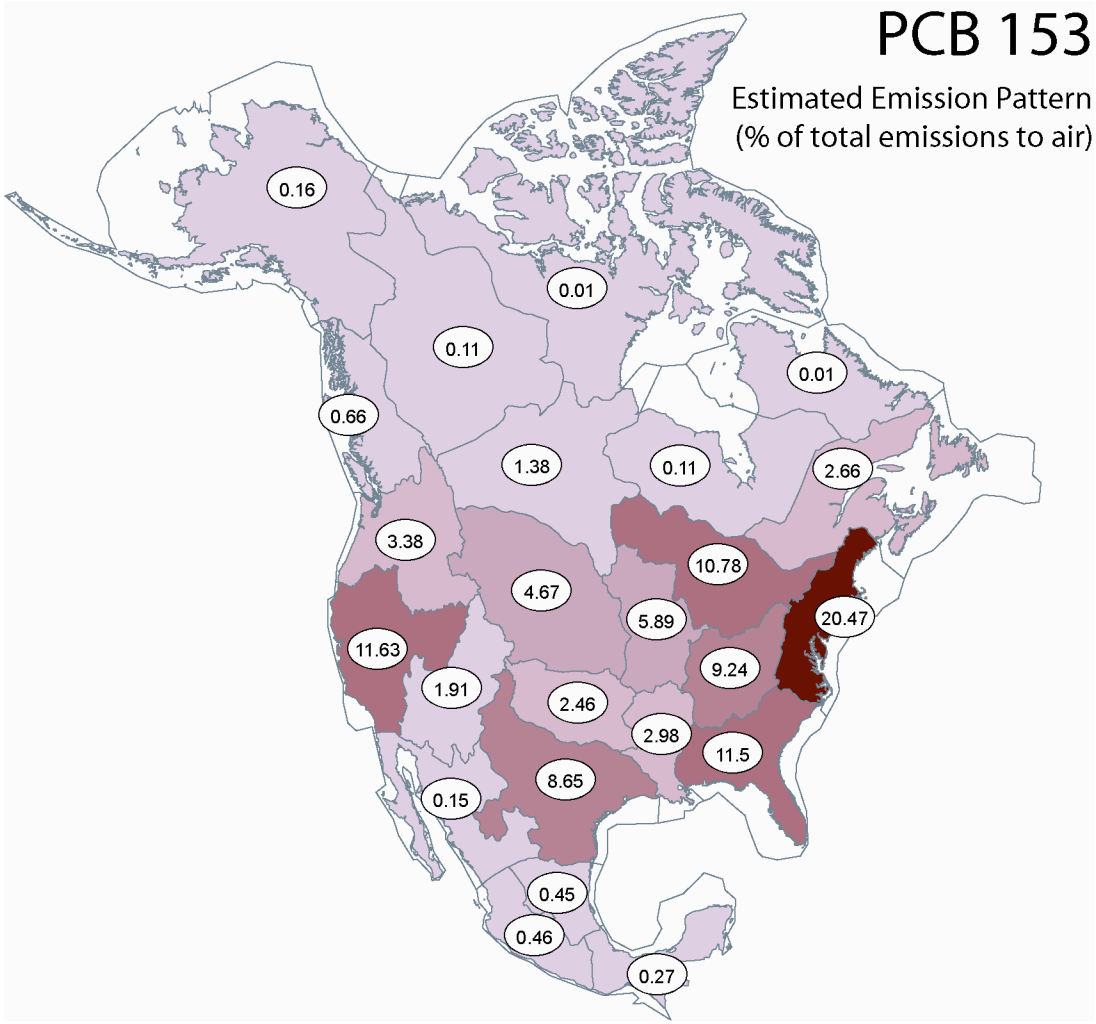

Figure 5.1.6. Estimated percentage of cumulative emissions of PCB 153 to air in North America occurring in each region of the BETR North America model.

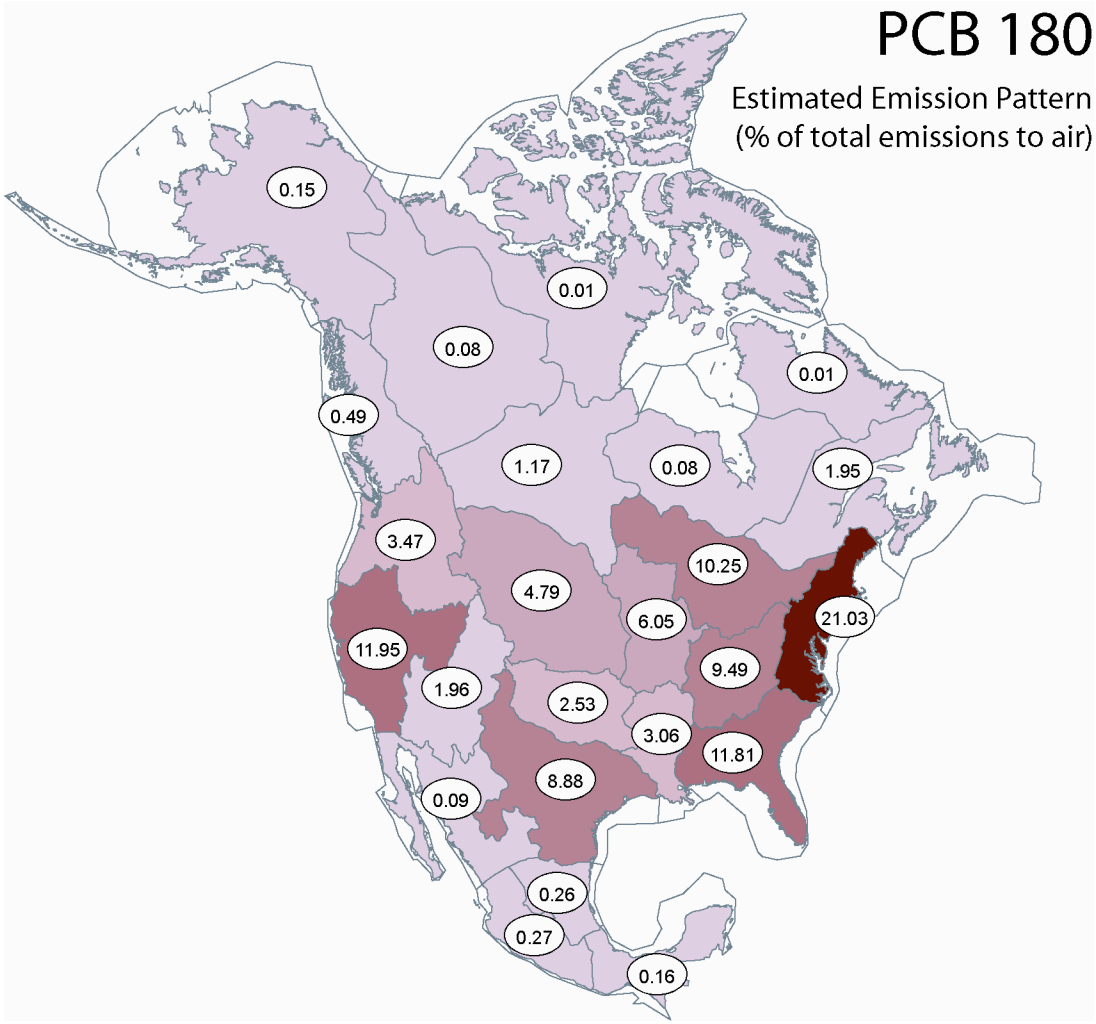

Figure 5.1.7. Estimated percentage of cumulative emissions of PCB 180 to air in North America occurring in each region of the BETR North America model.

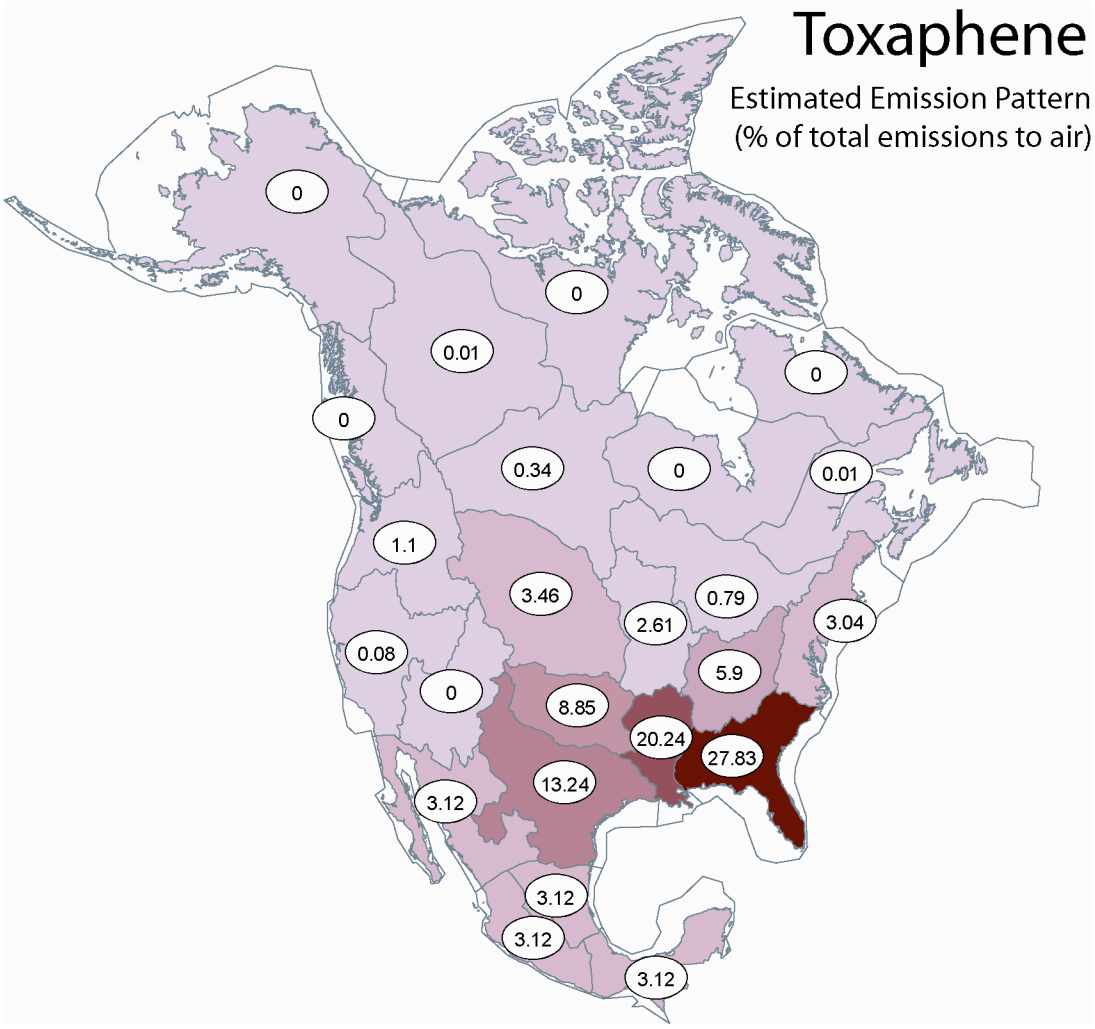

Figure 5.1.8. Estimated percentage of cumulative emissions of toxaphene to air in North America occurring in each region of the BETR North America model.

5.2 Global Emissions of PCBs and α-Hexachlorocyclohexane (α-HCH)

Breivik and al. [16,17] have compiled global estimates of emissions to air for individual PCB congeners on a country by country basis between 1930 and 2000. As emissions input for the BETR Global model, we have apportioned these emissions into individual model regions based on population distribution exploiting the geographically referenced population data available from Environment Canada [18]. As discussed above, there are three emission scenarios (*maximum*, *default*, and *minimum*) that reflect the uncertainty range of the emissions estimates. In Figures 5.1.1 – 5.1.14, we present emissions data from the *default* scenario in two ways: (1) as the fraction of cumulative emissions between 1930 and 2000 that occurred in each model region, and (2) as the fraction of emissions in the year 2000 in each region.

In reviewing these figures, we note that the proportion of global PCB emissions taking place in close proximity to the Great Lakes was much lower in 2000 than over the entire use-history of PCBs. The geographic profile of PCB emissions in 2000 has shifted much more toward Eastern Europe and Asia, and away from North America and Western Europe. This pattern reflects the aggressive emission reduction programs that have been pursued in Canada, the United States and Western European countries.

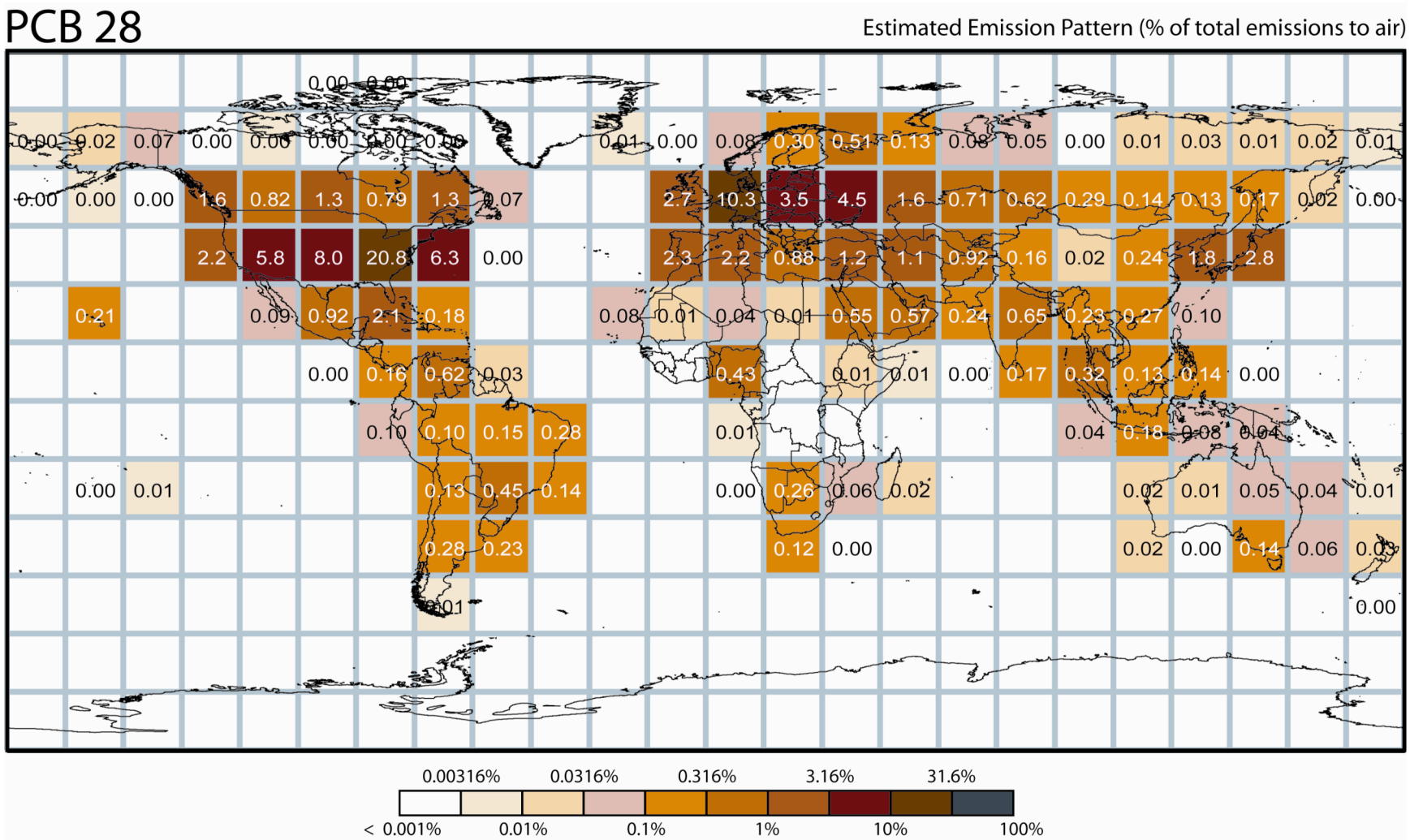

Figure 5.2.1. Estimated percentage of cumulative emissions of PCB 28 to air occurring in each region of the BETR Global model under the default emission scenario.

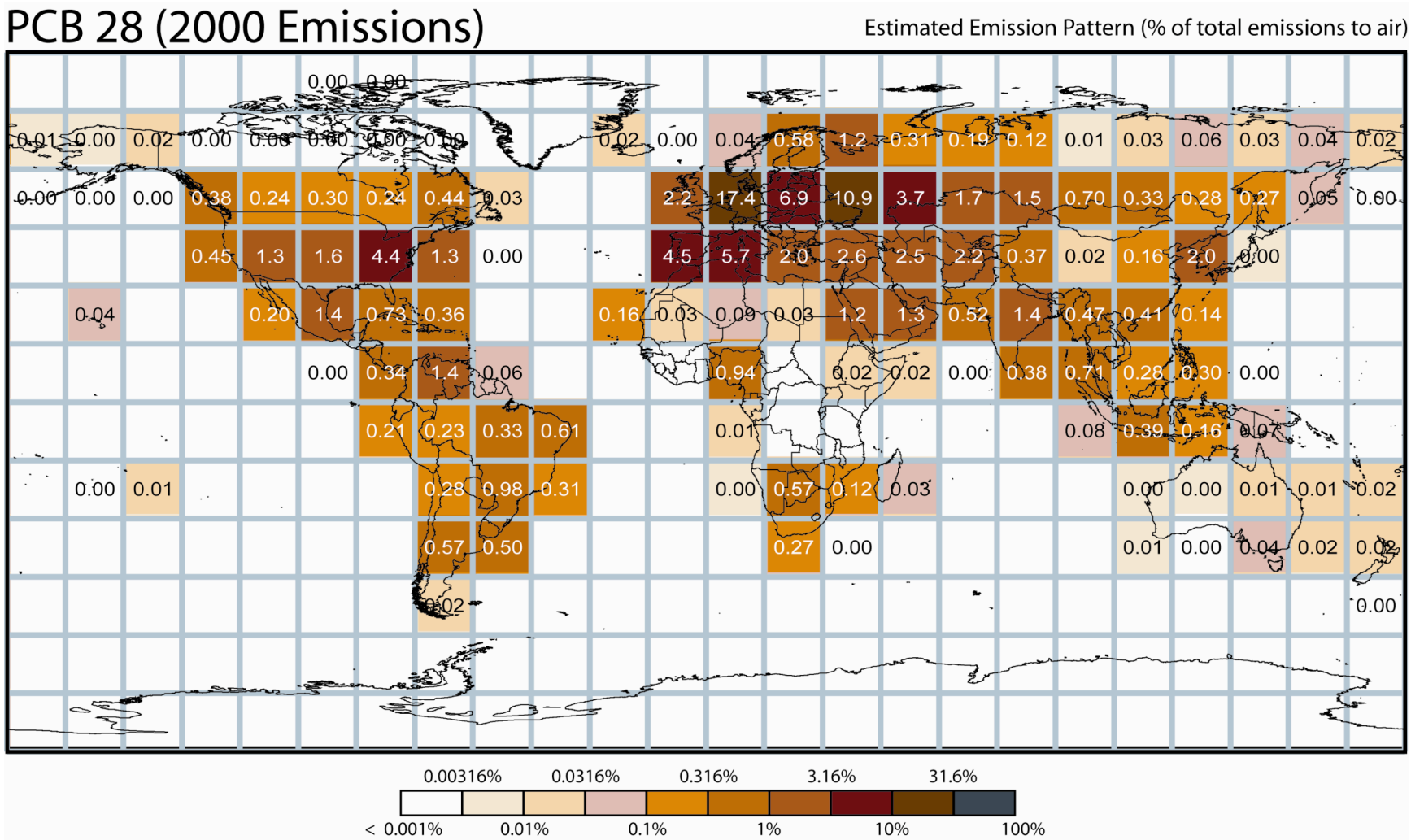

Figure 5.2.2. Estimated percentage of emissions of PCB 28 to air occurring in each region of the BETR Global model in the year 2000 under the default emission scenario.

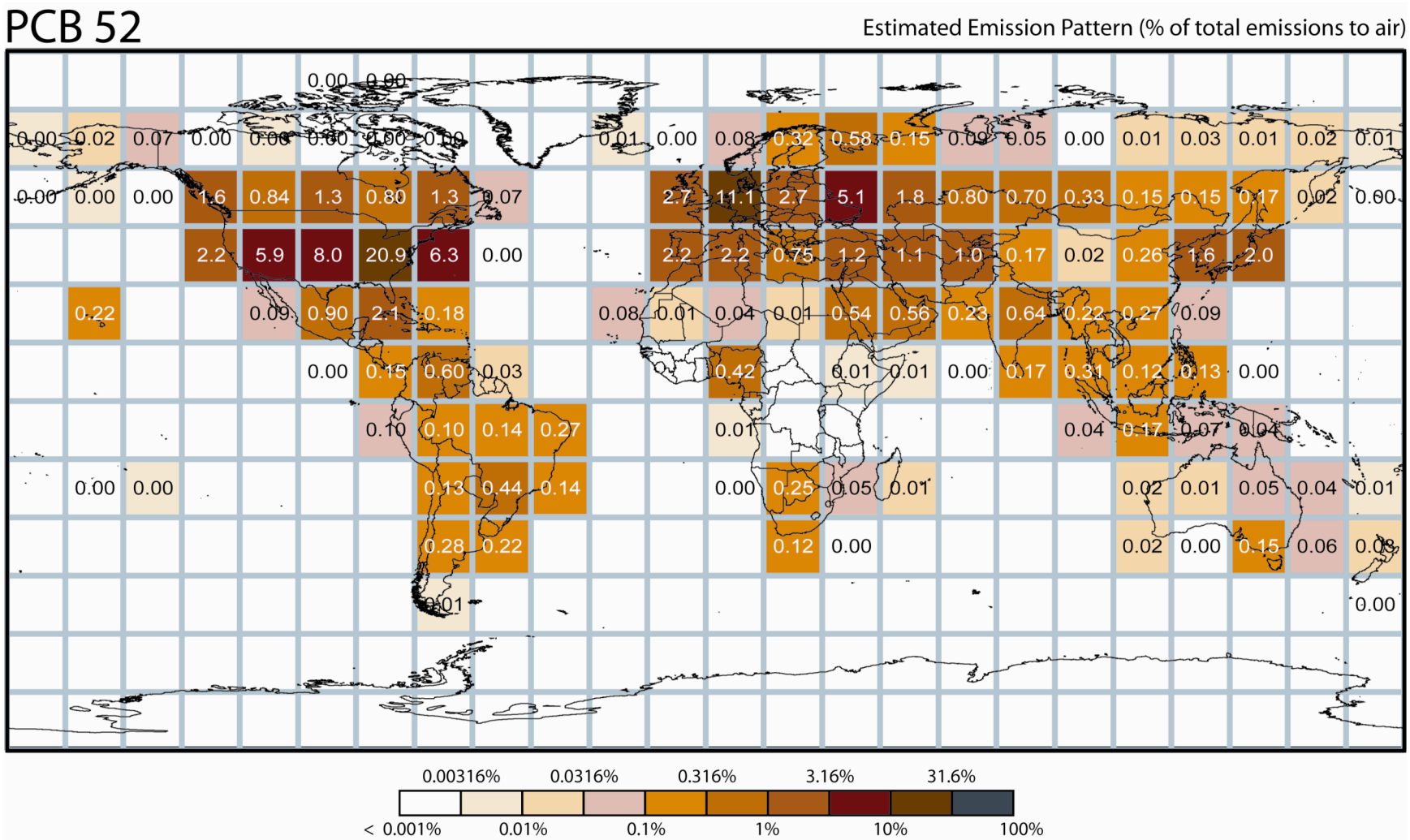

Figure 5.2.3. Estimated percentage of cumulative emissions of PCB 52 to air occurring in each region of the BETR Global model under the default emission scenario.

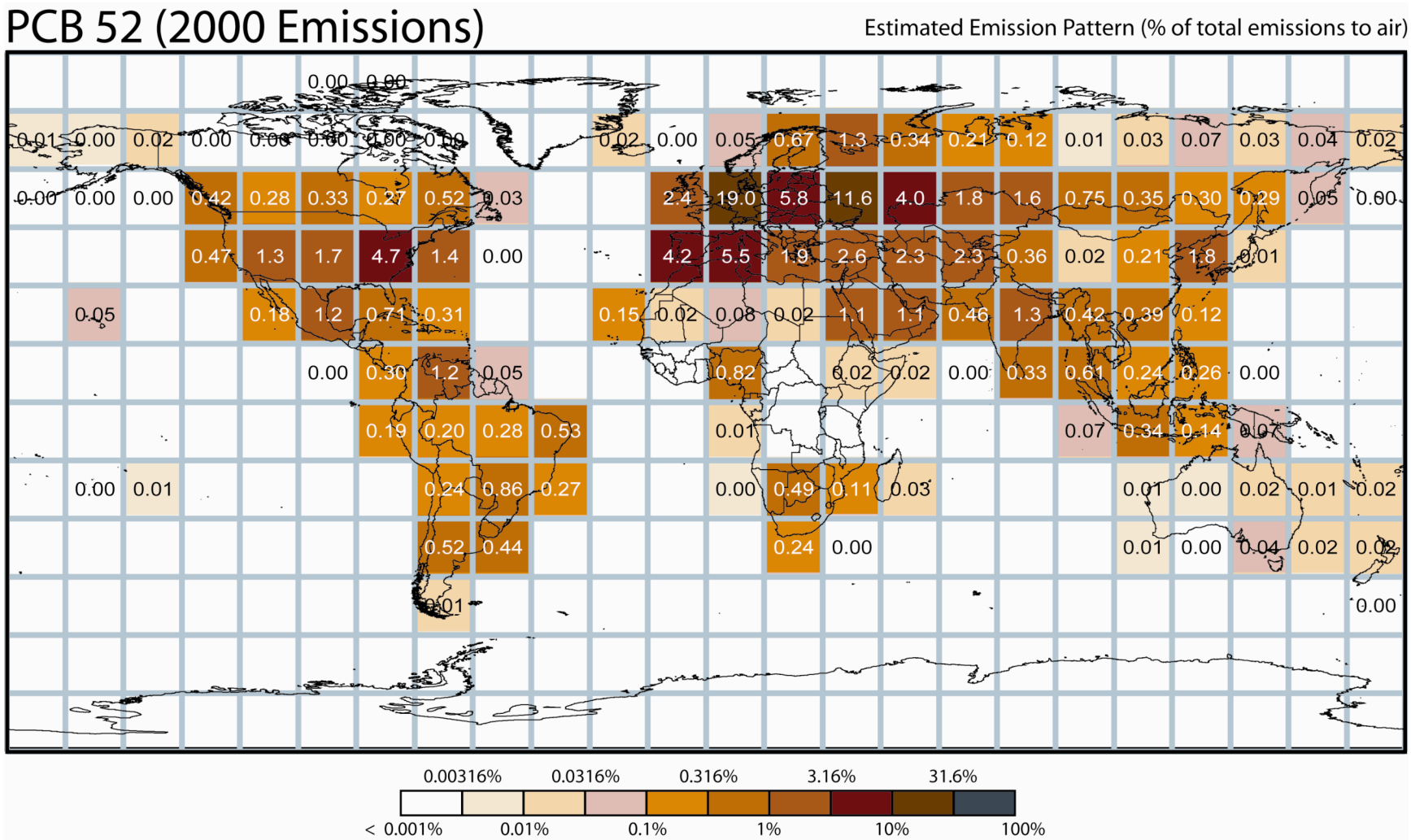

Figure 5.2.4. Estimated percentage of emissions of PCB 52 to air occurring in each region of the BETR Global model in the year 2000 under the default emission scenario.

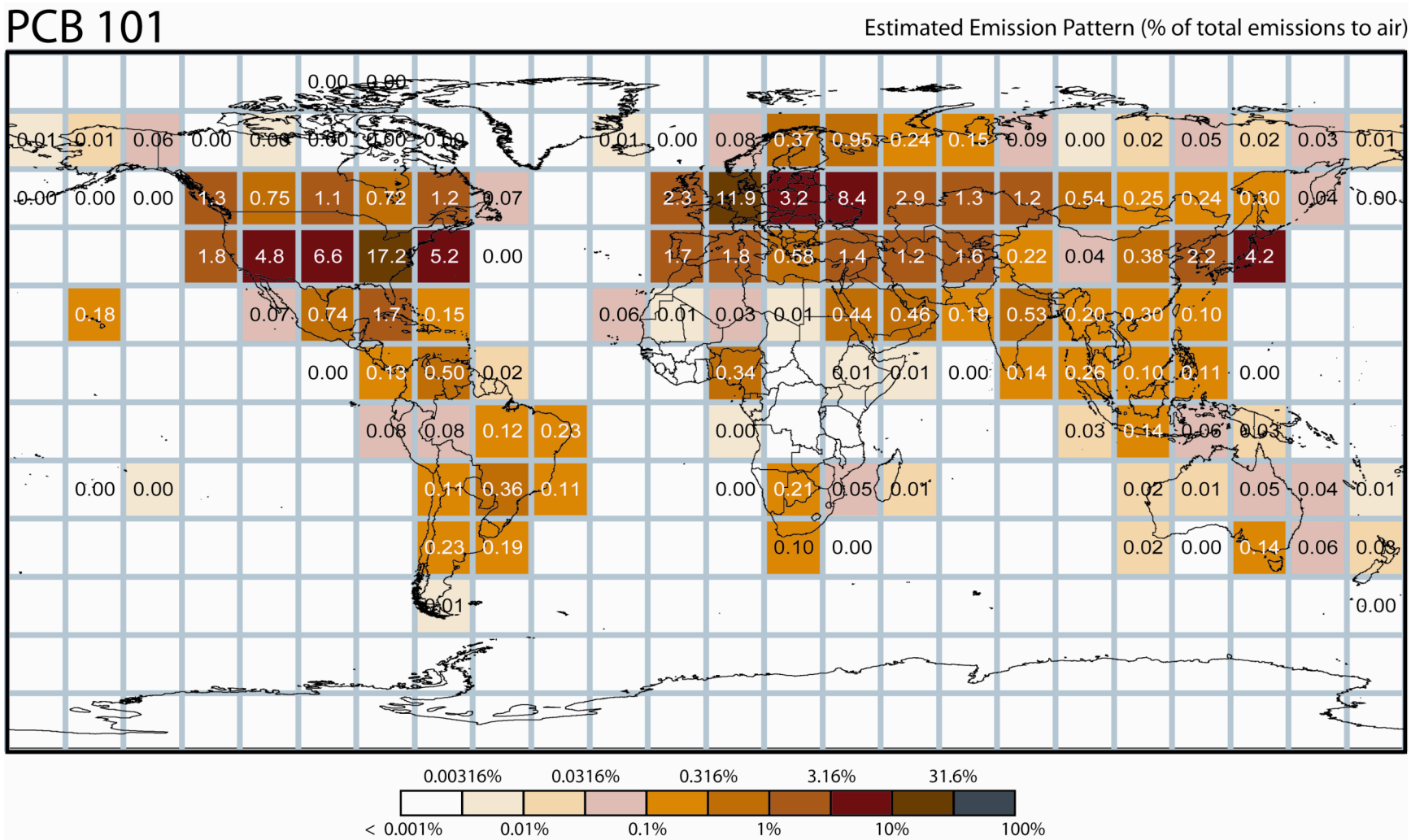

Figure 5.2.5. Estimated percentage of cumulative emissions of PCB 101 to air occurring in each region of the BETR Global model under the default emission scenario

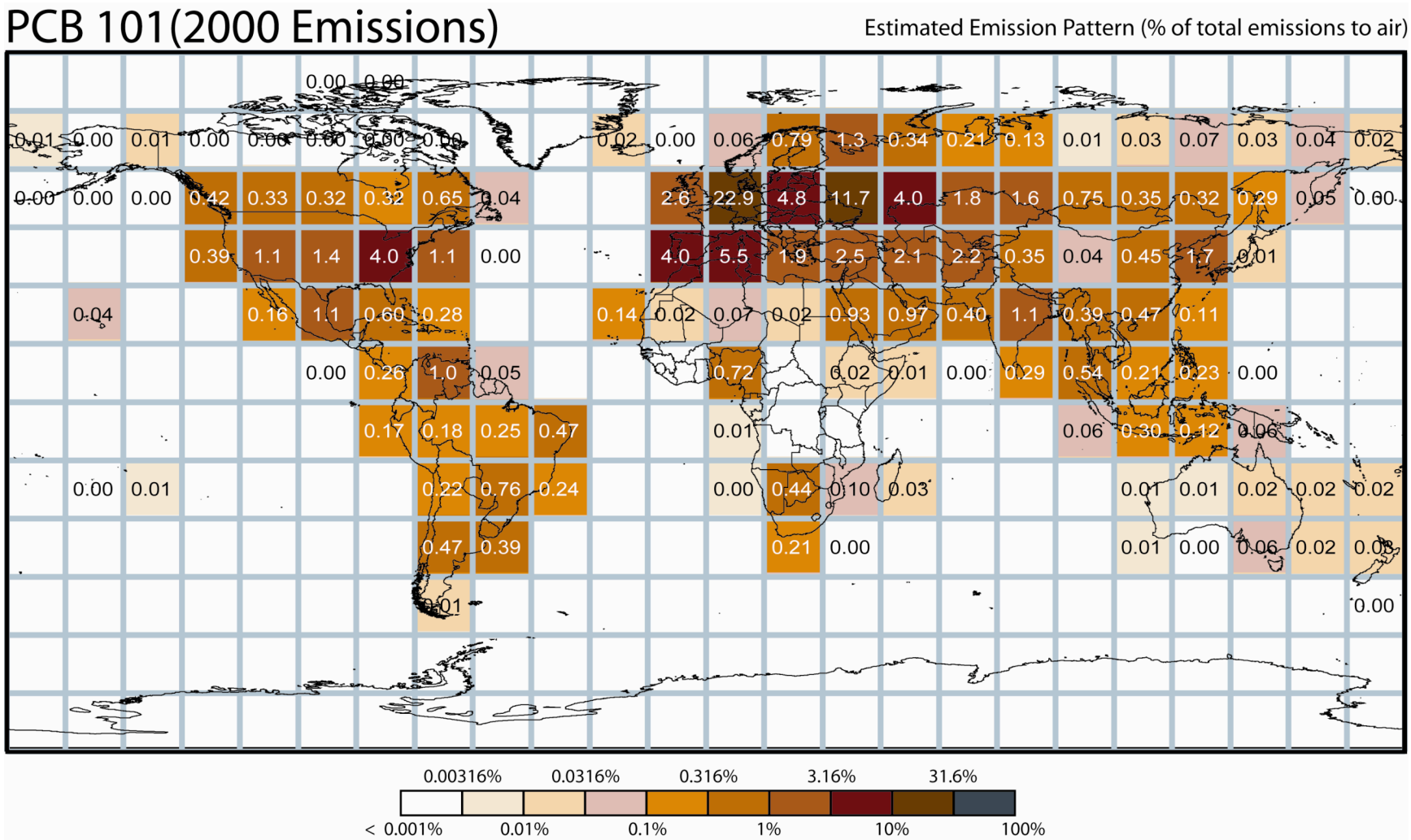

Figure 5.2.6. Estimated percentage of emissions of PCB 101 to air occurring in each region of the BETR Global model in the year 2000 under the default emission scenario.

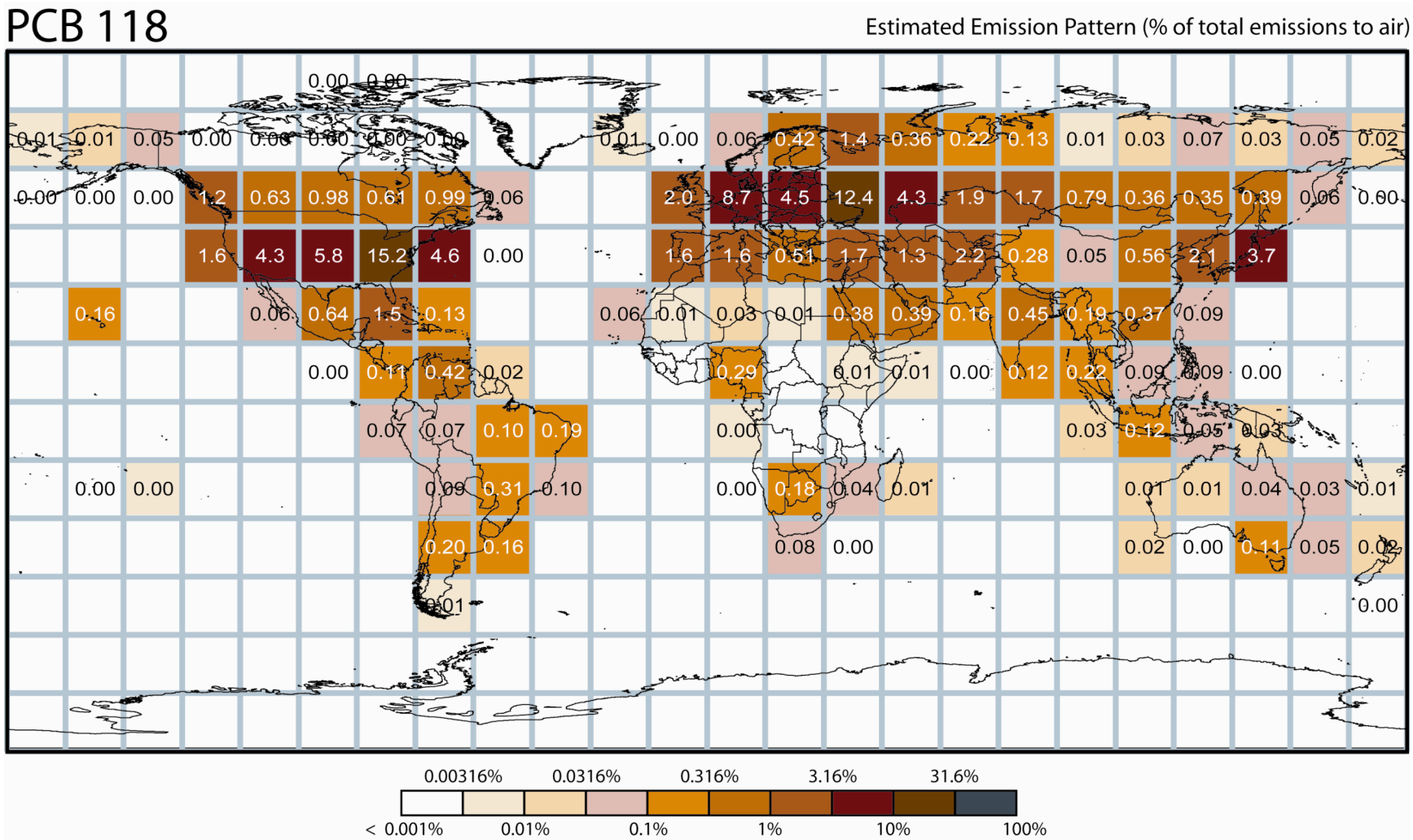

Figure 5.2.7. Estimated percentage of cumulative emissions of PCB 118 to air occurring in each region of the BETR Global model under the default emission scenario

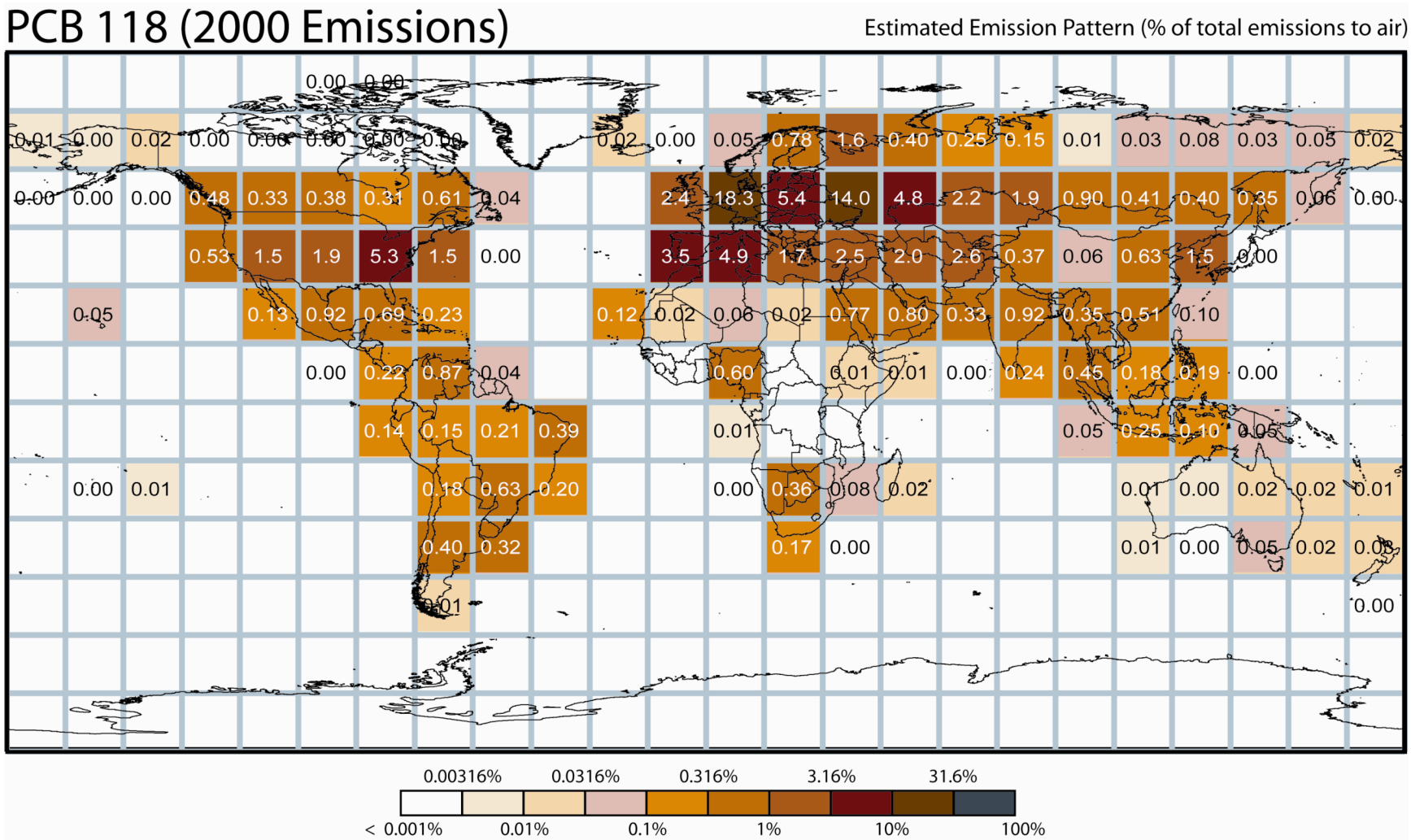

Figure 5.2.8. Estimated percentage of emissions of PCB 118 to air occurring in each region of the BETR Global model in the year 2000 under the default emission scenario.

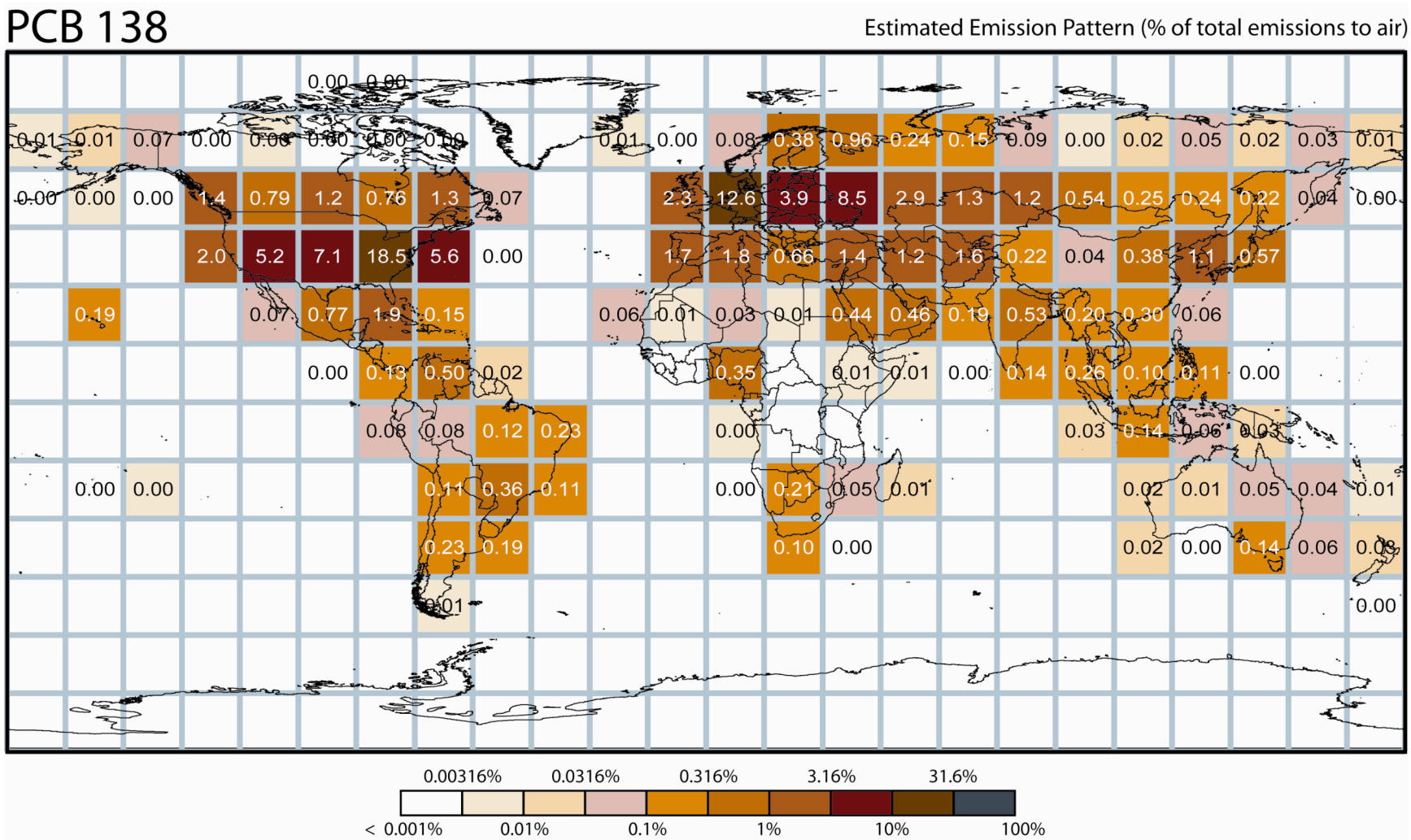

Figure 5.2.9. Estimated percentage of cumulative emissions of PCB 138 to air occurring in each region of the BETR Global model under the default emission scenario

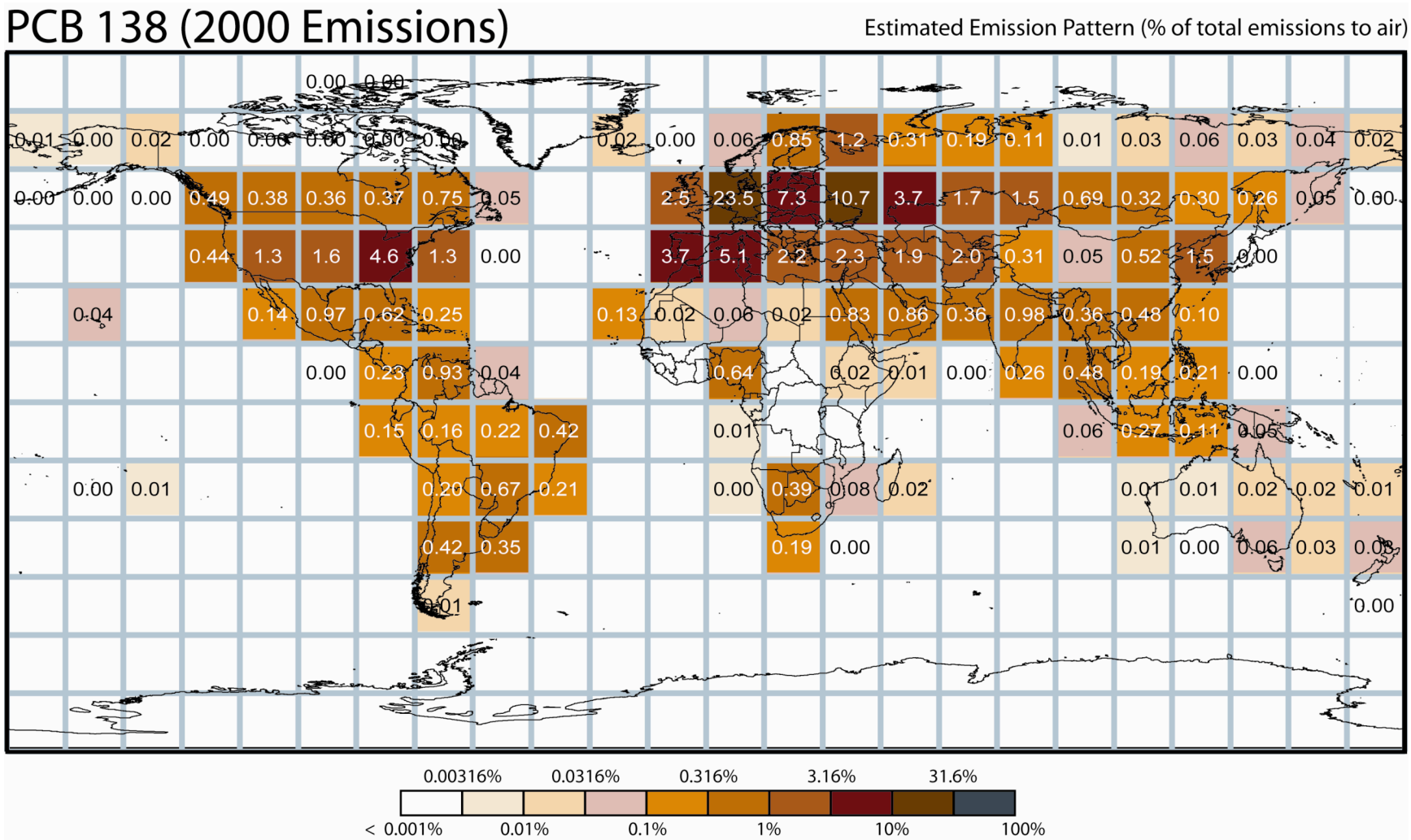

Figure 5.2.10. Estimated percentage of emissions of PCB 138 to air occurring in each region of the BETR Global model in the year 2000 under the default emission scenario.

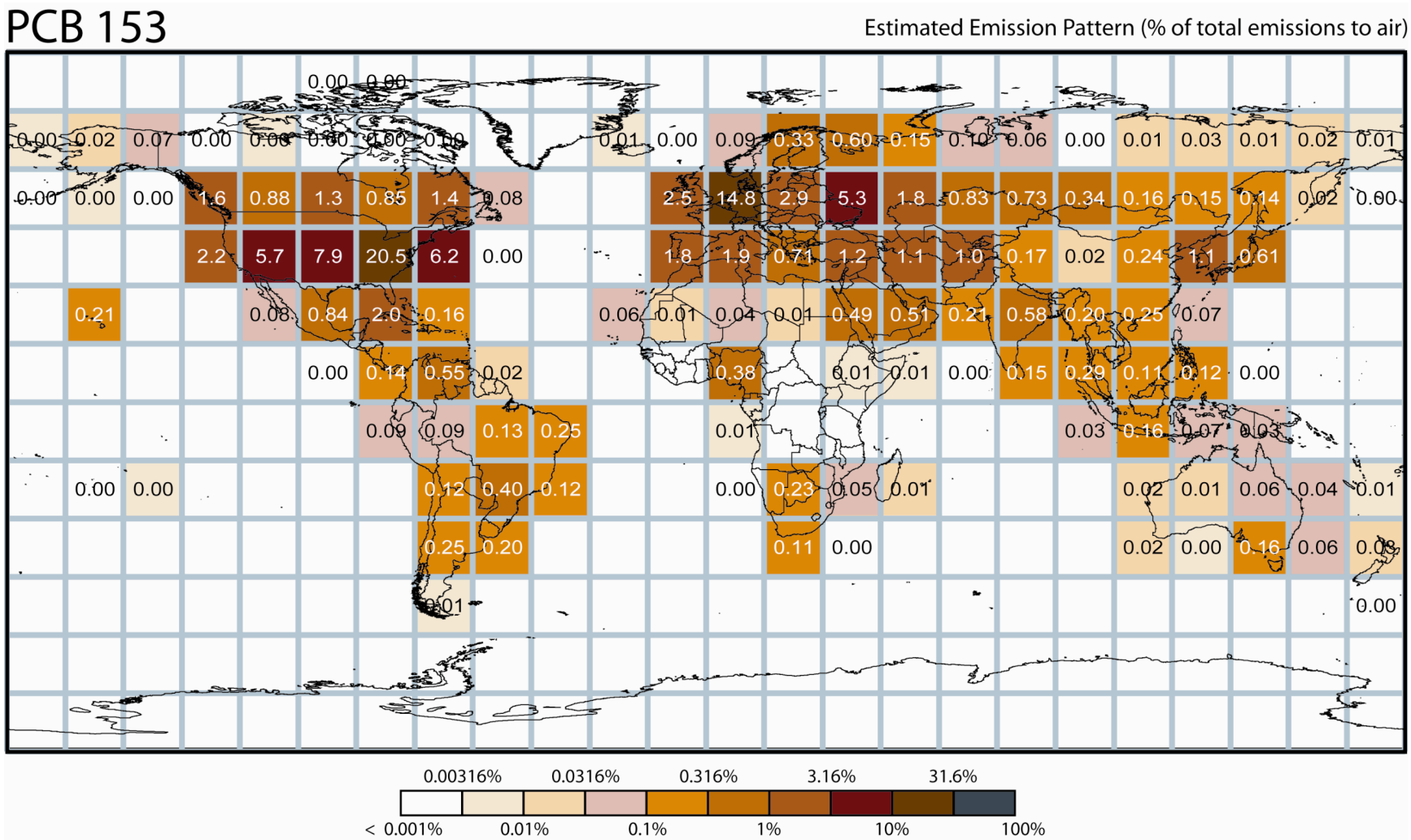

Figure 5.2.11. Estimated percentage of cumulative emissions of PCB 153 to air occurring in each region of the BETR Global model under the default emission scenario

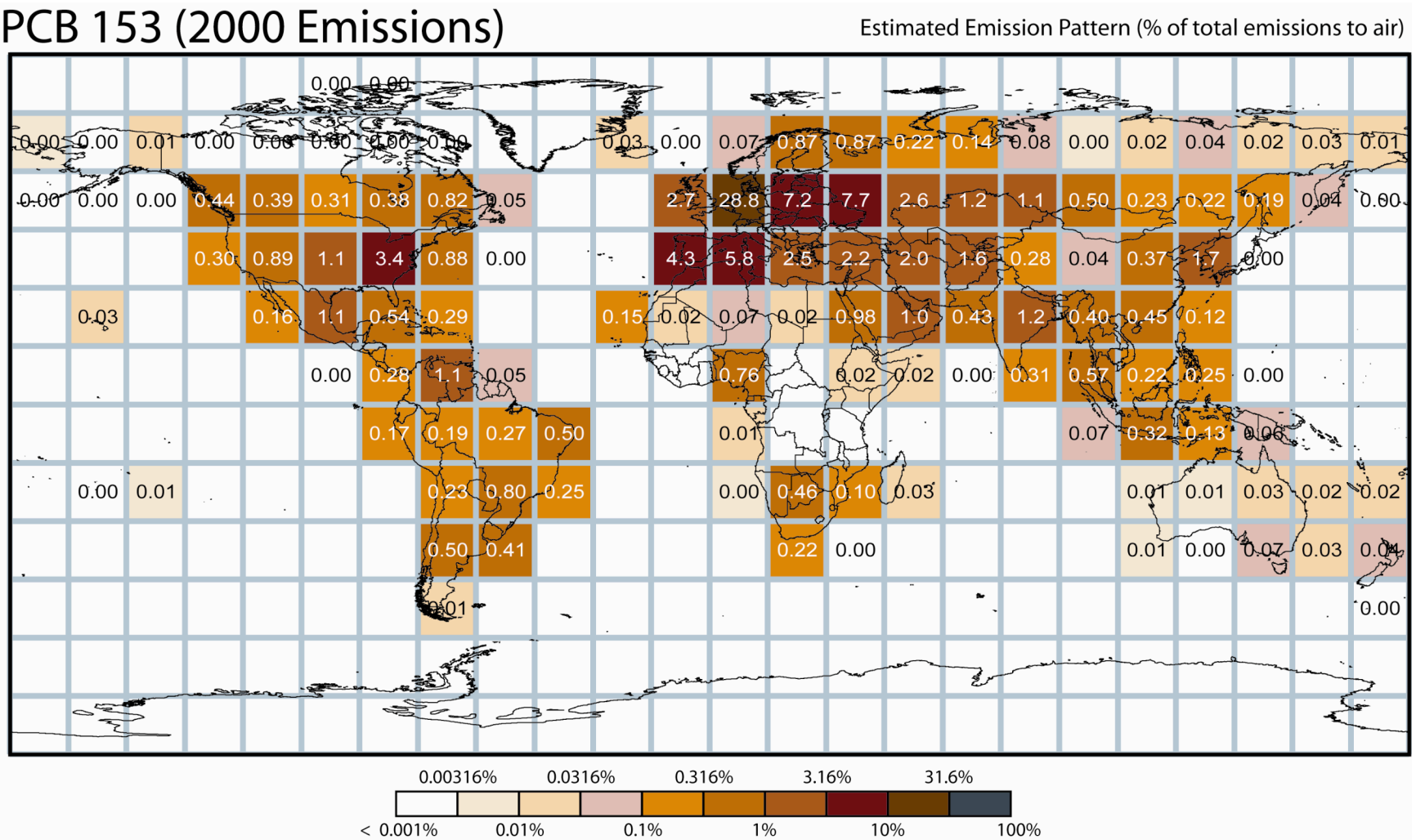

Figure 5.2.12. Estimated percentage of emissions of PCB 153 to air occurring in each region of the BETR Global model in the year 2000 under the default emission scenario.

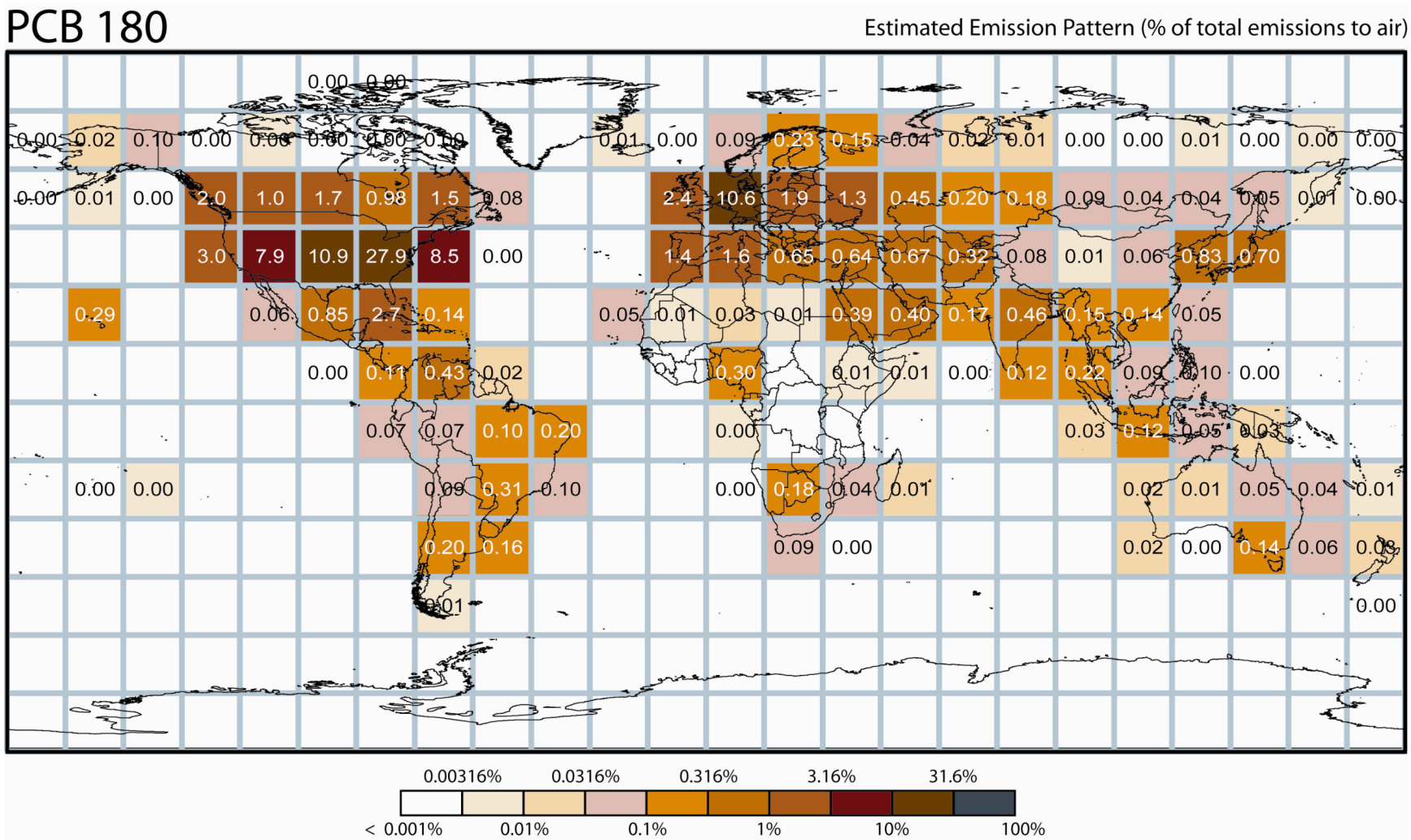

Figure 5.2.13. Estimated percentage of cumulative emissions of PCB 180 to air occurring in each region of the BETR Global model under the default emission scenario

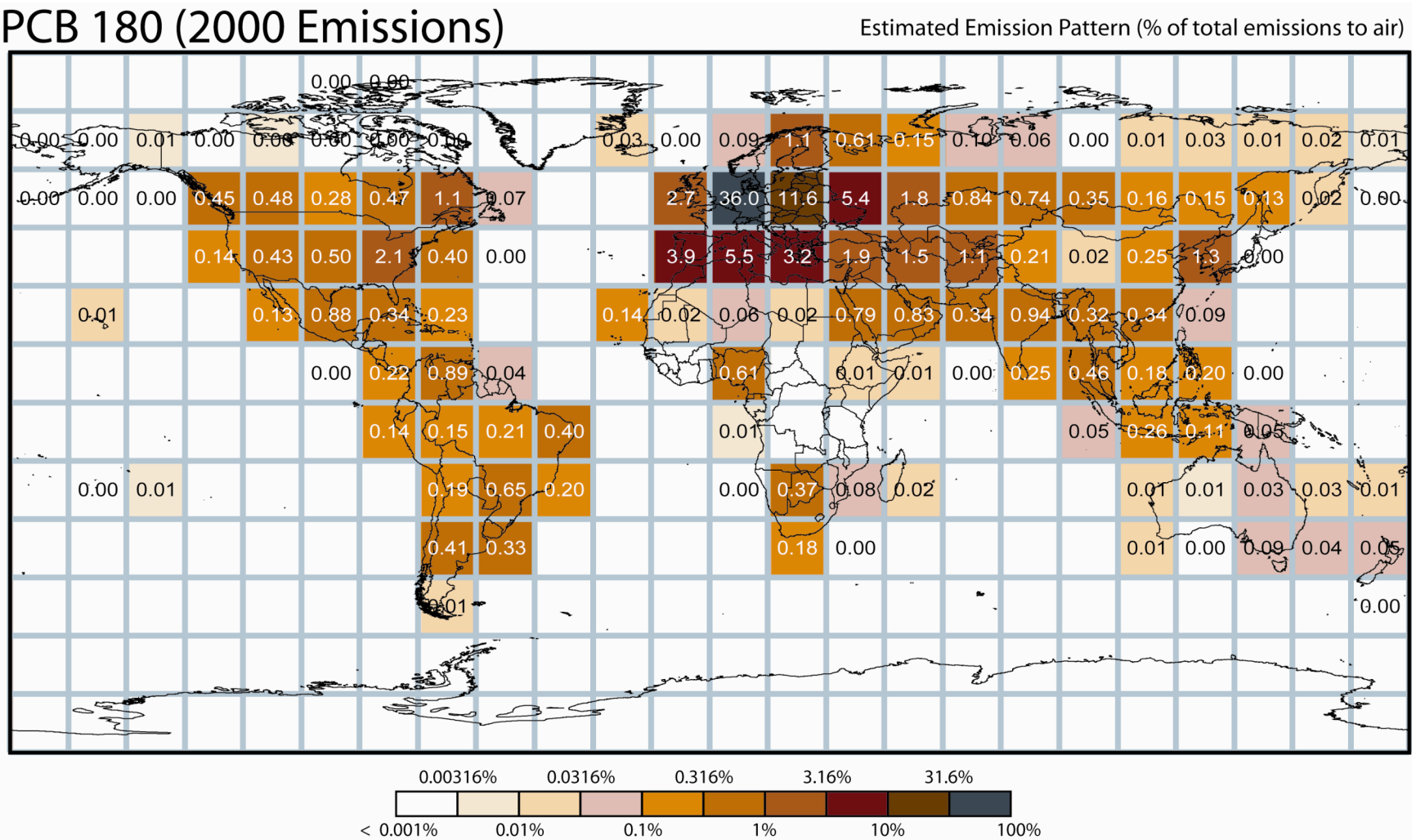

Figure 5.2.14. Estimated percentage of emissions of PCB 180 to air occurring in each region of the BETR Global model in the year 2000 under the default emission scenario.

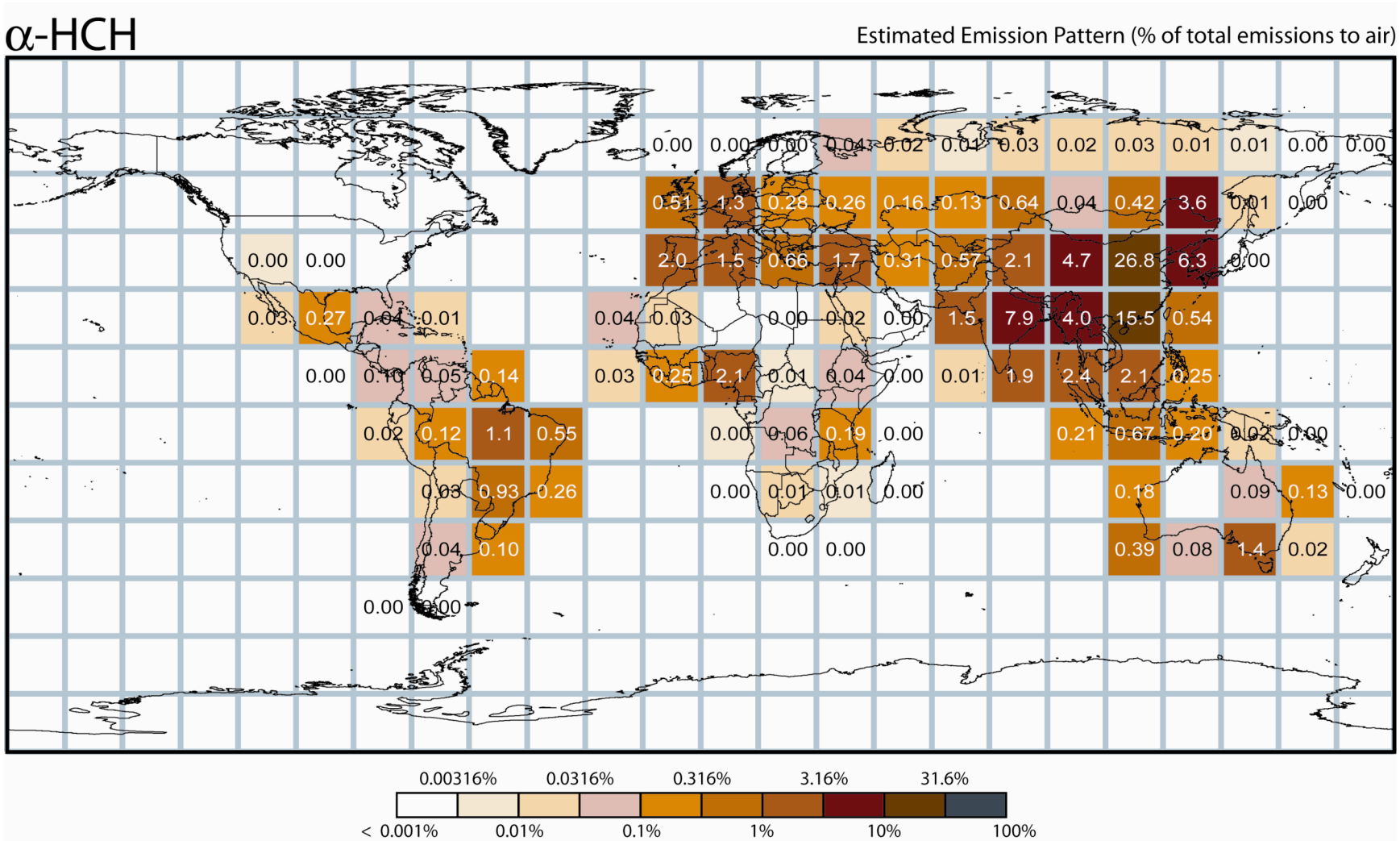

Figure 5.2.15. Estimated percentage of cumulative emissions of a-HCH to air occurring in each region of the BETR Global model.

5.3 Global-scale Modeling of PCB Concentrations in Air

We evaluate the performance of the BETR Global model as a descriptor of chemical fate by comparing model results with measured concentrations of persistent contaminants at eleven locations in the global environment. A complete description of our work on development and evaluation of the BETR Global model can be found in the paper by MacLeod et al. [6]. We focus here on the model results for the PCB congeners. We gathered reported measurements of atmospheric PCB concentrations from eleven long-term monitoring sites located in seven different model regions, including data from the International Atmospheric Deposition Network in the Great Lakes region (See Table 5.3.1 for details). We calculated the corresponding atmospheric concentrations of the PCB congeners with the model by simulating a 70-year period using each of the three emissions scenarios proposed by Breivik et al. [16,17] for the period 1930 - 2000.

Figures 5.3.1 – 5.3.3 compare modeled and measured concentrations of the seven selected PCB congeners in air at the eleven monitoring sites for the two emission scenarios. The diagonal lines are provided for comparison, representing perfect agreement between the model and measurements, agreement within a factor of 3.16 ($=10^{0.5}$), and agreement within a factor of 10. Correlation coefficients between observed and modeled concentrations are statistically significant under all three emission scenarios. Inspection of these figures indicates that concentrations are dramatically under-predicted using the "*minimum*" emission scenario, slightly under-predicted using the "*default*" emission scenario, and slightly over-predicted by the "*maximum*" scenario. When we use the "*maximum*" scenario, 60% of the 479 modeled concentrations are within a factor of 3.16 of the measured concentration and 96% are within a factor of 10. Therefore the residual error that represents the difference between modeled and measured concentrations has a 96% confidence interval of ± 1 order of magnitude. This means that 96% of the measured concentration data is within and order of magnitude or less of the corresponding modeled concentration. From this we conclude that agreement between

modeled and measured PCB concentrations in air is satisfactory. This exercise demonstrates that the model is providing a verifiable description of PCB concentrations in the atmosphere of the Northern Hemisphere.

In the global scale modeling of PCBs, the most important aspect of the emissions profile is the geographical distribution of emissions to air, and the relationship between emissions of the different congeners, and not the absolute amount emitted. Recognizing our goals, we have selected the "*default*" emission scenario as most appropriate for use in our model assessments since it produces modeled concentrations with slopes between modeled and measured data closest to unity. The "*default"* emissions scenario therefore produces model results that are most representative of the temporal, spatial, and congener-to-congener variability in air concentrations that are observed at long-term monitoring stations.

Table 5.3.1. Sources of information for long-term monitoring data of atmospheric PCB concentrations.

Abbreviation	Site Name	BETR-Global Model Region	Location	Data period Used in Analysis	Data availability
Zeppelin	Zeppelin Station	14	Svalbard, Norway	1998 – 2000	[a]
IADN EGH	IADN - Eagle Harbour	55	Michingan, USA	1991 – 2000	[b]
IADN BNT	IADN - Burnt Island	55	Ontario, Canada	1993 – 2000	[b]
Hazelrigg	Hazelrigg Weather Station	60	Lancaster, England	1994 – 2000	[c]
CZK	Kosetice Observatory	61	Czech Republic	1999 – 2000	[a]
IVL Rorvik	Rorvik	61	Rorvik, Sweden	1995 – 2000	[d]
IVL Aspvreten	Aspvreten	62	Aspvreten, Sweden	1996 – 2000	[d]
IVL Pallas	Pallas	62	Pallas, Sweden	1996 – 2000	[d]
IADN SBD	IADN - Sleeping Bear Dunes	79	Michigan, USA	1992 – 2000	[b]
IADN STP	IADN - Sturgeon Point	79	New York, USA	1992 – 2000	[b]
IADN PPT	IADN - Point Petre	79	Ontario, Canada	1992 – 2000	[b]

[a] – by request from Dr. Weche Aas, Norwegian Institute for Air Research (NILU), waa@nilu.no

[b] – by request from Environment Canada, http://www.msc-smc.ec.ca/iadn/Data/form/form_e.html

[c] – by request from Dr. Robert G. M. Lee, Institute of Environmental and Natural Sciences, Lancaster University, r.g.lee@lancaster.ac.uk

[d] – available for download from IVL Swedish Environmental Research Institute, http://www.ivl.se/miljo/db/startkart.asp

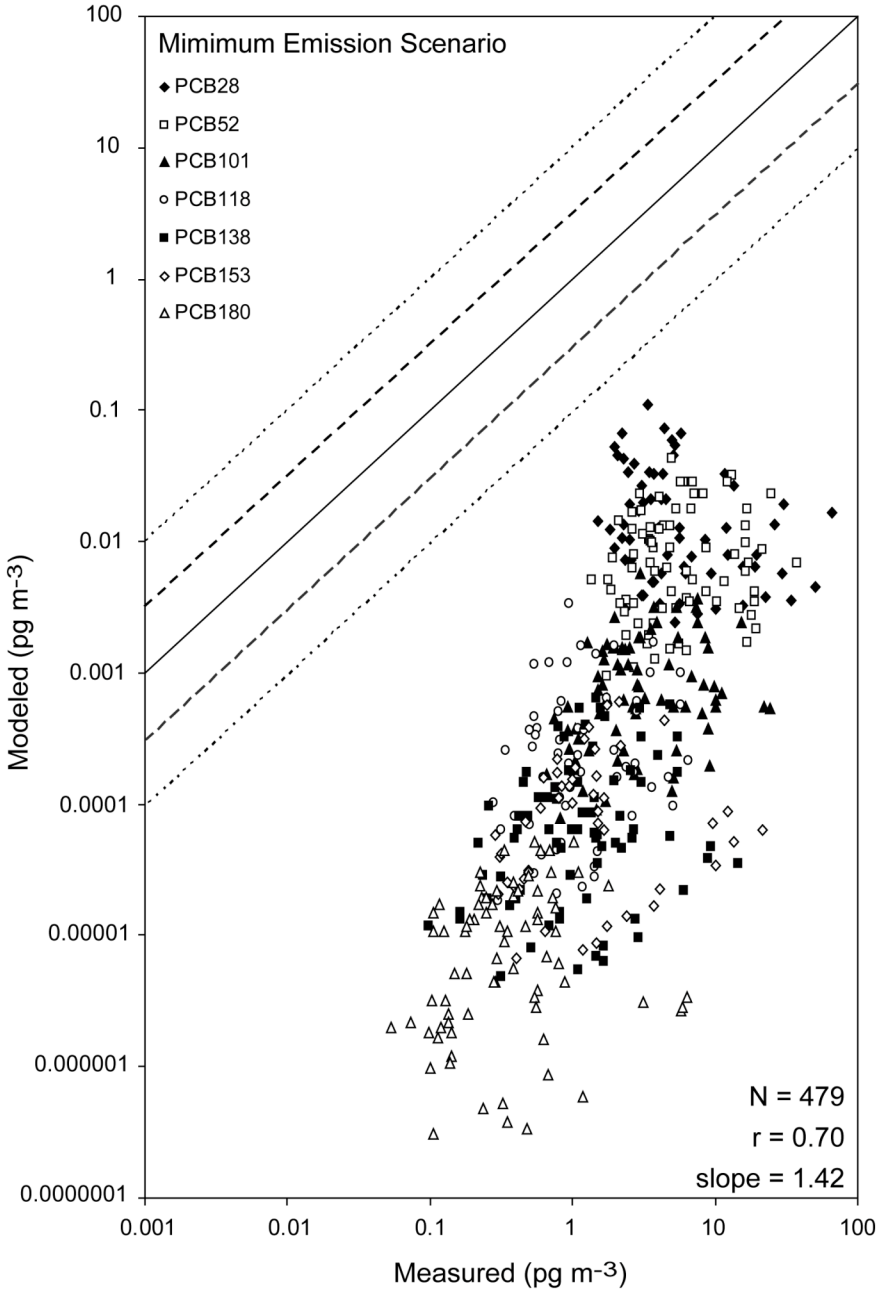

Figure 5.3.1. Comparison of yearly averaged measured and modeled atmospheric PCB congener concentrations for the "*minimum*" emission scenario reported by Breivik et al. [16,17] Measurement data are from eleven long-term monitoring stations located in seven different model regions.

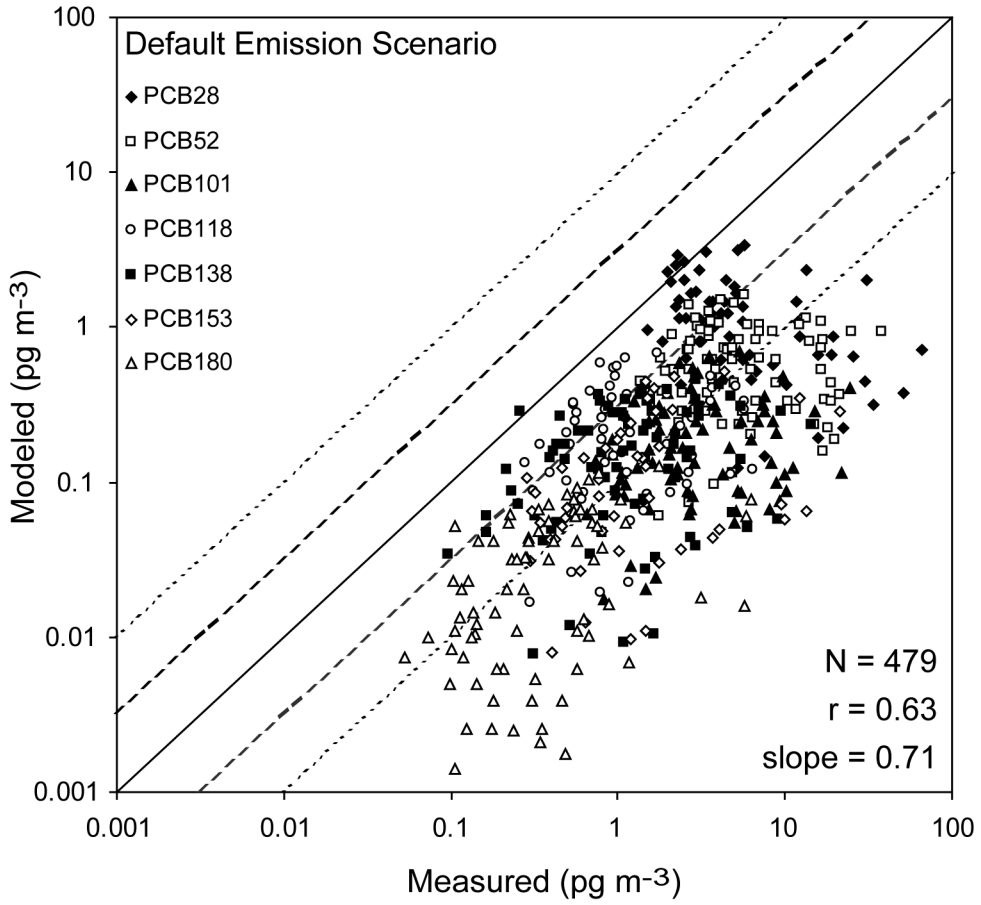

Figure 5.3.2. Comparison of yearly averaged measured and modeled atmospheric PCB congener concentrations for the "*default*" emission scenario reported by Breivik et al. [16,17] Measurement data are from eleven long-term monitoring stations located in seven different model regions.

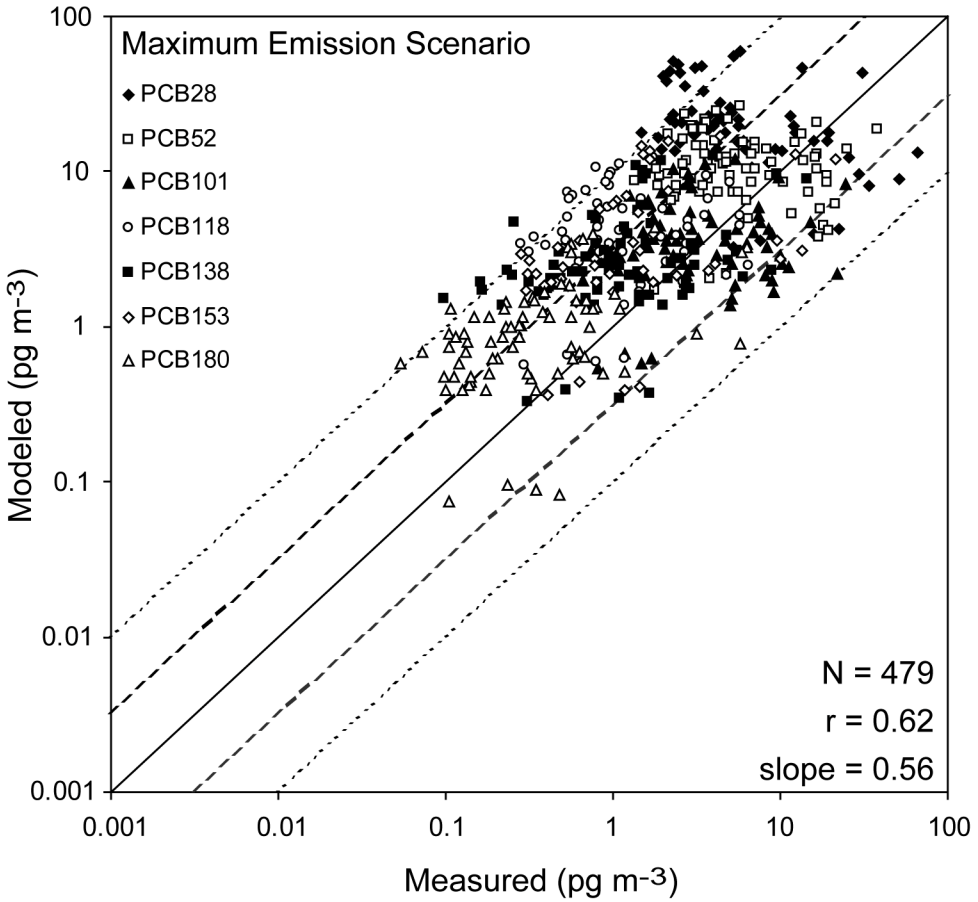

Figure 5.3.3. Comparison of yearly averaged measured and modeled atmospheric PCB congener concentrations for the "*maximum*" emission scenario reported by Breivik et al. [16,17] Measurement data are from eleven long-term monitoring stations located in seven different model regions.

6.0 REGIONAL CONTRIBUTIONS TO ATMOSPERIC LOADINGS OF LEVEL I SUBSTANCES

In this section we combine information from the generic modeling and emissions estimates to calculate the fraction of total loading from the atmosphere that is attributable to sources in different regions of North America and the world.

6.1 North American Contributions to Loadings of PCBs and Toxaphene

Using the Great Lakes Transfer Efficiencies presented in Section 4.0 and the North American-scale emissions estimates in Section 5.0, we derive here the relative contribution from different regions of North America to atmospheric deposition of PCBs and toxaphene to the Great Lakes water shed. We provide results of this analysis in Figures 6.1.1 – 6.1.8.

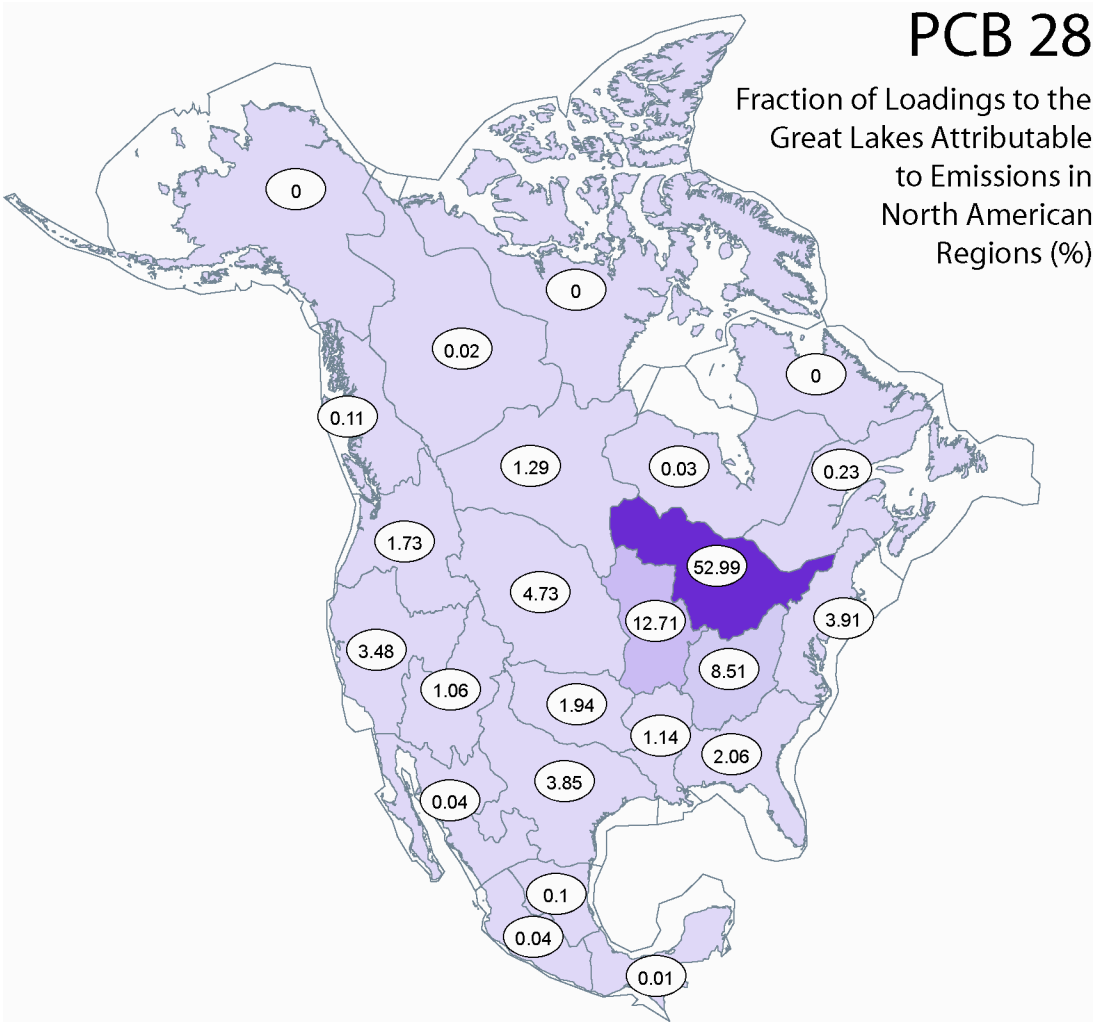

Figure 6.1.1. Fraction of atmospheric loading of PCB 28 to the Great Lakes attributable to emissions in each region of the BETR North America model.

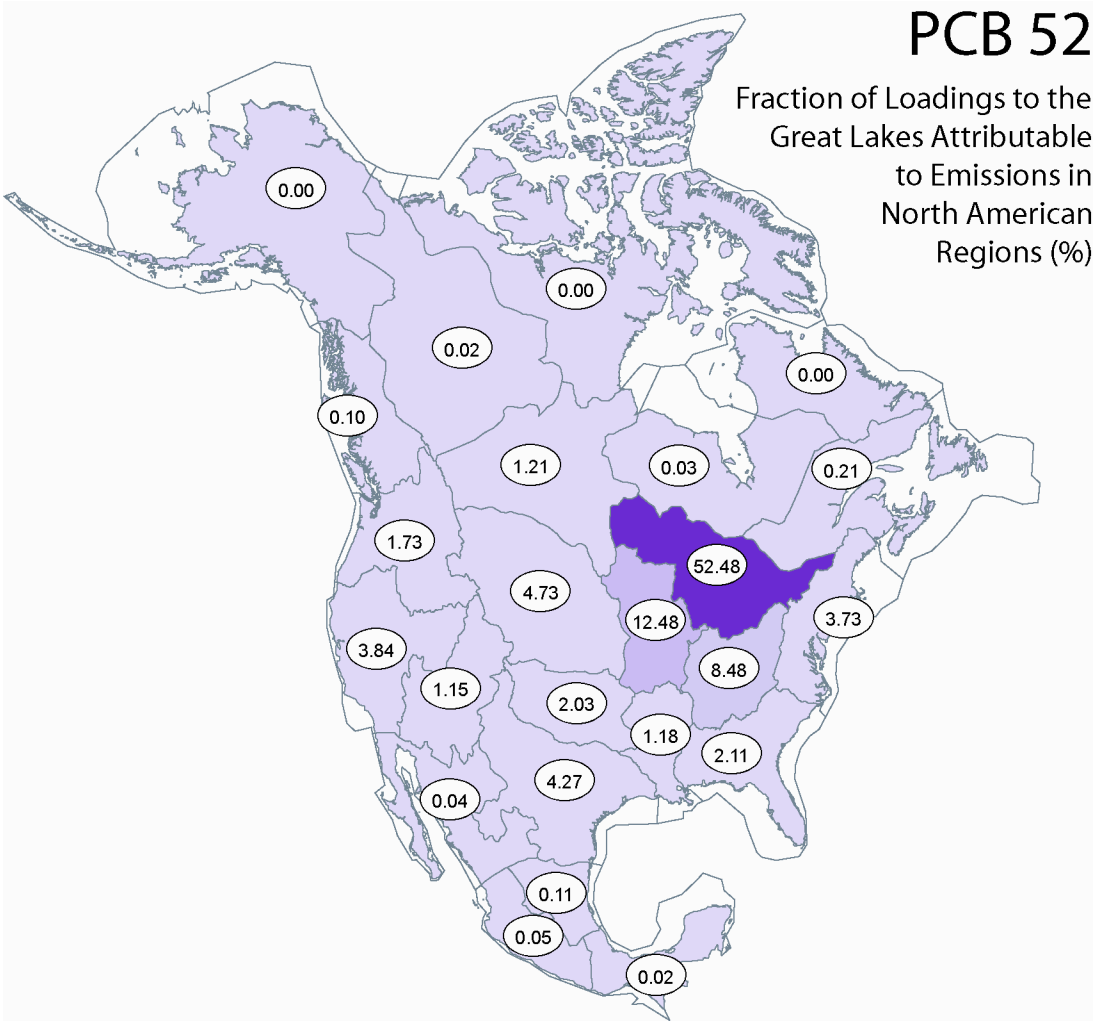

Figure 6.1.2. Fraction of atmospheric loading of PCB 52 to the Great Lakes attributable to emissions in each region of the BETR North America model.

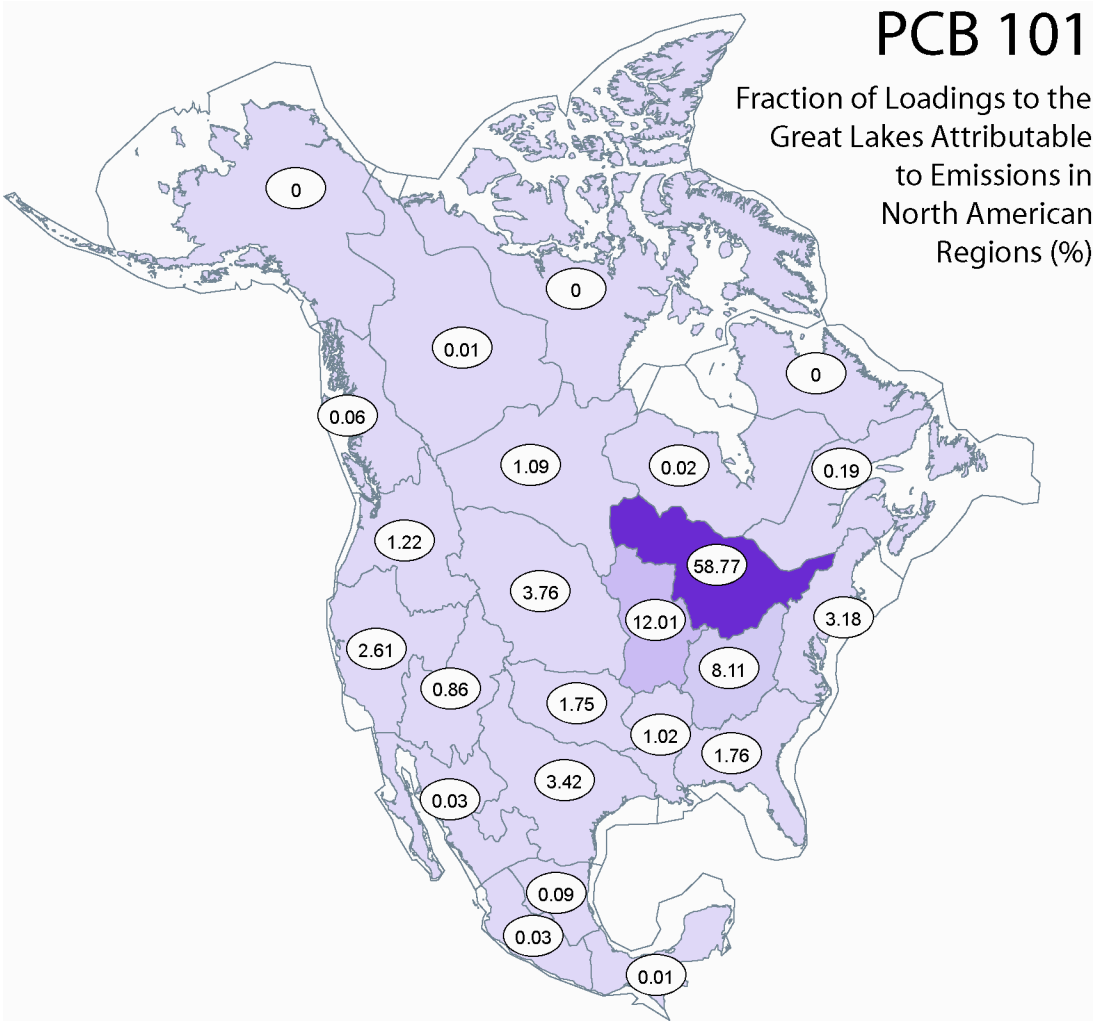

Figure 6.1.3. Fraction of atmospheric loading of PCB 101 to the Great Lakes attributable to emissions in each region of the BETR North America model.

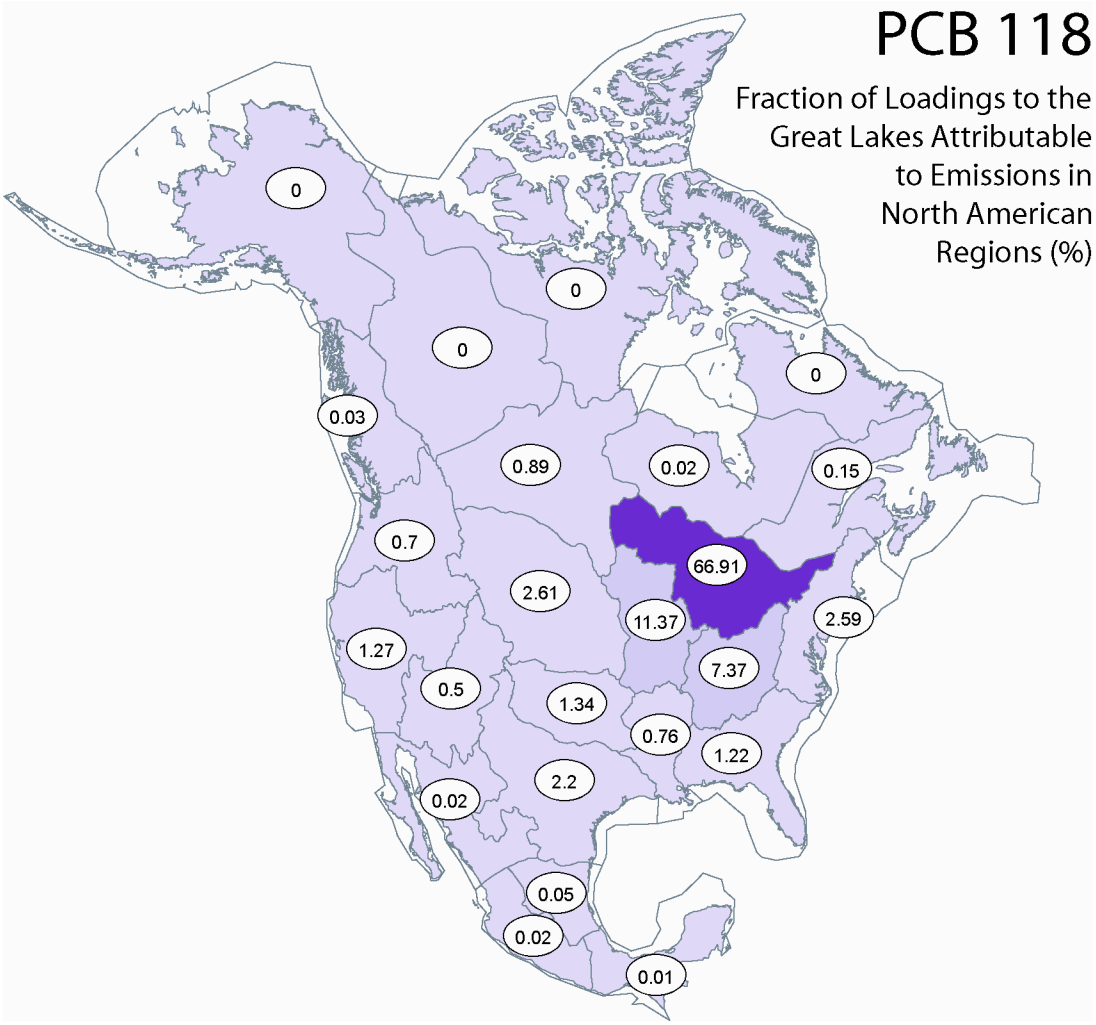

Figure 6.1.4. Fraction of atmospheric loading of PCB 118 to the Great Lakes attributable to emissions in each region of the BETR North America model.

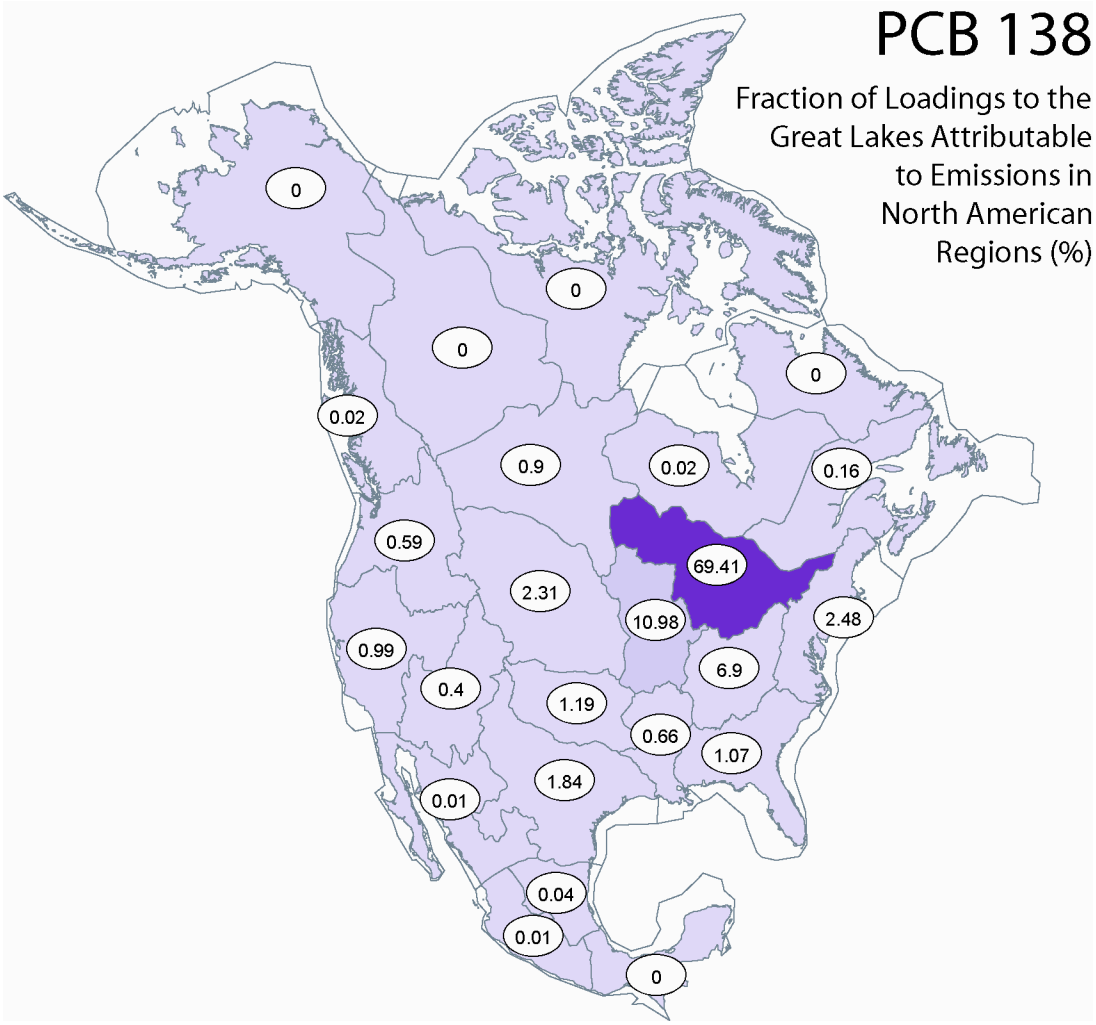

Figure 6.1.5. Fraction of atmospheric loading of PCB 138 to the Great Lakes attributable to emissions in each region of the BETR North America model.

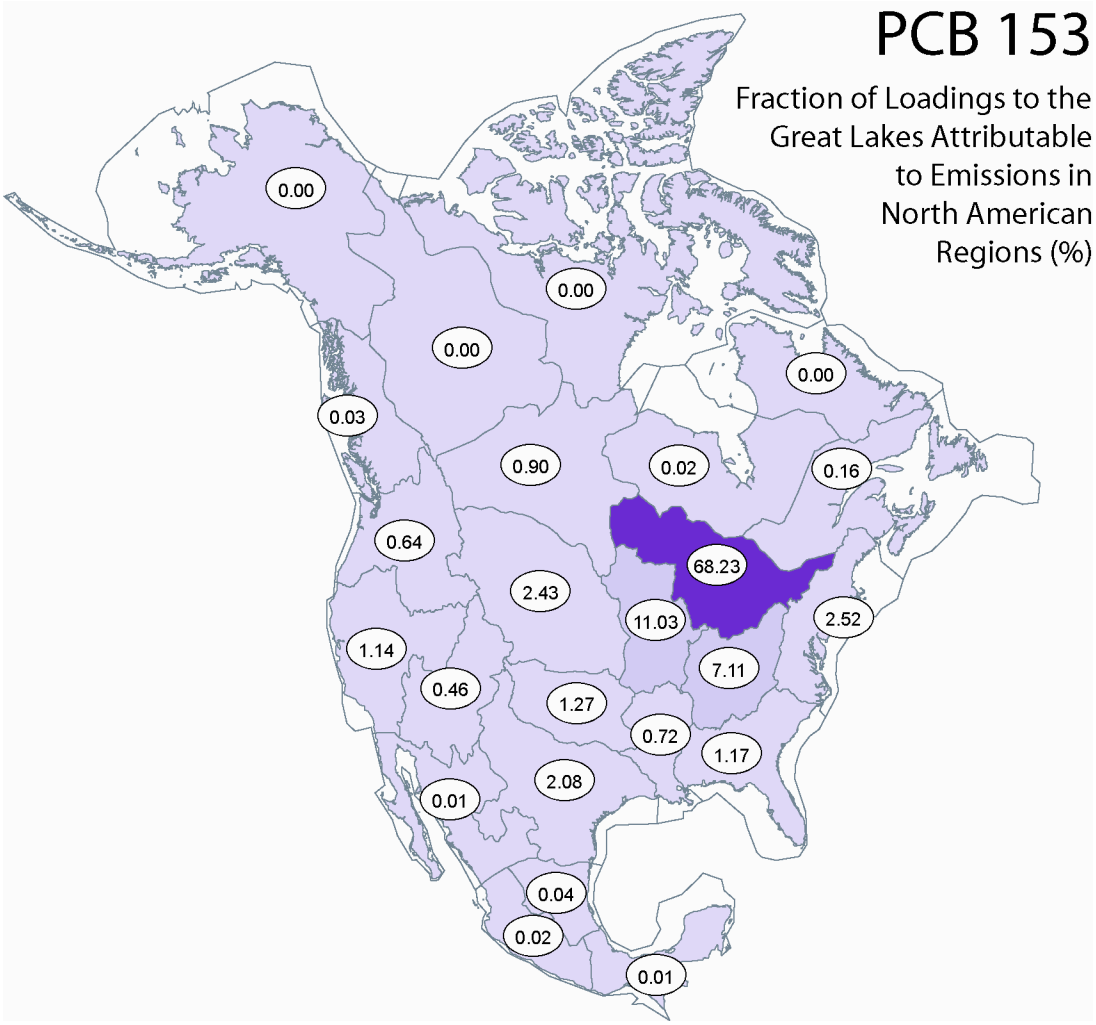

Figure 6.1.6. Fraction of atmospheric loading of PCB 153 to the Great Lakes attributable to emissions in each region of the BETR North America model.

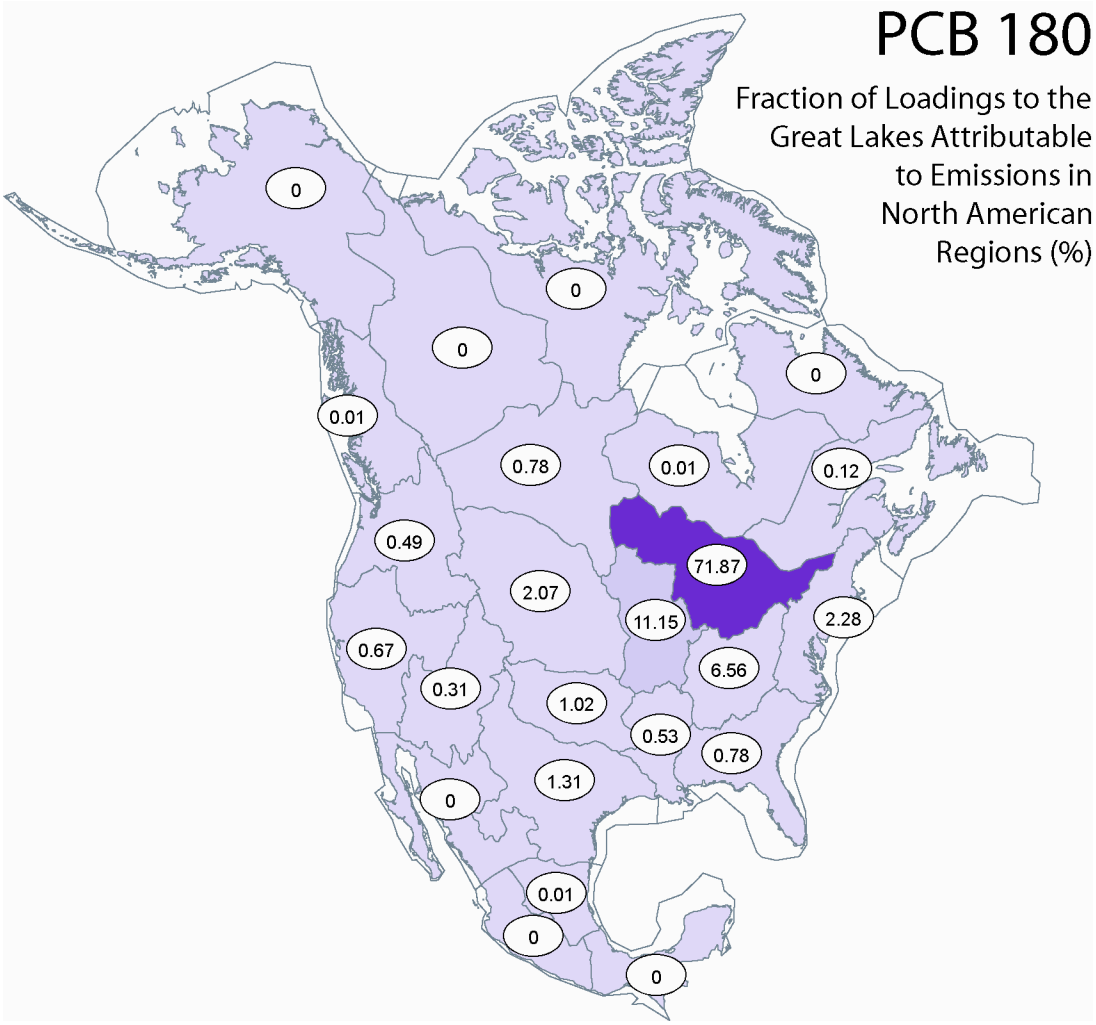

Figure 6.1.7. Fraction of atmospheric loading of PCB 180 to the Great Lakes attributable to emissions in each region of the BETR North America model.

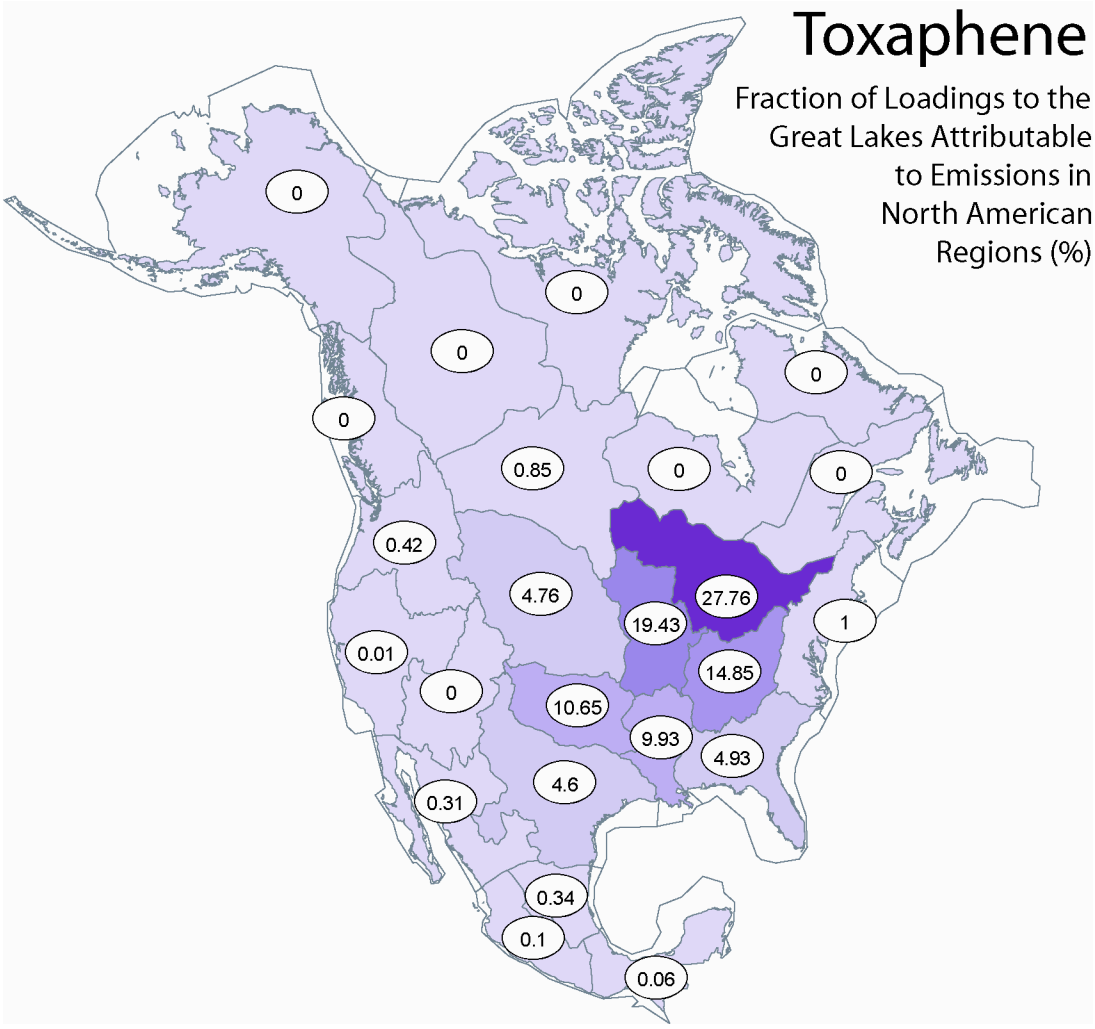

Figure 6.1.8. Fraction of atmospheric loading of toxaphene to the Great Lakes attributable to emissions in each region of the BETR North America model.

As can be seen from Figures Figures 6.1.1 – 6.1.7, the majority of PCB deposition from the atmosphere to the Lakes for all of the congeners examined is due to emissions within the Great Lakes Basin. Moreover, the relative contribution of local sources increases with increasing chlorination level, and ranges from 53% for PCB 28 and PCB 52 to 72% for PCB 180.

In interpreting these results it is important to consider issues that impact their reliability. First of all, we note that our estimates of contributions to Great Lakes loadings reflect the cumulative emissions of PCBs to the atmosphere over the entire use history of these compounds. Because of data limitations associated with applying the country-specific global-scale emissions estimates of Breivik et al. [16,17] at the North American scale, we have not examined the relative contributions to loadings at the end of the emission scenario in the North American model. The emissions inventory only provides an estimate of total emissions in the United States, Canada and Mexico, and these emissions are then apportioned based on population density. Therefore we lack spatially resolved information on the relative rate of PCB emission reductions in different parts of North America. A spatially resolved emissions inventory for North America that included information about the relative rates of emission reductions in different parts of the continent would be required to perform such an analysis.

As discussed in detail by MacLeod et al.[19] the contribution of local sources of toxaphene to atmospheric deposition to the Lakes due to emissions in North America is approximately 30%. Differences between the results for toxaphene in Figure 6.1.8 and those presented by MacLeod et al. are due to different assumptions about emission patterns. MacLeod and Mackay assumed 70% emissions to soil, 25% to air, and 5% to surface water to represent typical usage of toxaphene, while this study assumes 100% emissions to air to focus on atmospheric transport and deposition explicitly, and to allow direct comparison between toxaphene and the PCB congeners.

6.2 Global Contributions to Loadings of PCBs and α-HCH

We use the BETR Global model and the data and methods described in Sections 3 through 5 to derive the relative contribution from different global regions to atmospheric loading of the PCB congeners and α-HCH. We present the results of these analyses in Figures 6.2.1 – 6.2.15. The results for the PCB congeners reflect an emission scenario representing the cumulative emissions from 1930 – 2000 under the Breivik et al. [16,17] "*default"* emission scenario, and for emissions representative of the pattern in 2000 under the "*default"* scenario.

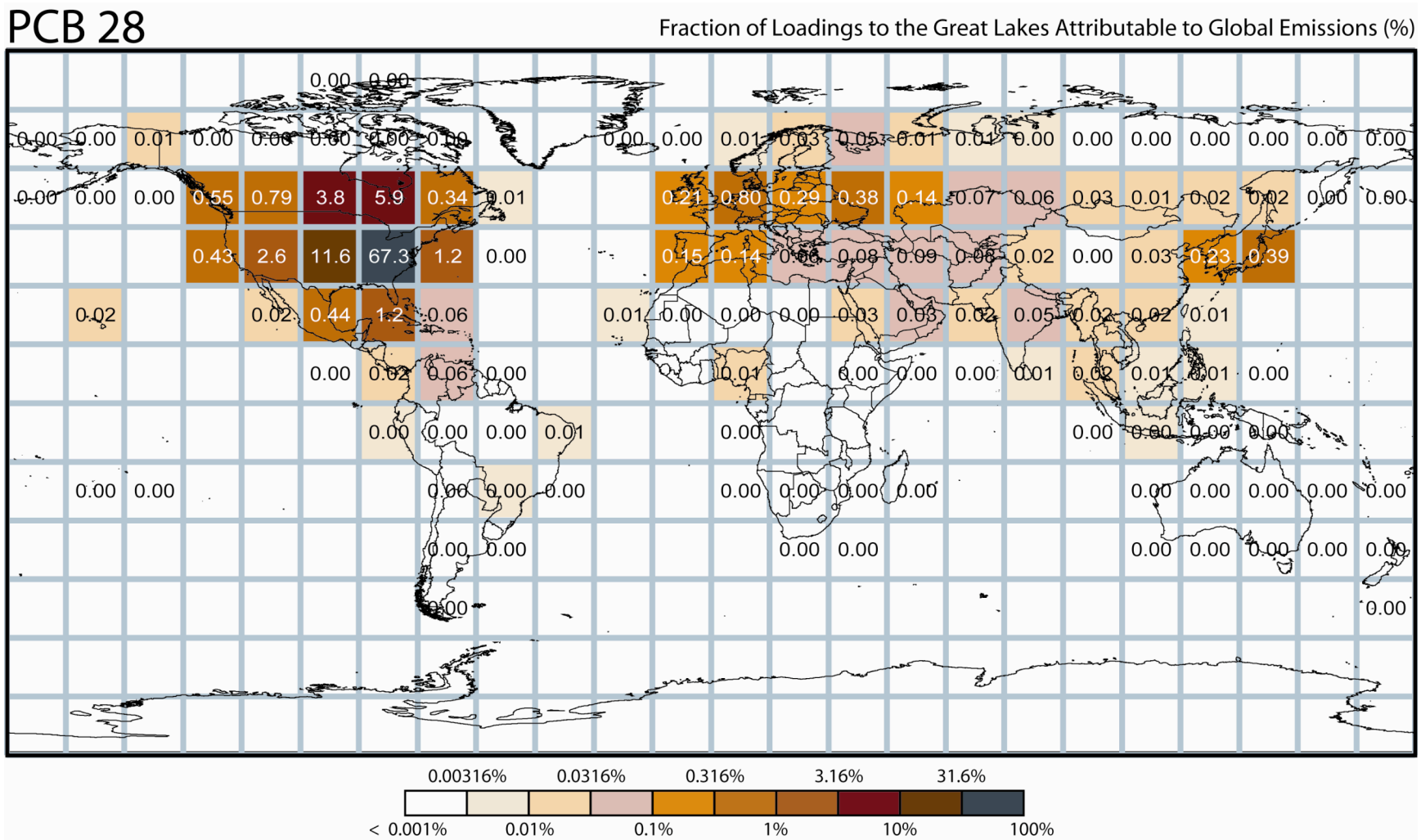

Figure 6.2.1. Estimated fraction of atmospheric loading of PCB 28 to the Great Lakes attributable to emissions in each region of the BETR Global model under the cumulative default emission scenario.

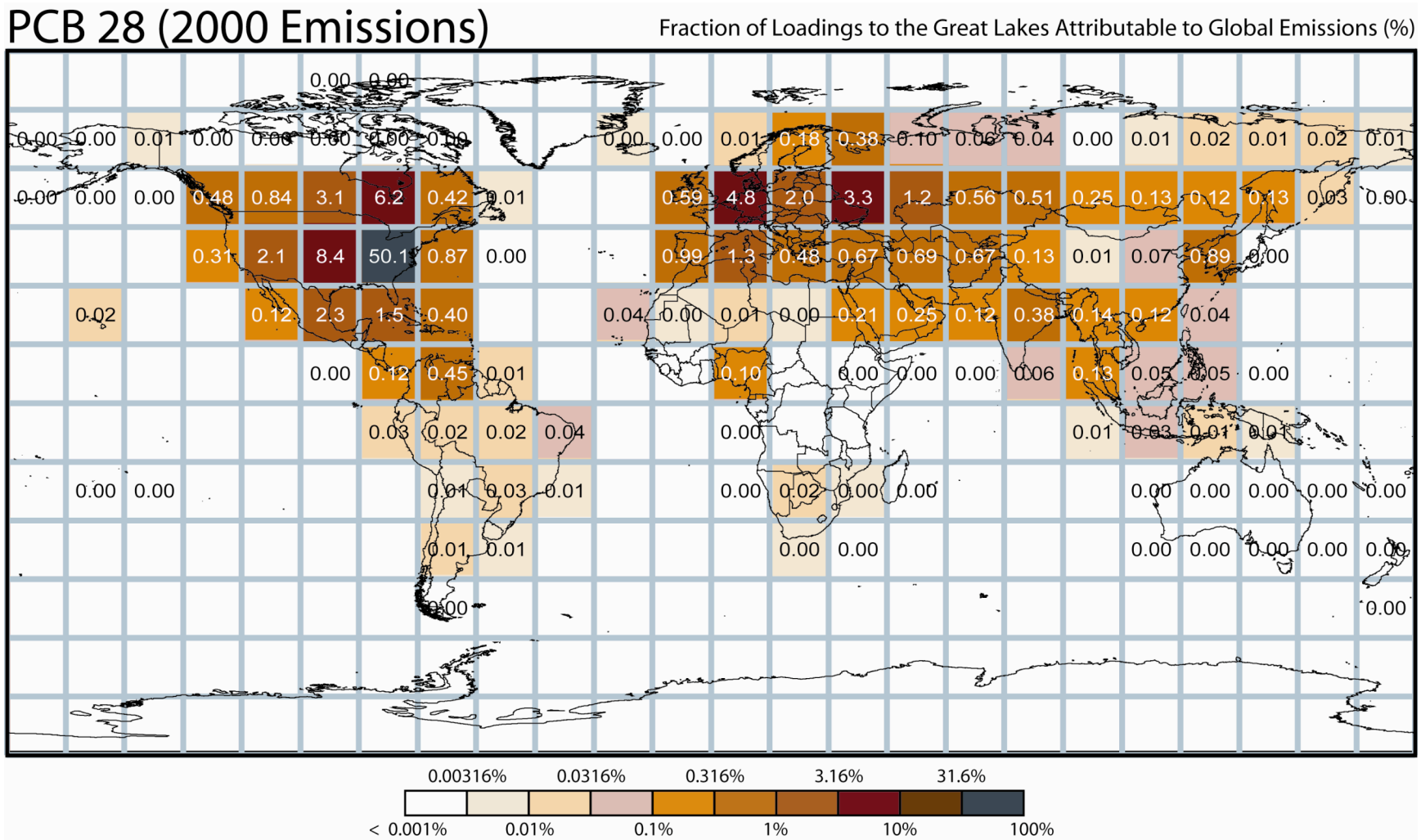

Figure 6.2.2. Estimated fraction of atmospheric loading of PCB 28 to the Great Lakes attributable to emissions in each region of the BETR Global model due to year 2000 emissions under the default emission scenario.

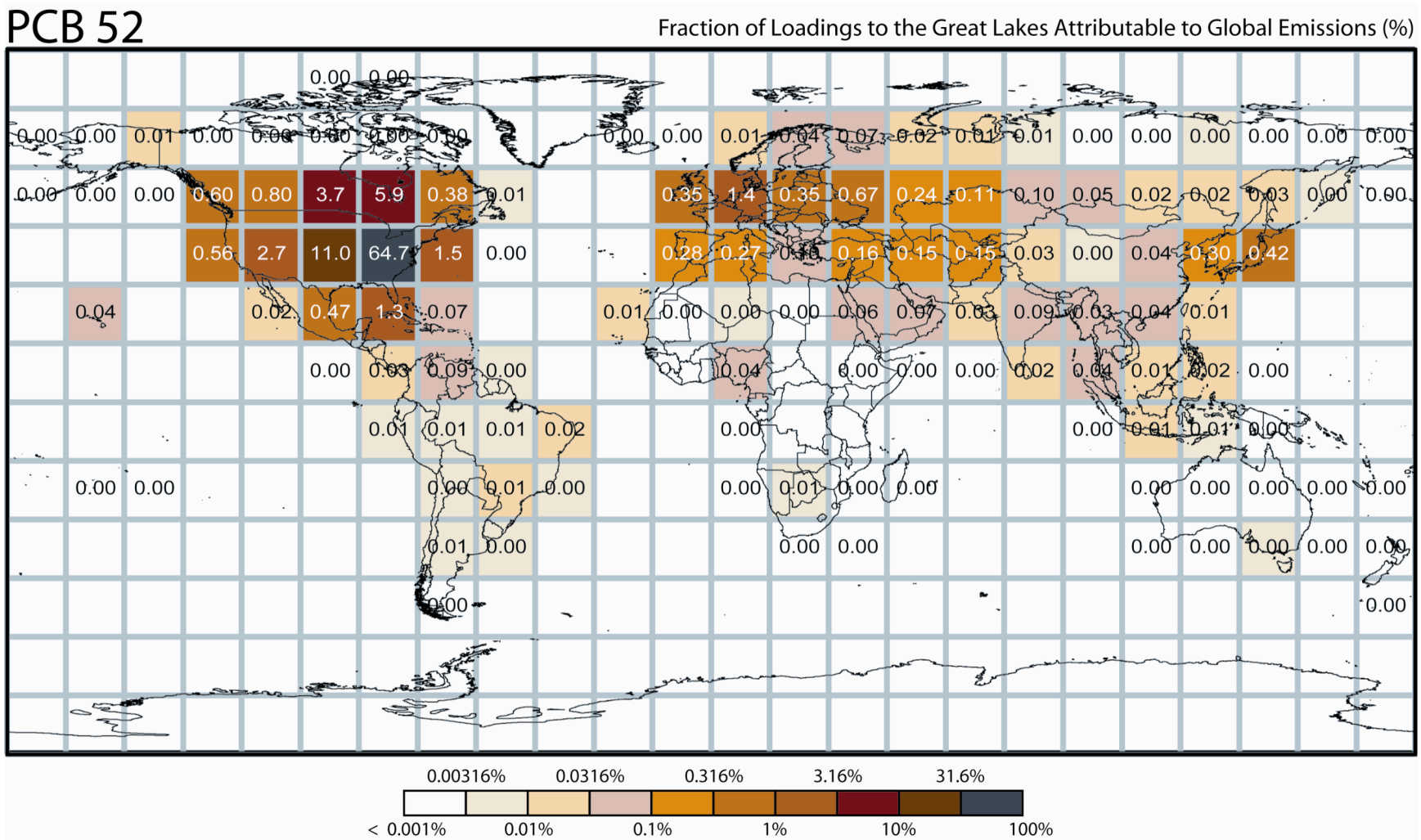

Figure 6.2.3. Estimated fraction of atmospheric loading of PCB 52 to the Great Lakes attributable to emissions in each region of the BETR Global model under the cumulative default emission scenario.

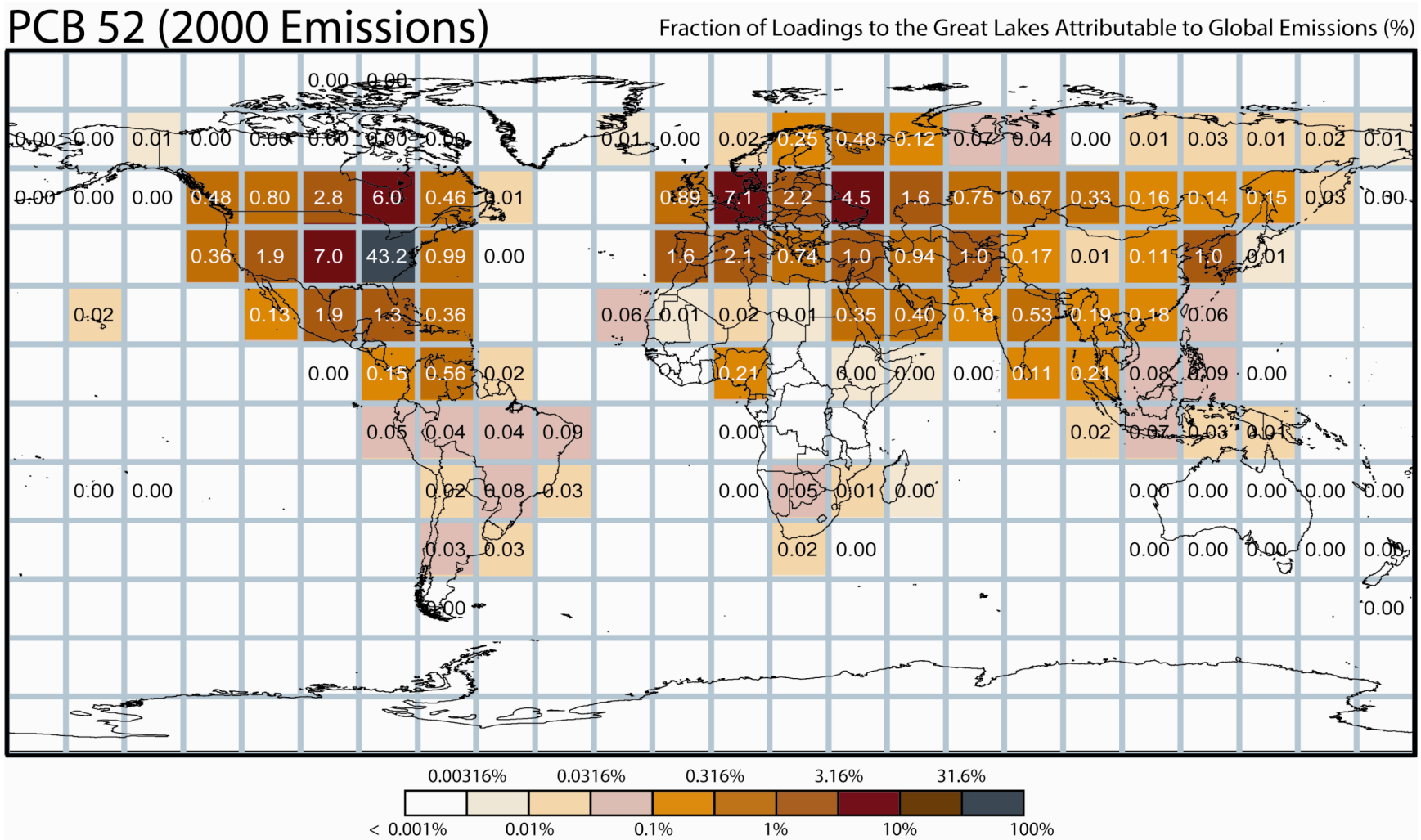

Figure 6.2.4. Estimated fraction of atmospheric loading of PCB 52 to the Great Lakes attributable to emissions in each region of the BETR Global model due to year 2000 emissions under the default emission scenario.

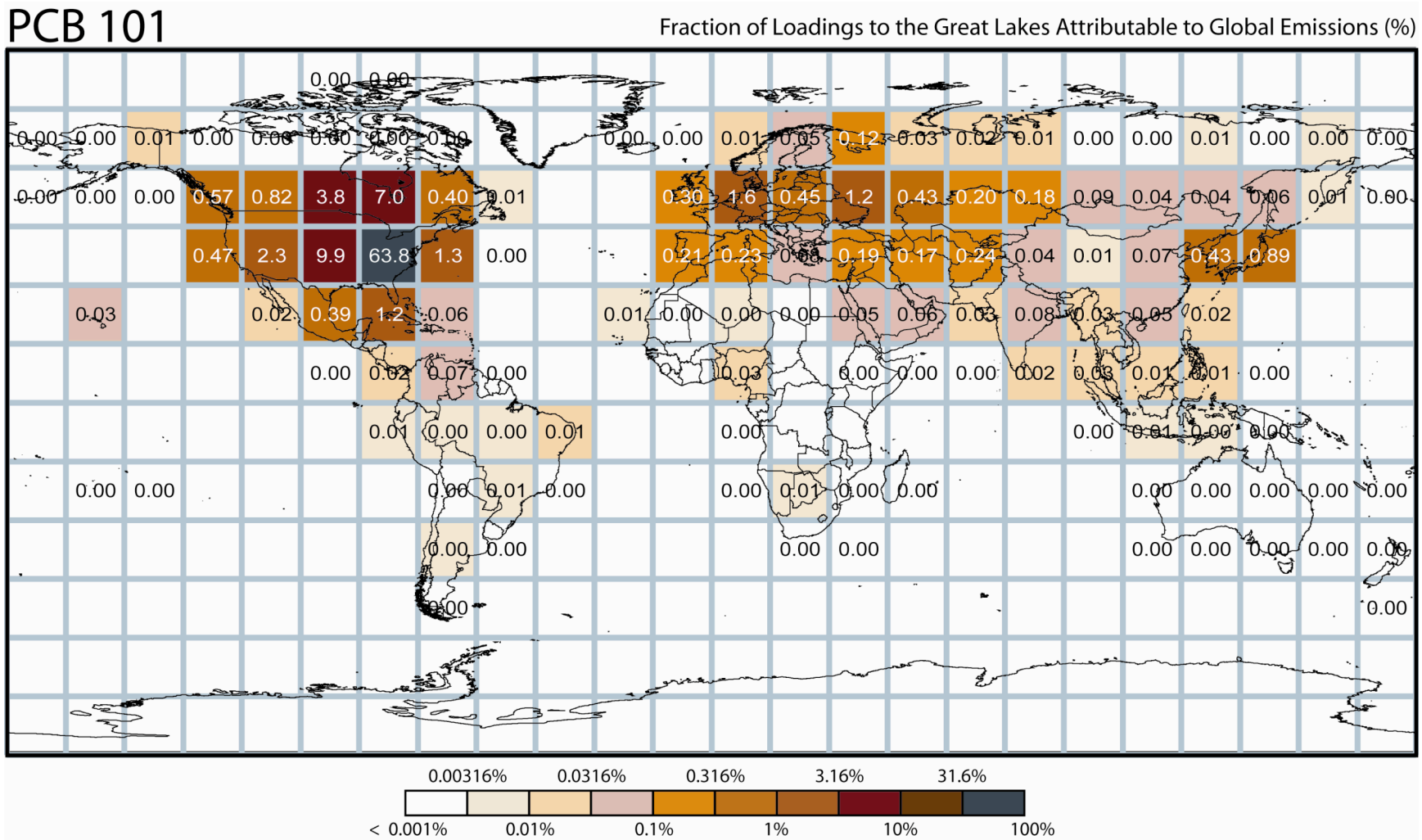

Figure 6.2.5. Estimated fraction of atmospheric loading of PCB 101 to the Great Lakes attributable to emissions in each region of the BETR Global model under the cumulative default emission scenario.

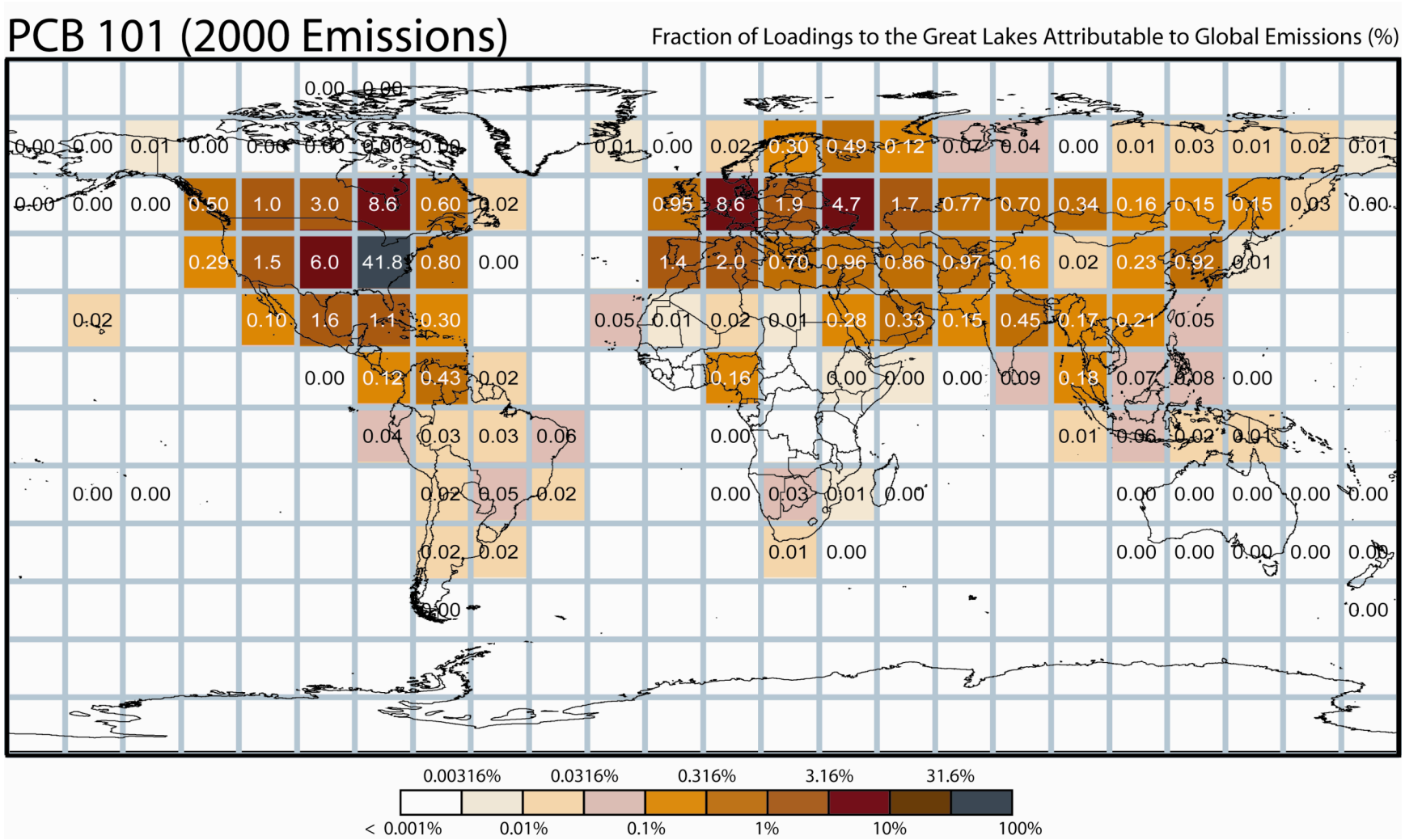

Figure 6.2.6. Estimated fraction of atmospheric loading of PCB 101 to the Great Lakes attributable to emissions in each region of the BETR Global model due to year 2000 emissions under the default emission scenario.

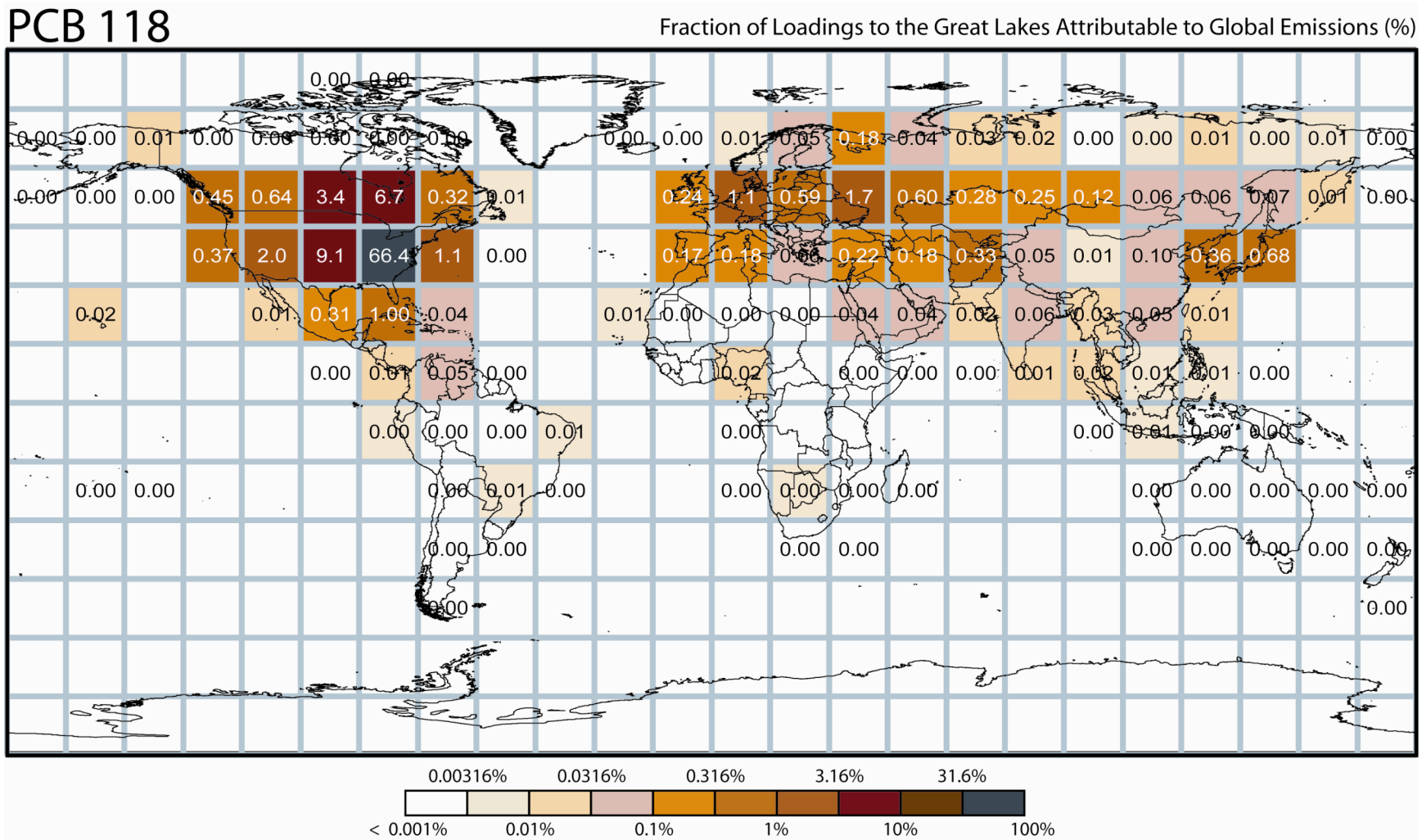

Figure 6.2.7. Estimated fraction of atmospheric loading of PCB 118 to the Great Lakes attributable to emissions in each region of the BETR Global model under the cumulative default emission scenario.

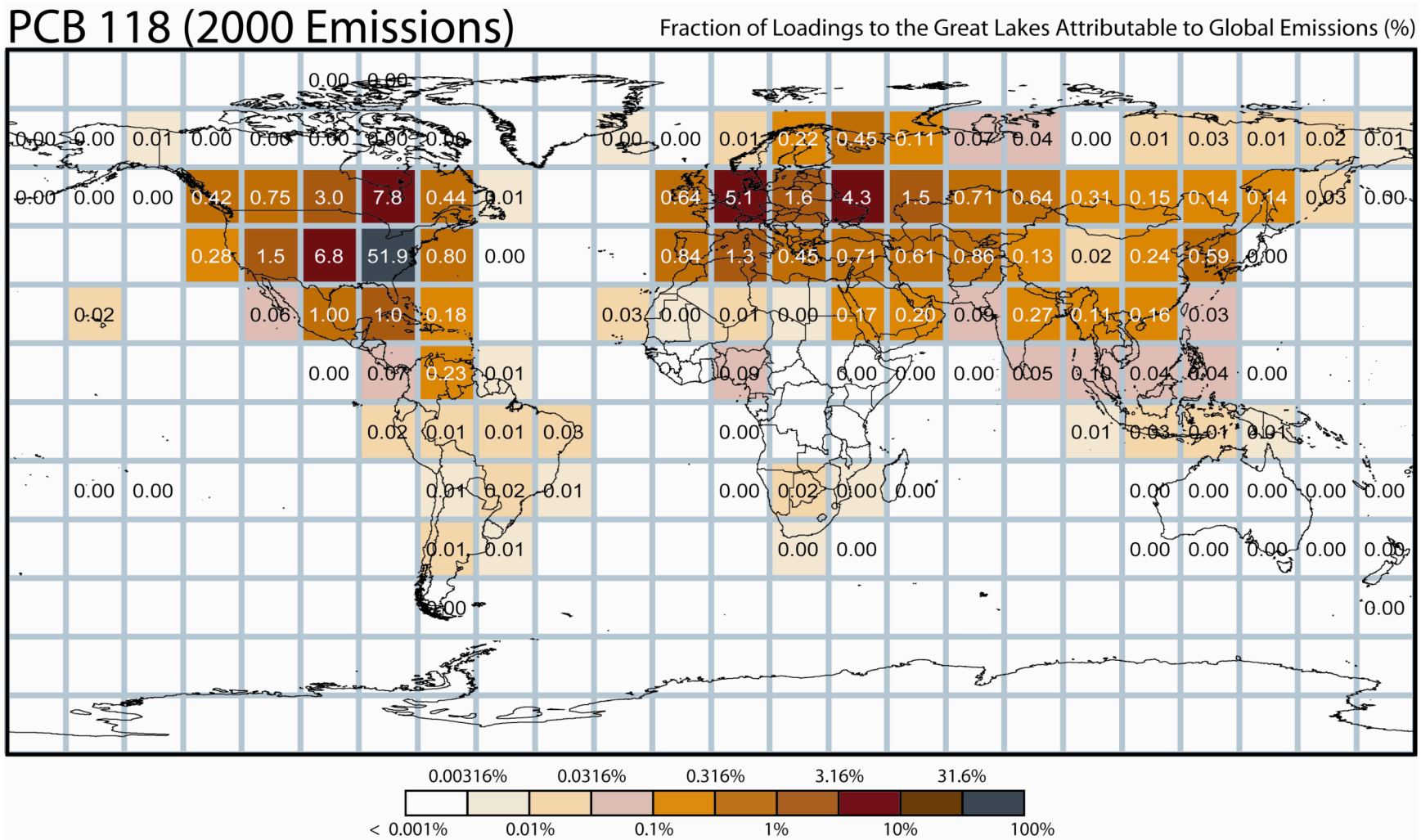

Figure 6.2.8. Estimated fraction of atmospheric loading of PCB 118 to the Great Lakes attributable to emissions in each region of the BETR Global model due to year 2000 emissions under the default emission scenario.

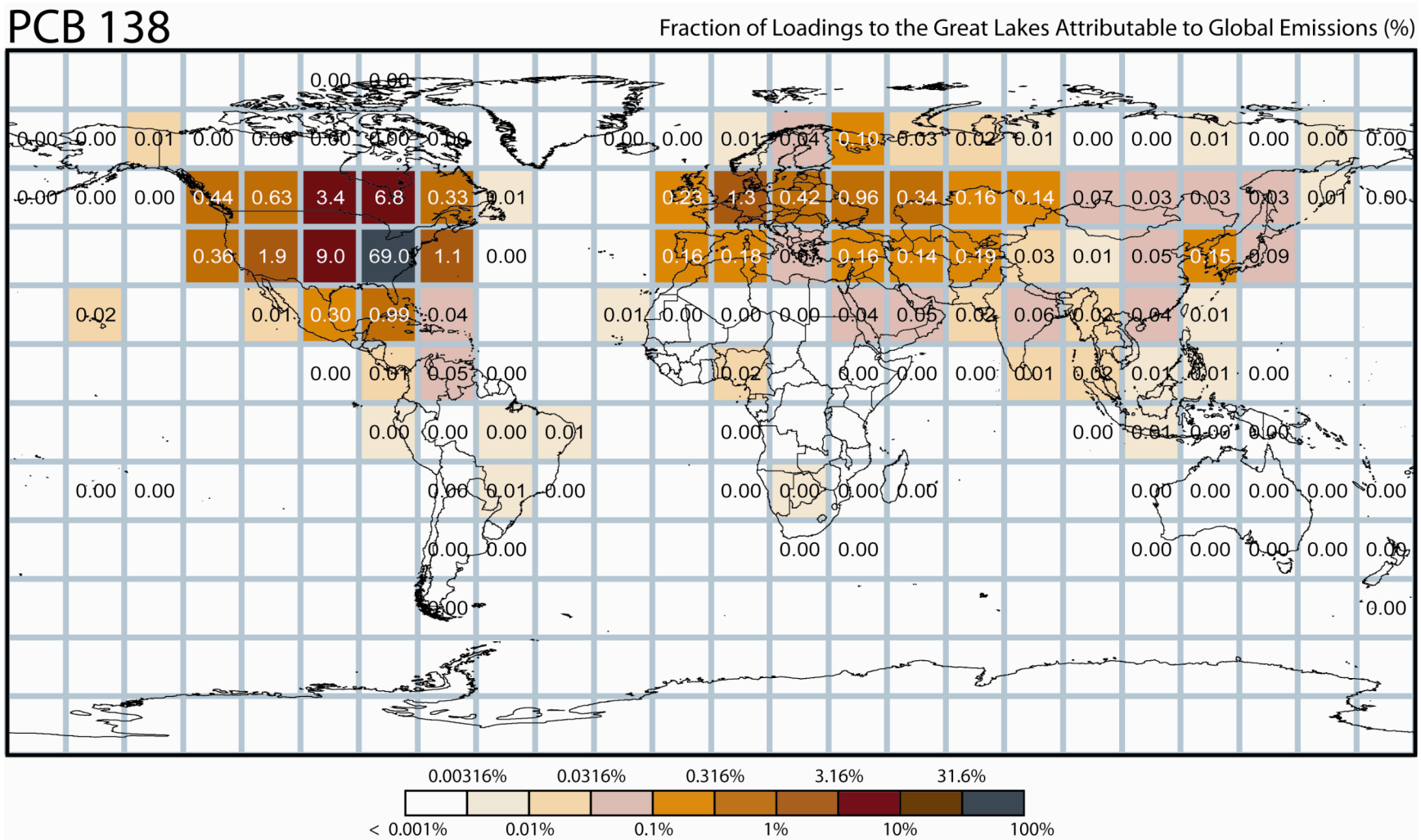

Figure 6.2.9. Estimated fraction of atmospheric loading of PCB 138 to the Great Lakes attributable to emissions in each region of the BETR Global model under the cumulative default emission scenario.

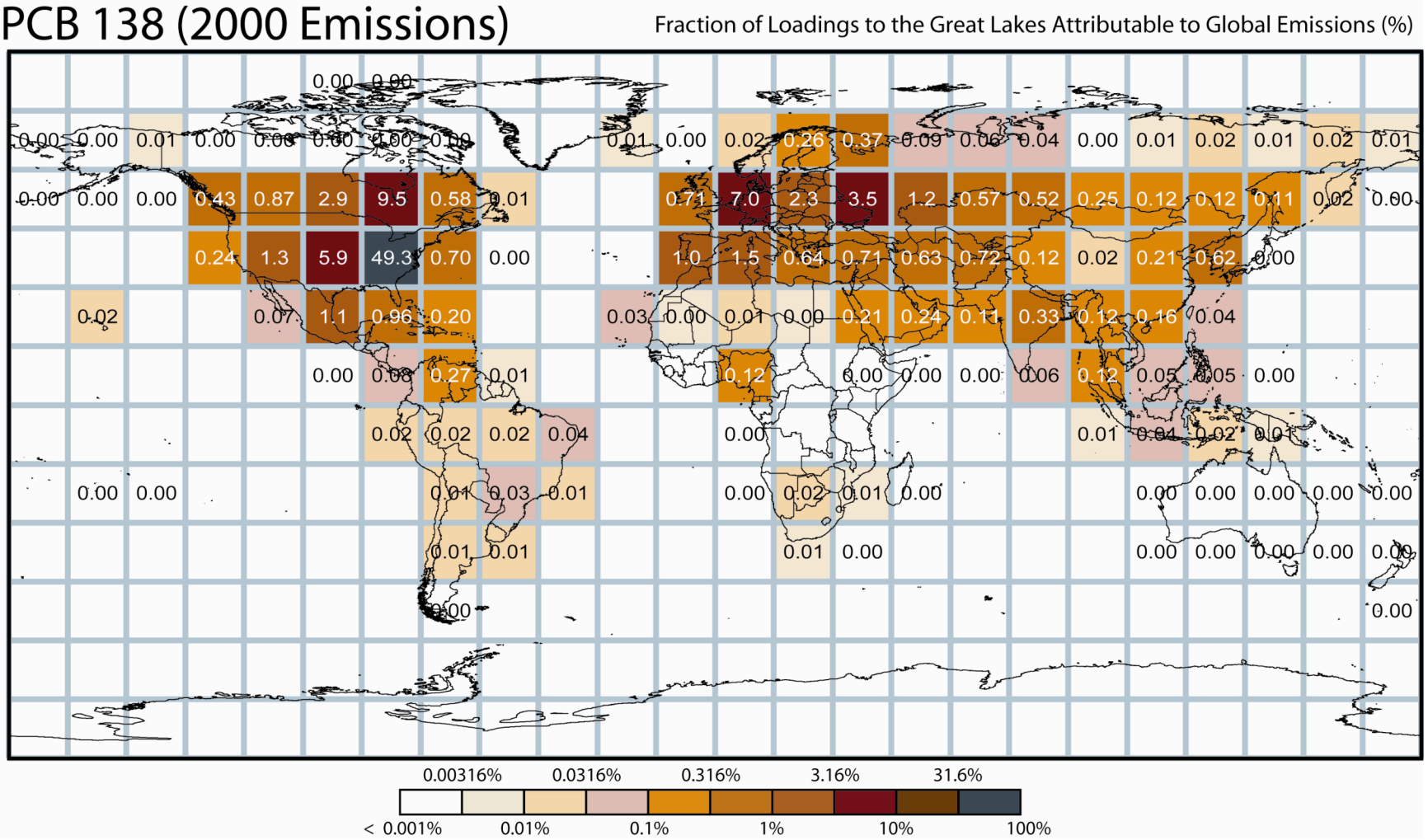

Figure 6.2.10. Estimated fraction of atmospheric loading of PCB 138 to the Great Lakes attributable to emissions in each region of the BETR Global model due to year 2000 emissions under the default emission scenario.

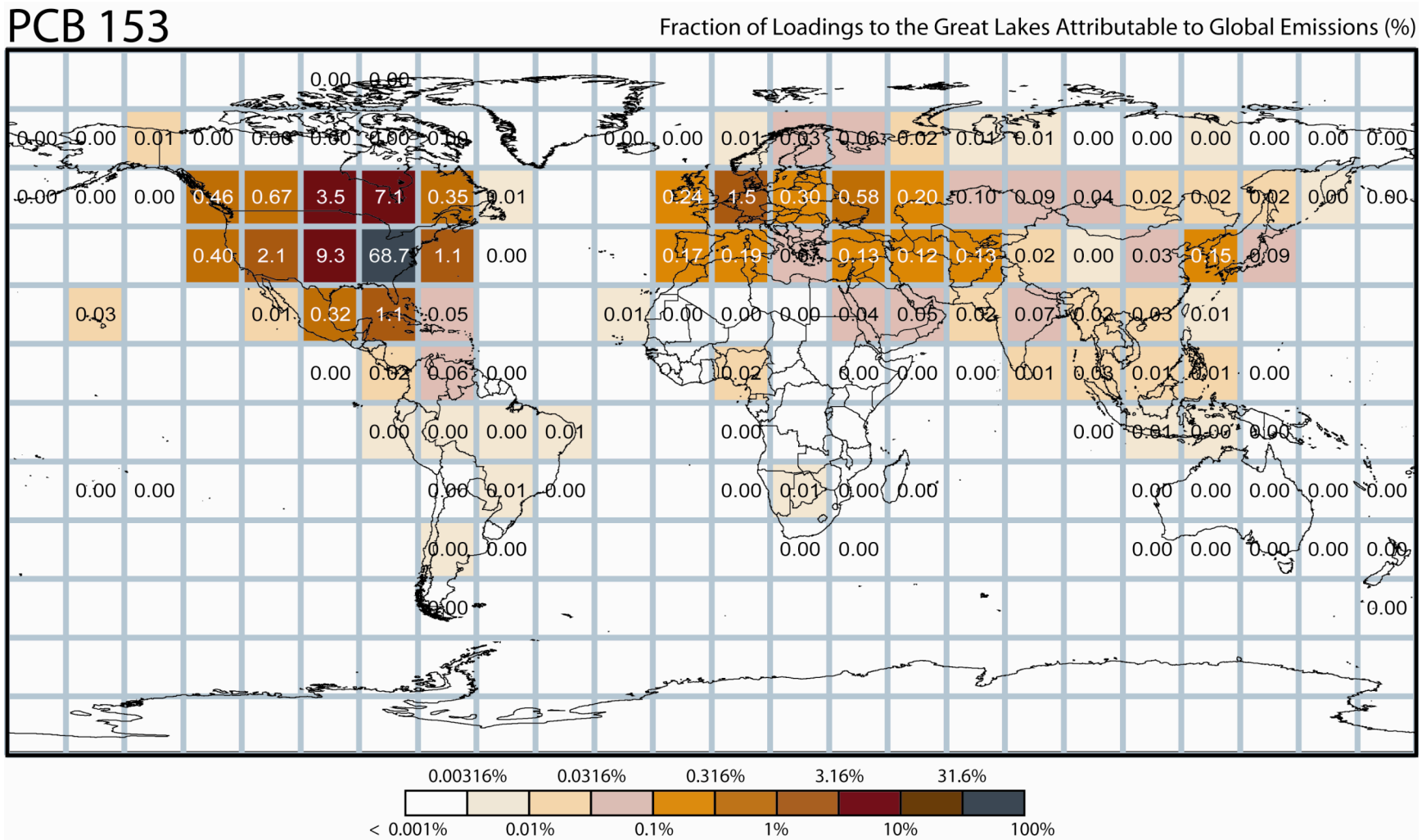

Figure 6.2.11. Estimated fraction of atmospheric loading of PCB 153 to the Great Lakes attributable to emissions in each region of the BETR Global model under the cumulative default emission scenario.

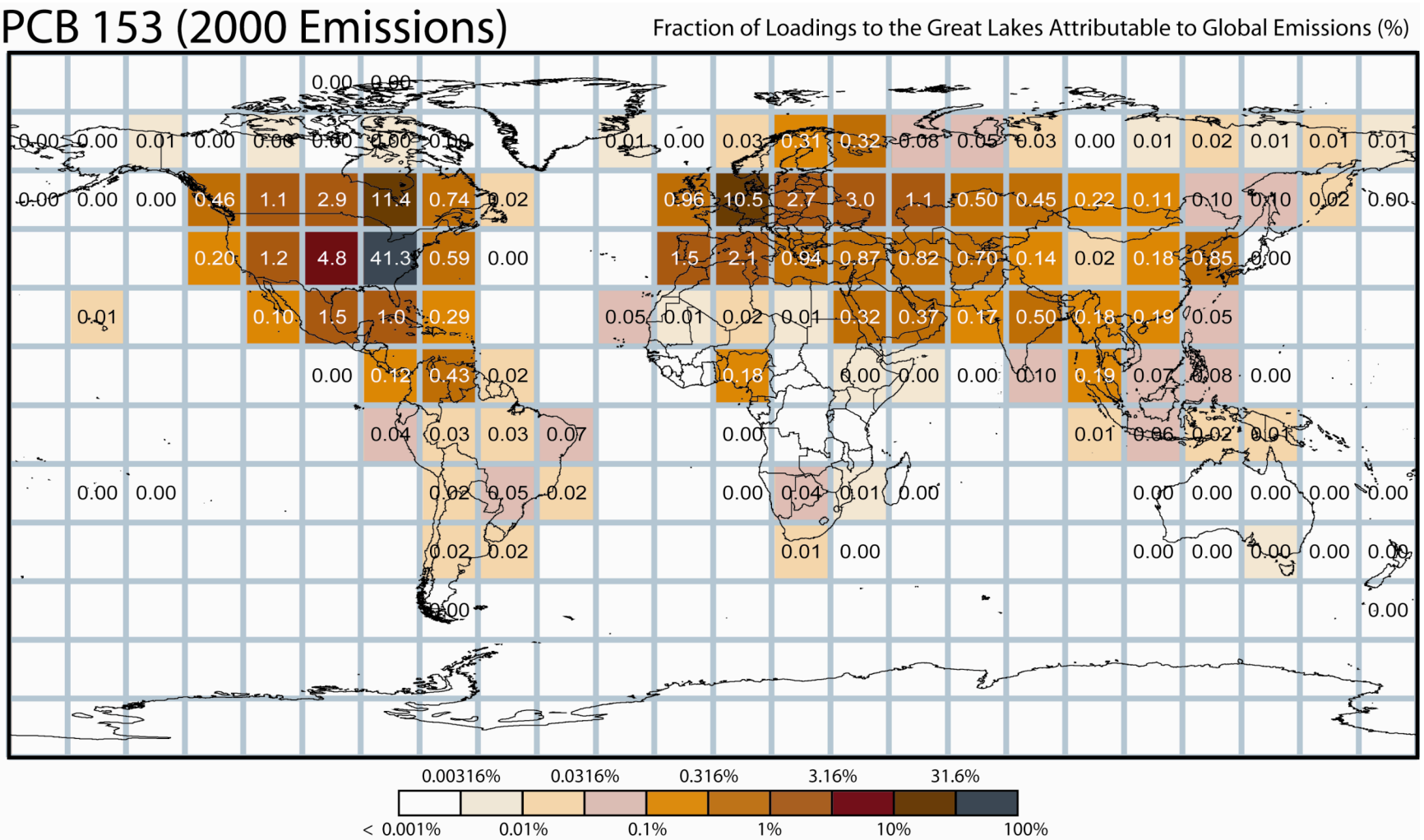

Figure 6.2.12. Estimated fraction of atmospheric loading of PCB 153 to the Great Lakes attributable to emissions in each region of the BETR Global model due to year 2000 emissions under the default emission scenario.

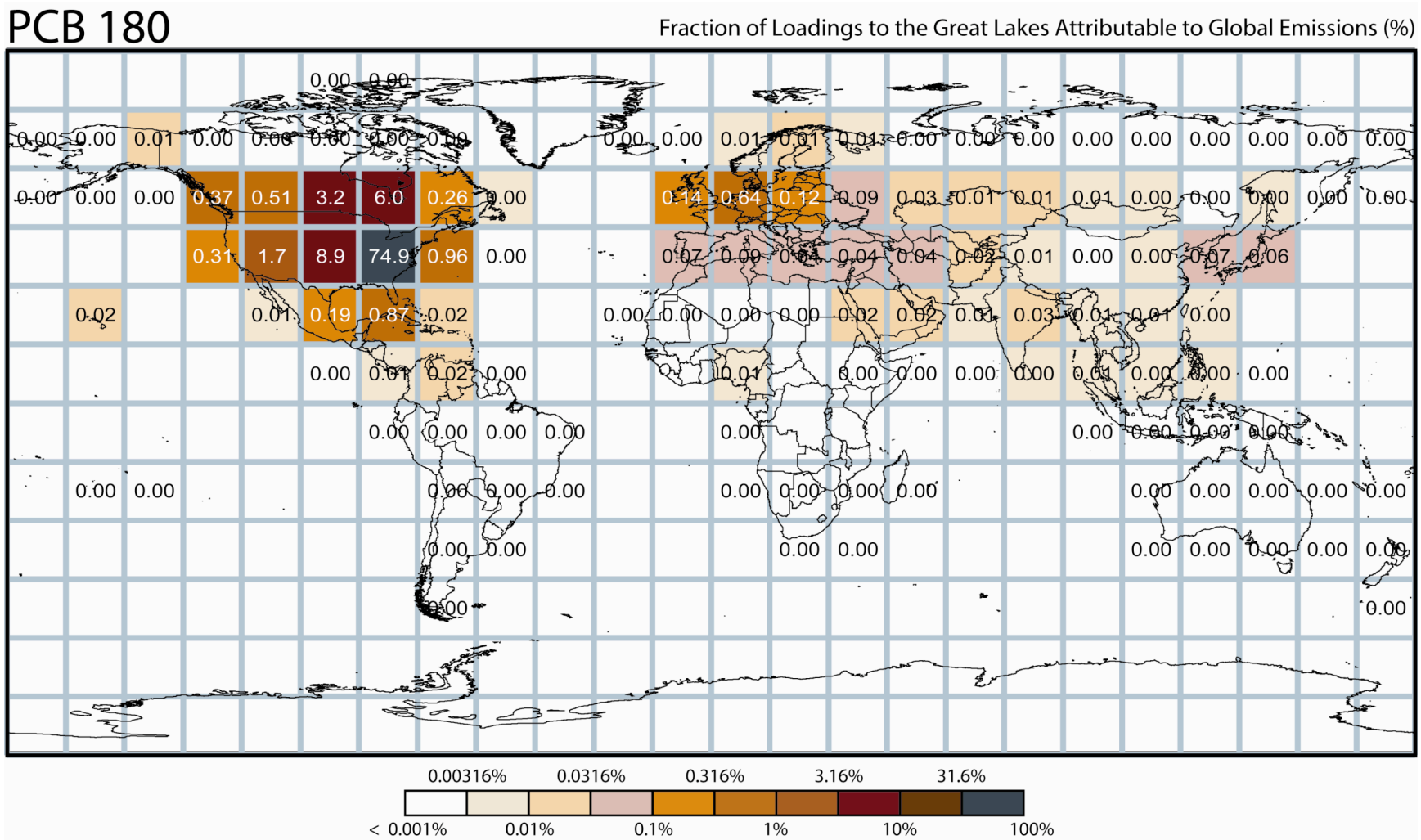

Figure 6.2.13. Estimated fraction of atmospheric loading of PCB 180 to the Great Lakes attributable to emissions in each region of the BETR Global model under the cumulative default emission scenario.

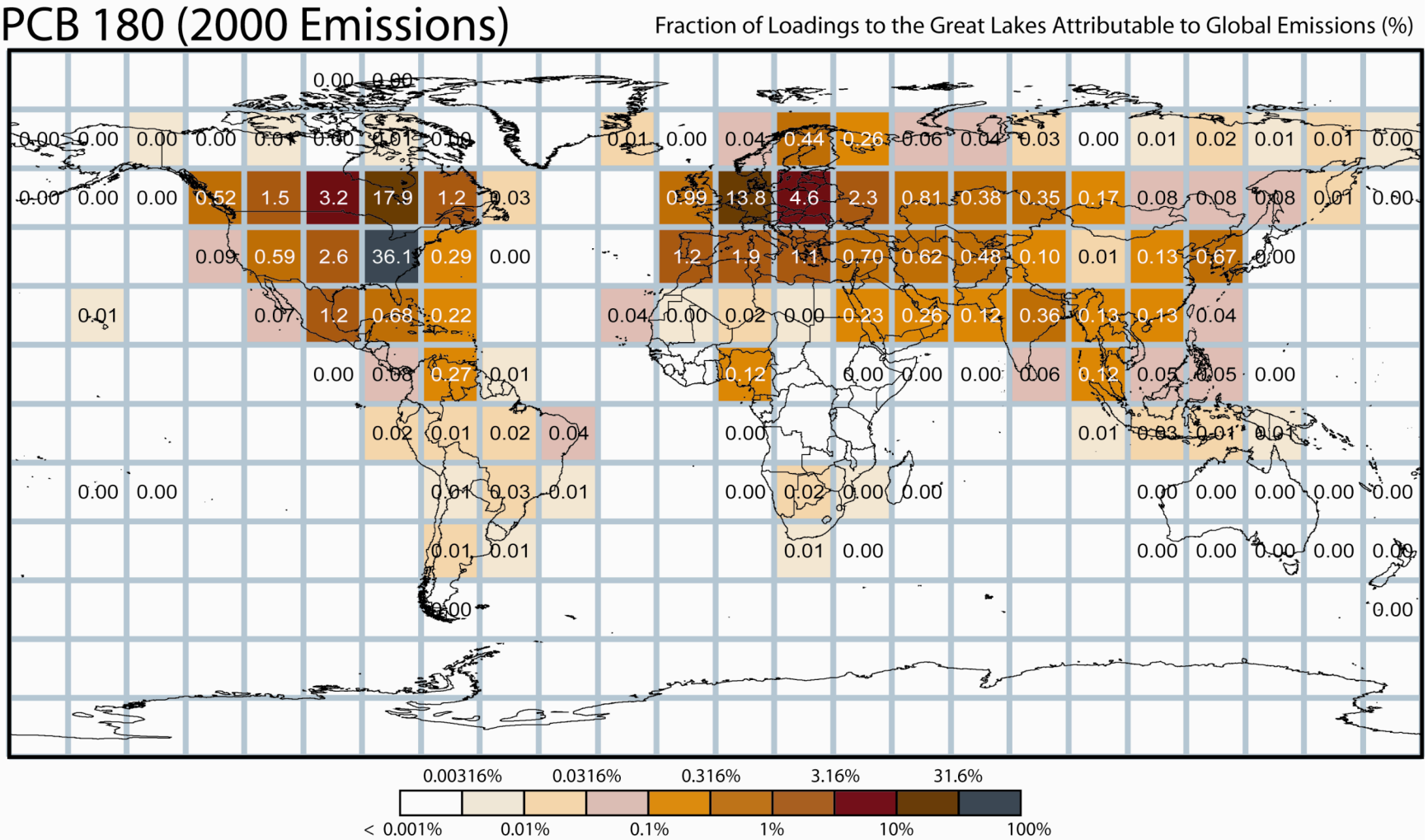

Figure 6.2.14. Estimated fraction of atmospheric loading of PCB 180 to the Great Lakes attributable to emissions in each region of the BETR Global model due to year 2000 emissions under the default emission scenario.

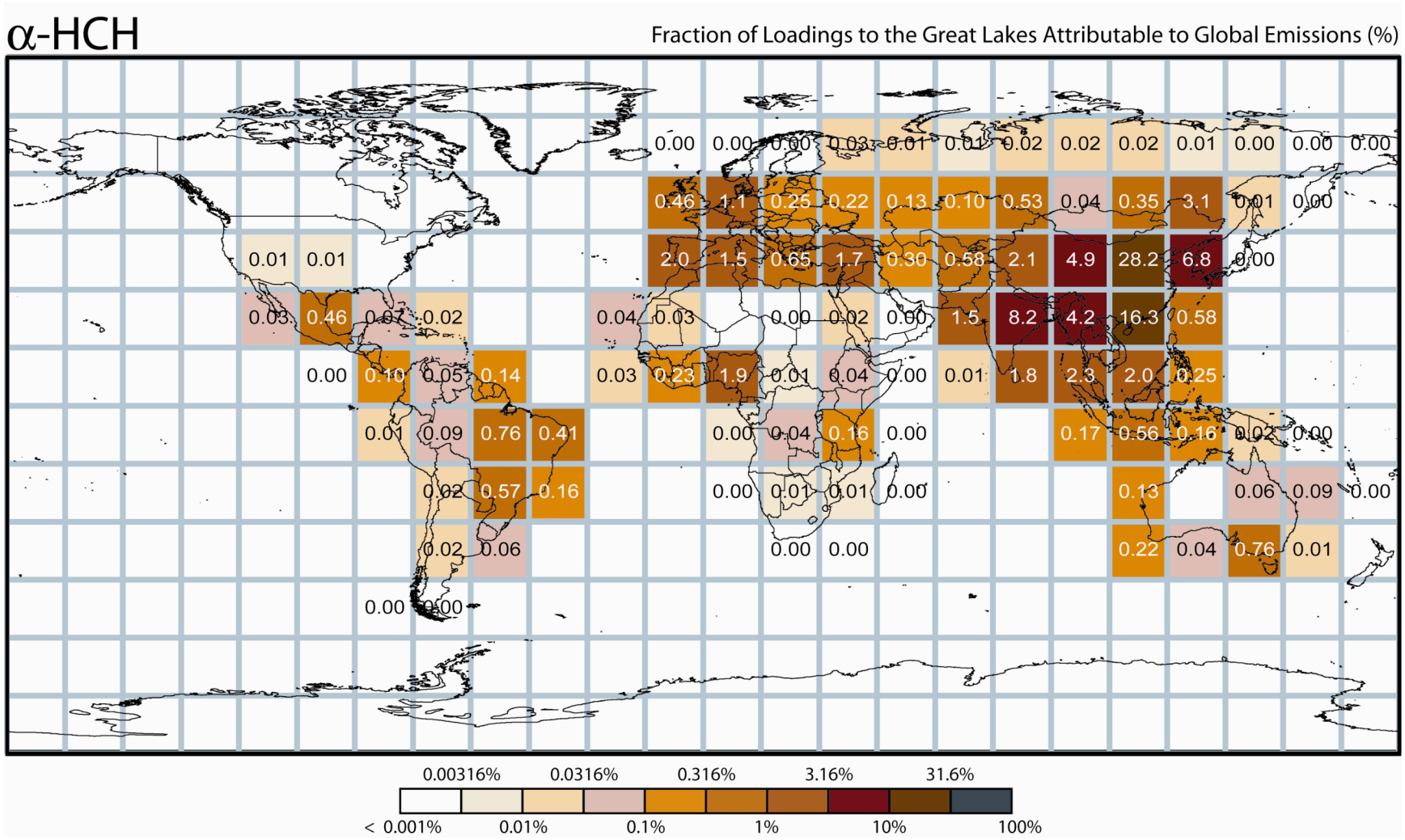

Figure 6.2.15. Estimated fraction of atmospheric loading of α-HCH to the Great Lakes attributable to emissions in each region of the BETR Global model.

In the case of the global-scale assessment for year 2000 releases, we find that the modeled contributions to atmospheric deposition to the Great Lakes for the PCB congeners shift from local sources toward more distant contributions. When cumulative (1930-2000) emissions are considered, local sources tend to dominate overall loading to the Great Lakes. But under the year 2000 scenario, there is a shift toward a larger influence of sources in Asia and particularly Eastern Europe to Great Lakes loading. Because the GLTE from all locations is identical under both emission scenarios, this shift is directly attributable to the more rapid rate of emission reductions in the United States and Canada relative to Asia and Eastern Europe.

As an example of the shift to distant sources of PCB deposition to the Great Lakes, we consider PCB 52. When we consider cumulative emissions between 1930 and 2000, greater than 70% of atmospheric loadings of PCB 52 to surface water in model regions including the Great Lakes are attributable to sources in close proximity to the Lakes, and sources in North America account for 90% of loadings. Under the year 2000 emission scenario the contribution of local sources of PCB 52 is less than 50%, the North American contribution is less than 70 %, and the bulk of the balance is made up of contributions from sources in Eastern Europe.

Atmospheric loadings of α-HCH to the Great Lakes are mostly attributable to emissions in Asia, consistent with very low usage in North America and efficient transport over the global scale.

7.0 CONCLUSIONS AND RECOMENDATIONS

In this section, we present overall conclusions from the study and suggest avenues for future research. We recommend actions to further improve our ability to identify sources of atmospherically derived persistent pollutants in the Great Lakes and to more accurately quantify the relative contributions of these sources to total loadings.

7.1 Conclusions

The first component of our assessment as reported here was to demonstrate a screening-level analysis to evaluate Level I substances for persistence and long-range transport potential. We selected all the organic chemicals among the Level I substances as identified in the Great Lakes Binational Toxics Strategy. Using a suite of mass balance contaminant fate models, we evaluated these chemicals for both persistence and potential for long-range transport and deposition to the Great Lakes. We compiled physicochemical properties and carried out generic modeling for 18 individual chemicals representing the Level I substances. Based on a screening analysis of partitioning properties alone, all of the substances examined demonstrated the potential for continental-scale transport and deposition to the Lakes provided they are sufficiently persistent. Modeling of Characteristic Travel Distance and Great Lakes Transfer Efficiency using generic emission scenarios indicated that the majority of the substances were sufficiently persistent to undergo significant continental, hemispheric or global-scale transport to the Great Lakes.

Generic transport and deposition efficiency modeling of the Level I substances over continental and global scales allowed us to categorize them according to the likely spatial scale of emissions that could significantly impact the Great Lakes. Our results are as follows:

(1) Local or regional scale: Dieldrin, Aldrin, benzo[a]pyrene

(2) Continental scale:	Chlordane, 2,3,7,8-TCDD, *p*,*p*'-DDT, toxaphene, octachlorostyrene, mirex
(3) Hemispheric scale:	PCBs
(4) Global scale:	hexachlorobenzene, α-HCH.

In order to calculate total atmospheric loading to the Lakes, we used available emissions estimates and the contribution of Level I substance emissions in different regions of North America and the world. The estimates of regional contributions to atmospheric loading are subject to large uncertainties most notably because of uncertainties in emission scenarios. There are also uncertainties attributable to chemical property inputs and to conceptual assumptions of multimedia fate models. Examples are the assumption that partitioning among environmental media is fast relative to inter-regional transfer and uncertainty in the empirical relationships between partition coefficients and environmental partitioning used in the model. However, these conceptual restrictions have been evaluated in a number of model evaluation studies and shown not be significant limitations on model performance. A more important source of uncertainty in these assessments is the limited quality, quantity, and relevance of data available on rates of chemical transformation in environmental media among the large and diverse landscapes considered in the BETR model applications. But in spite of the key uncertainties contributed by emissions and reaction rate uncertainties, based on available emissions estimates for seven PCB congeners we have assembled mass budgets for the period 1930 to 2000 that exhibit satisfactory agreement with observed atmospheric concentrations in the late 1990s at long term monitoring stations in the Northern Hemisphere. The uncertainty in the comparison between modeled and observed concentrations demonstrates the extent of our overall understanding of the sources and long-term fate and transport of PCBs in the global environment.

Calculated loadings attributable to different regions under emissions scenarios representing total historical PCB emissions and emissions in the year 2000 suggest that more rapid reductions of emissions in the United States and Canada relative to other parts of the world are shifting atmospheric deposition of PCBs to more distant sources.

However, as of the year 2000 the majority of PCBs deposited to the Lakes can still be attributed to sources to the atmosphere within the Great Lakes Basin and neighboring regions in North America. Therefore, our analysis suggests efforts aimed at further reductions in atmospheric loading to the Lakes should still be focused primarily on identifying and eliminating sources of PCBs within the Great Lakes Basin and neighboring regions.

We offer a hypothetical example to illustrate how model results can be used to support management decisions and to allocate resources. Consider an EPA official with a fixed allocation of funds to spend on eliminating emissions of PCBs to the atmosphere with the goal of maximizing cost-effectiveness in reducing atmospheric loading to the Great Lakes. Inspection of Figures 4.4.1 – 4.4.7 indicates that on average one kilogram of PCB emitted to air in the immediate vicinity of the Great Lakes will result in approximately 60 times as much atmospheric loading to the Lakes as one kilogram emitted in China, and approximately 100 times as much loading as one kilogram emitted in Eastern Europe. Therefore, to be cost effective, 60 – 100 times greater emission reduction per dollar spent would be required in China or Eastern Europe, relative to possible emission reductions in the Great Lakes region.

7.2 Recommendations

The model results presented here for PCBs and toxaphene at the North American spatial scale and for PCBs and α-HCH at the global scale provide a quantitative synthesis of current knowledge about the sources, transport, and ultimate fate of these persistent pollutants. Compiling these mass balances is a challenging task because information from a variety of sources must be gathered and harmonized into a coherent picture. We found that mass balances for many of the Level I substances could not be assembled because of a lack of quantitative information on emissions. This limitation confirms the need for further work on developing emission inventories. This effort should be made a priority to improve understanding of source-receptor relationships for all the Level 1 substances. We did, however, discover that even without information from emission

estimates it is possible to learn a great deal from the generic modeling evaluations of persistence and long-range transport, and to gain insight into the important processes controlling transport and deposition of persistent substances.

With regard to uncertainties, we have not conducted a systematic uncertainty analysis of the assessments, however considering both model uncertainty and input uncertainty it is apparent that the key contributors to uncertainties in model calculations for the Level I substances derive from incomplete emissions data and from unreliable chemical properties data —primarily transformation rates. Further refinements to the models to introduce more detailed descriptions of environmental conditions or higher spatial resolution will not reduce these uncertainties [(6)]. Only more accurate emissions inventories and additional studies to characterize the partitioning properties and degradability of the Level I substances in various environmental media will reduce this fundamental uncertainty. Uncertainties in physico-chemical properties are likely highest for octachlorostyrene, for which estimated values where used because no measured property values could be found. Once emissions and degradability uncertainties are reduced, the next phase in reducing overall model uncertainties will be addressing spatial and temporal heterogeneity in land-surface properties, degradation mechanisms and atmospheric transport.

In considering future model development work to build on the assessments presented here, we recommend additional modeling exercises to examine the importance of fate and transport processes that are not described in the current model, and continued work to improve the reliability of the empirical equations used in the model. For example, the models do not treat chemical fate processes associated with snow and ice, which dominate the landscape for a significant portion of the year, and the current version of BETR Global includes a highly simplified description of the circulation of ocean water. Additional model-based studies of fate and transport processes will help to refine the existing models and eventually contribute to reducing uncertainties in the overall assessments.

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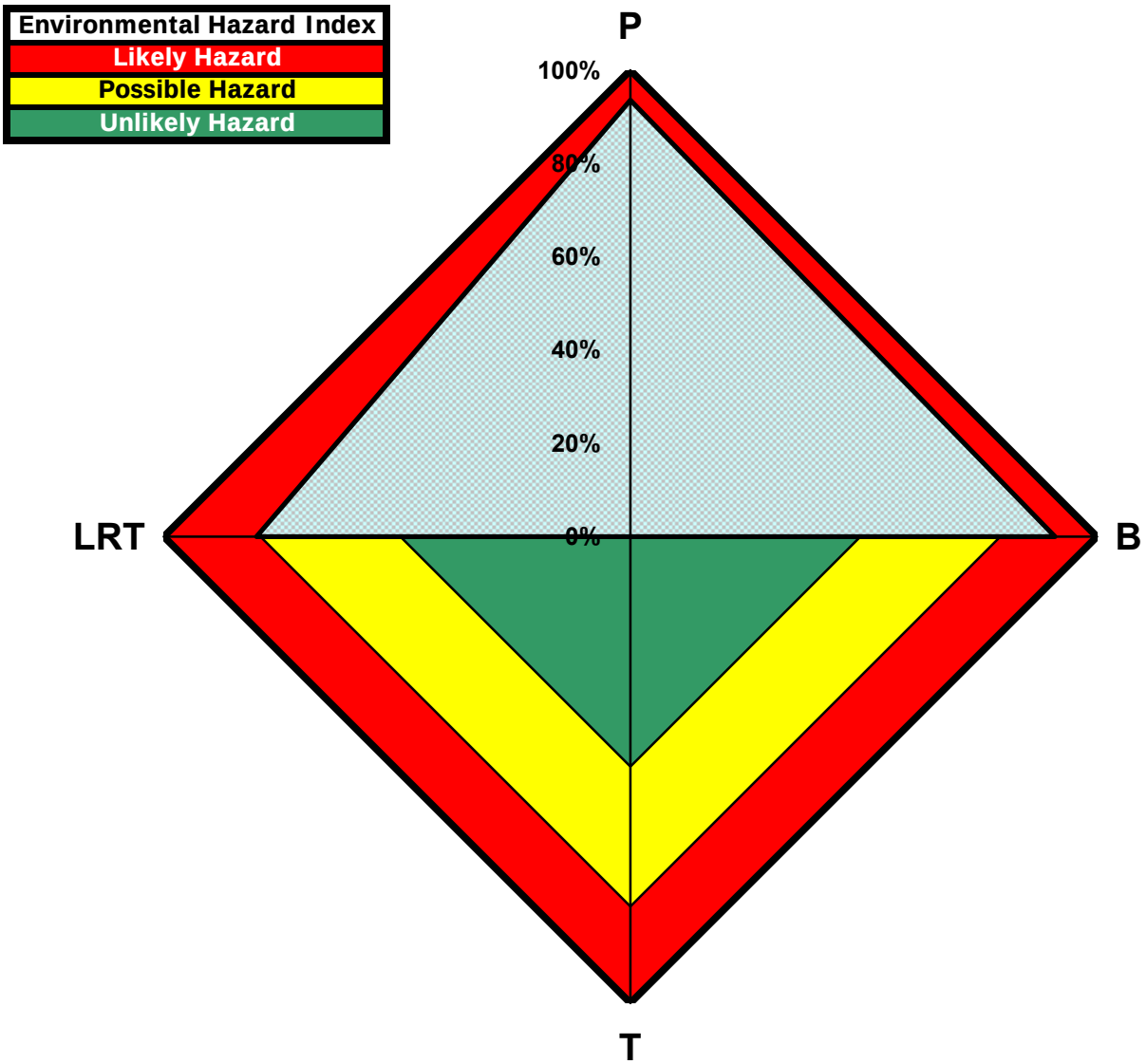
APPENDIX A: ChemSCORER Hazard Profiles for the Level 1 Substances

ChemSCORER Beta101 Assessment - Summary Ranking

EPA PCB28



Summary Rankings for: EPA PCB28

This chemical ...

is more PERSISTENT (P) than **94 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **91 %** of chemicals in the reference set.

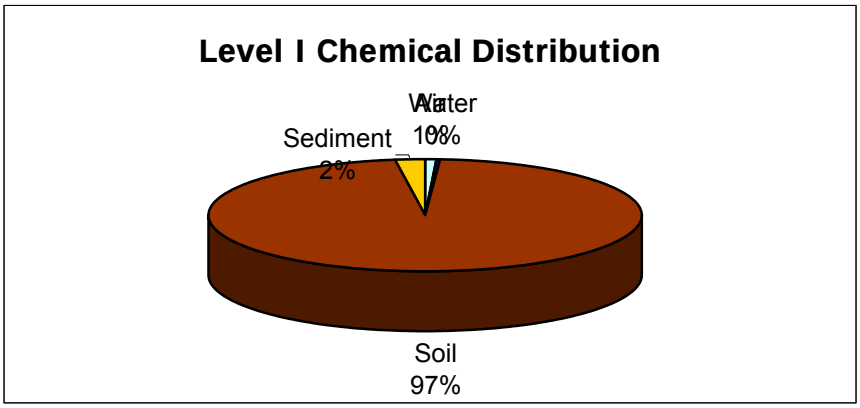
No data on mammalian toxicity was supplied.

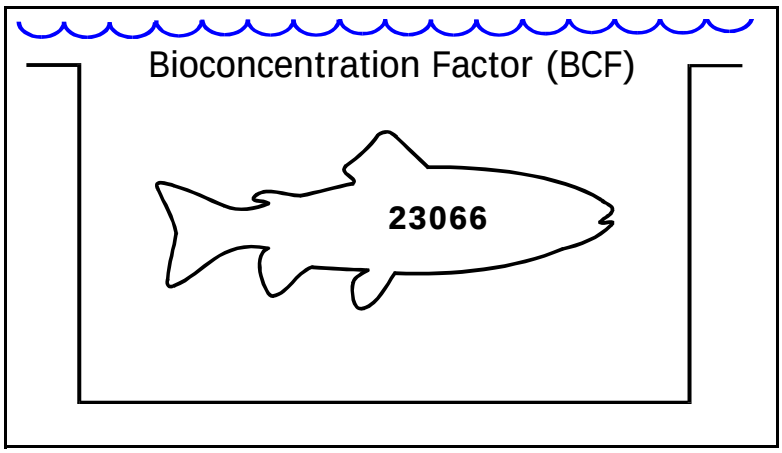
has greater LONG RANGE TRANSPORT (LRT) than **80 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA PCB28

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is greater than the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. In the absence of rapid metabolism by organisms, this substance is expected to bioaccumulate.

Details of Level I calculation for: EPA PCB28

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	3.00E-11	7.72E-09	6.51E-06	772	0.772
Water	6.19E-02	4.60E-09	1.18E-06	1.18E-06	237	0.237
Soil	5.62E+02	4.17E-05	1.08E-02	4.48E-03	96768	96.768
Sediment	1.12E+03	8.35E-05	2.15E-02	8.96E-03	2150	2.150
Suspended Sediment	3.51E+03	2.61E-04	6.72E-02	4.48E-02	67	0.067
Biota (Fish)	1.43E+03	1.06E-04	2.73E-02	2.73E-02	5	0.005
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

Input Parameters			Partition Coefficients		Three Solubilities	
					(g/m^3)	
Molar Mass	257.54	g/mol				
Vapor Pressure	1	Pa	Log Kow	5.66	Air	1.04E-01
Aqueous Solubility	15.94	g/m^3	Log Kaw	-2.19	Water	1.59E+01
Log Kow	5.664		Log Koa	7.85	Octanol	7.35E+06
Melting Point	-999	deg C				

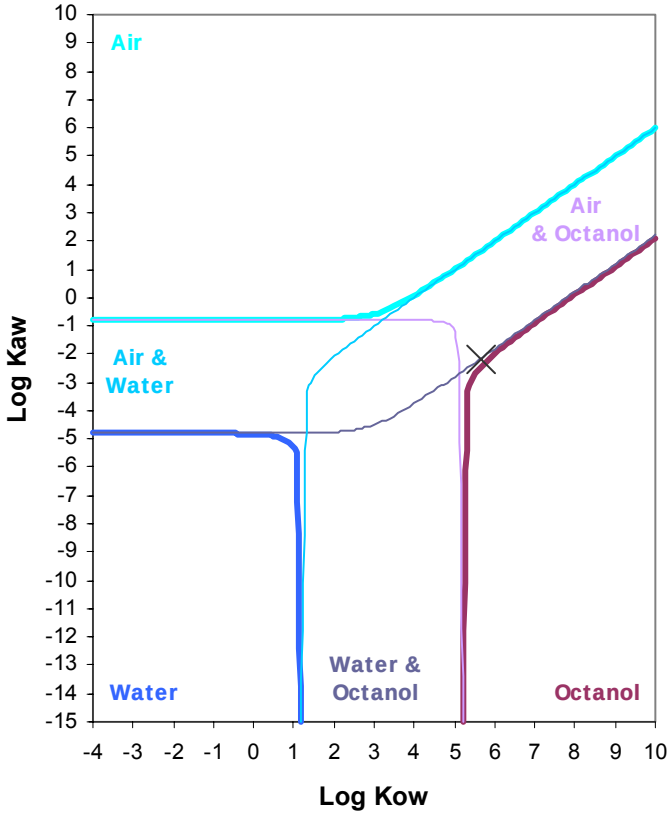
ChemSCORER Beta101 - Level II Model Results

EPA PCB28

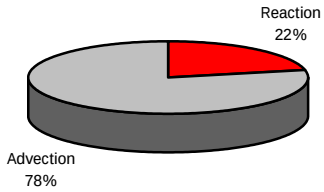
Equilibrium Partitioning Persistence Information

The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.

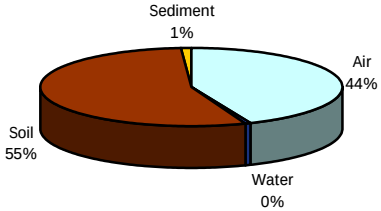
The equilibrium distribution reaction residence time calculated for this substance can be measured in years, and is comparable to that of pentachlorobenzene (2 years). Reactive and advective residence times are comparable, indicating the substance may be mobile to other regions.



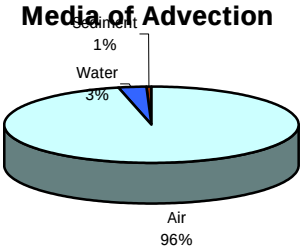
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	407	days	1.12	years
Reaction Residence Time:	1870	days	5.12	years
Advection Residence Time:	521	days	1.43	years

Details of Level II calculation for: EPA PCB28

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	550	5.08E+07	4.03E+08	9.51E+01	7.55E+02	84.983
Water	17000	5.05E+05	1.24E+07	9.44E-01	2.32E+01	2.410
Soil	55000	6.37E+07	0	1.19E+02	0	11.921
Sediment	55000	1.42E+06	2.25E+06	2.65E+00	4.21E+00	0.685
Total		1.16E+08	4.18E+08	2.18E+02	7.82E+02	100.000
Reaction + Advection		5.35E+08		1000		

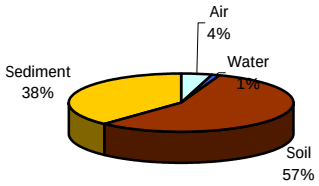
ChemSCORER Beta101 - Level III Model Results

EPA PCB28

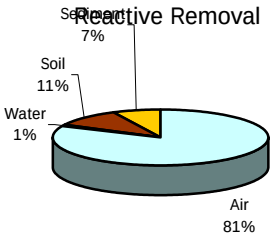
Emission to Air

Emissions to air partition significantly to soil and sediment.

Steady State Distribution



Reactive Removal



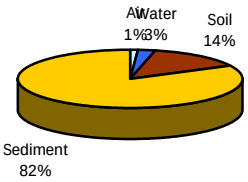
	Persistence
(hours)	14788.8
(days)	616.2
(years)	1.7

Persistence of air emissions is comparable to that of hexachlorobenzene (2200 days).

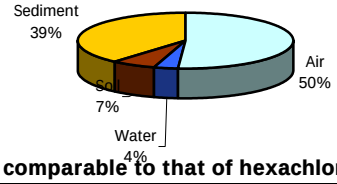
Emission to Water

Emissions to water partition significantly to sediment and may migrate to soil.

Steady State Distribution



Reactive Removal



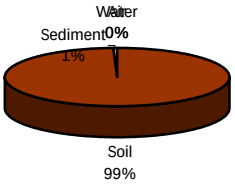
	Persistence
(hours)	37221.4
(days)	1550.9
(years)	4.2

Persistence of water emissions is comparable to that of hexachlorobenzene (2300 days).

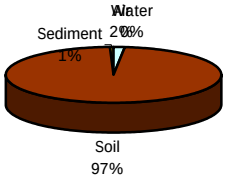
Emission to Soil

Emissions to soil remain predominantly in the soil compartment.

Steady State Distribution



Reactive Removal

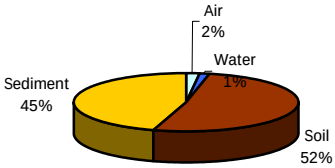


	Persistence
(hours)	78088.8
(days)	3253.7
(years)	8.9

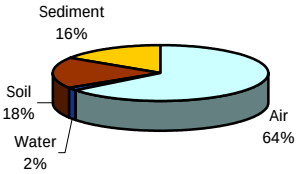
Persistence of soil emissions is comparable to that of hexachlorobenzene (3200 days).

Emission to All 3

Steady State Distribution



Reactive Removal



	Persistence
(hours)	27848.6
(days)	1160.4
(years)	3.2

Persistence under the standard emission scenario is comparable to that of hexachlorobenzene (2300 days).

Details of Level III calculation for: EPA PCB28

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	6.48E+05	1.71E+05	8.34E+06	5.63E+06	1.48E+07
Water	0	1000	0	4.05E+05	9.33E+05	5.20E+06	3.07E+07	3.72E+07
Soil	0	0	1000	1.26E+04	1.33E+04	7.76E+07	4.36E+05	7.81E+07
All 3	600	300	100	5.12E+05	3.84E+05	1.43E+07	1.26E+07	2.78E+07
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	817	7	105	71	1000
Water	0	1000	0	510	38	66	387	1000
Soil	0	0	1000	16	1	978	5	1000
All 3	600	300	100	645	16	181	159	1000

ChemSCORER Beta101 - Transport Model Results

EPA PCB28

TaPL II - Equilibrium distribution Characteristic Travel Distance

Under equilibrium partitioning conditions, this chemical is likely to be transported most effectively in air.

TaPL III - Mode of entry assessments

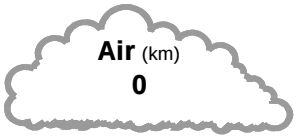
Emission to air - Characteristic Travel Distance in Air

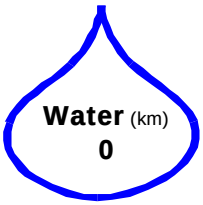
Characteristic Travel Distance in air is high, and is comparable to that of hexachlorinated PCBs (4200 km). This chemical may be subject to long range transport and deposition in the arctic.

Emission to water - Characteristic Travel Distance in Water

Characteristic Travel Distance in water is high, and is comparable to that of toxaphene (9700 km). This chemical may be subject to long range transport in surface and ocean waters.

Emission to soil - Effective Travel Distance





Emissions directly to soil are not expected to partition significantly to air or water, and are not likely to be subject to transport.

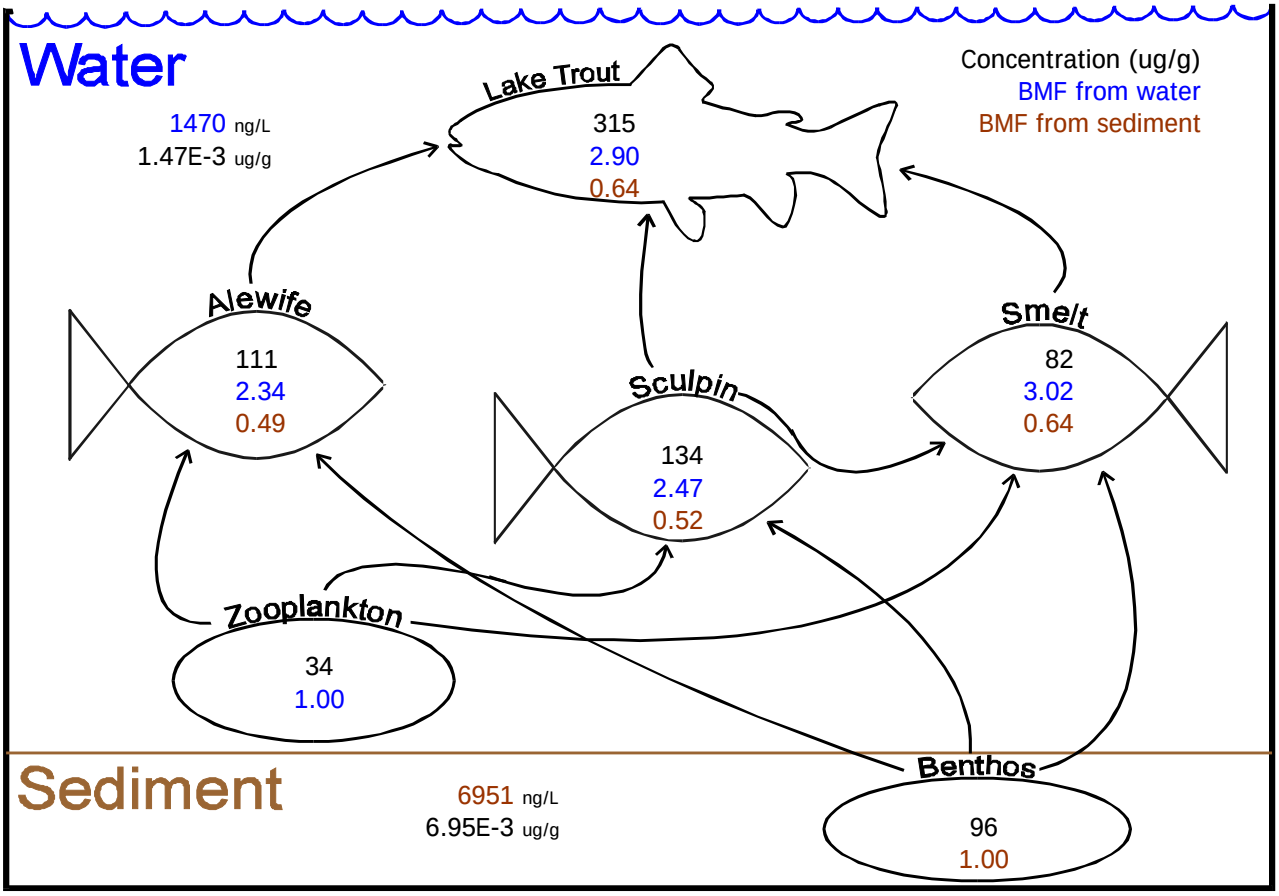
ChemSCORER Beta101 - Toxicity and Bioaccumulation
EPA PCB28

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



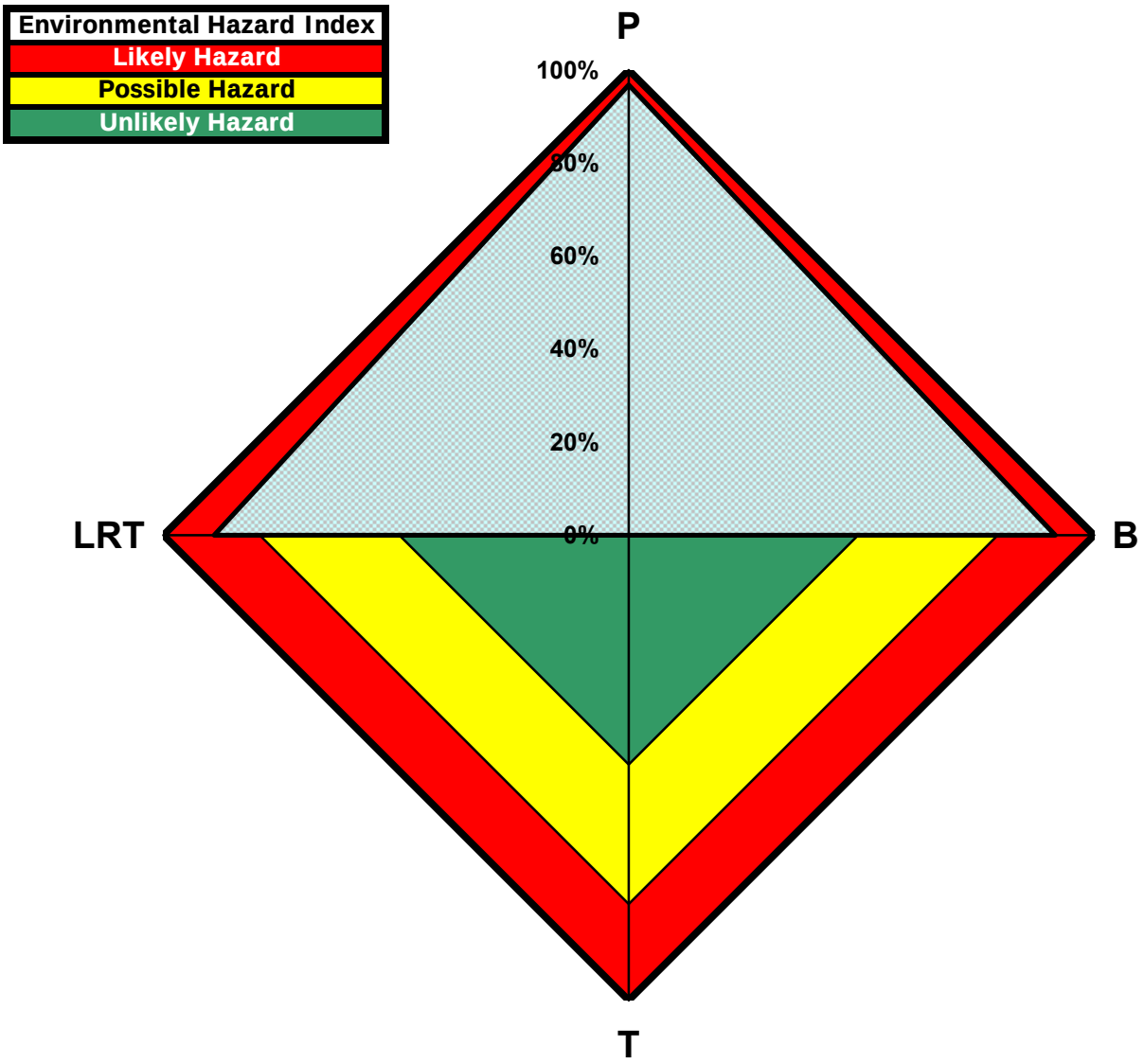
Overall Bioaccumulation Factor, Lake Trout / Water : 214341

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.

ChemSCORER Beta101 Assessment - Summary Ranking

EPA PCB52



Summary Rankings for: EPA PCB52

This chemical ...

is more PERSISTENT (P) than **97 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **92 %** of chemicals in the reference set.

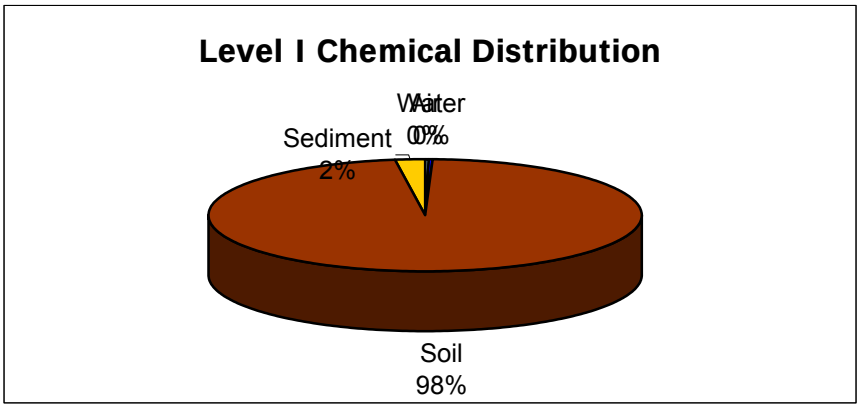
No data on mammalian toxicity was supplied.

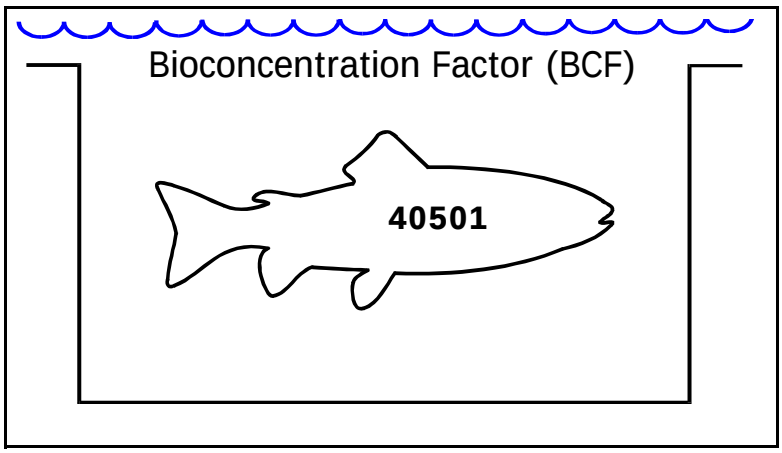
has greater LONG RANGE TRANSPORT (LRT) than **89 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA PCB52

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is substantially greater than the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. In the absence of metabolism by organisms, this substance may bioaccumulate similar to DDT (BCF 63000) or PCBs (BCFs up to 300000).

Details of Level I calculation for: EPA PCB52

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	1.13E-11	3.31E-09	2.79E-06	331	0.331
Water	8.27E-02	2.32E-09	6.78E-07	6.78E-07	136	0.136
Soil	1.32E+03	3.70E-05	1.08E-02	4.50E-03	97298	97.298
Sediment	2.64E+03	7.40E-05	2.16E-02	9.01E-03	2162	2.162
Suspended Sediment	8.23E+03	2.31E-04	6.76E-02	4.50E-02	68	0.068
Biota (Fish)	3.35E+03	9.41E-05	2.75E-02	2.75E-02	5	0.005
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

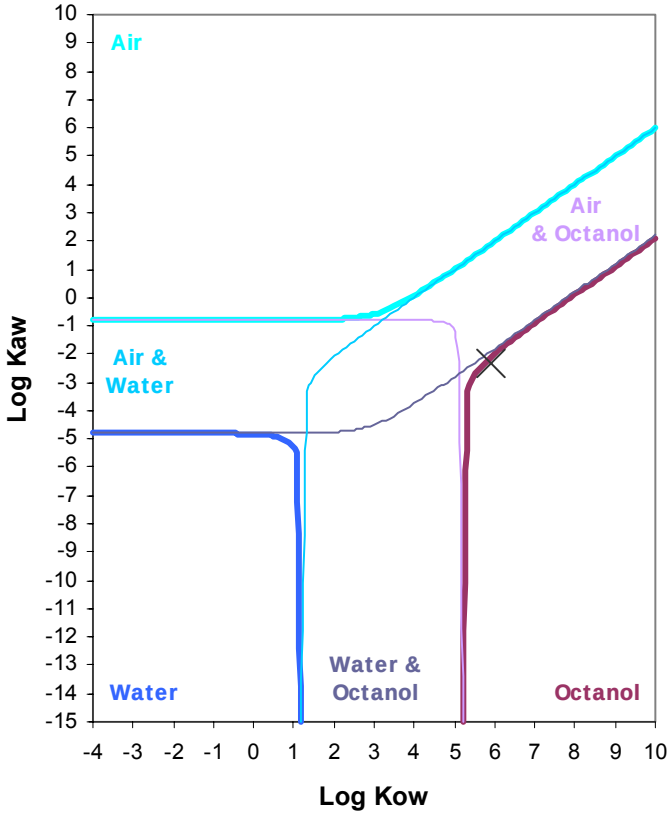
Input Parameters			Partition Coefficients		Three Solubilities	
					(g/m^3)	
Molar Mass	291.99	g/mol				
Vapor Pressure	1	Pa	Log Kow	5.91	Air	1.18E-01
Aqueous Solubility	24.13365746	g/m^3	Log Kaw	-2.31	Water	2.41E+01
Log Kow	5.9085		Log Koa	8.22	Octanol	1.95E+07
Melting Point	-999	deg C				

ChemSCORER Beta101 - Level II Model Results

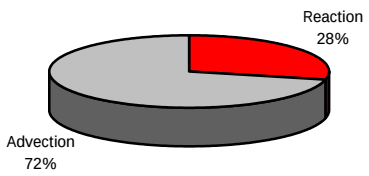
EPA PCB52

Equilibrium Partitioning Persistence Information

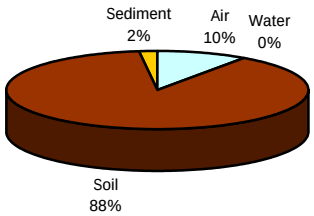
The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.
The equilibrium distribution reaction residence time calculated for this substance is greater than five years, and is comparable to that of hexachlorobenzene (7.6 years). Reactive and advective residence times are comparable, indicating the substance may be subject to long range transport.



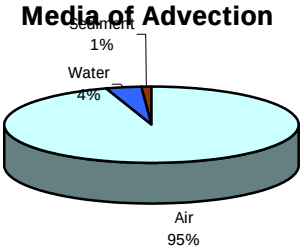
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	854	days	2.34	years
Reaction Residence Time:	2998	days	8.21	years
Advection Residence Time:	1194	days	3.27	years

Details of Level II calculation for: EPA PCB52

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	1700	1.64E+07	4.03E+08	2.77E+01	6.78E+02	70.612
Water	55000	2.08E+05	1.65E+07	3.50E-01	2.78E+01	2.815
Soil	55000	1.49E+08	0	2.51E+02	0	25.128
Sediment	55000	3.32E+06	5.27E+06	5.58E+00	8.86E+00	1.445
Total		1.69E+08	4.25E+08	2.85E+02	7.15E+02	100.000
Reaction + Advection		5.95E+08		1000		

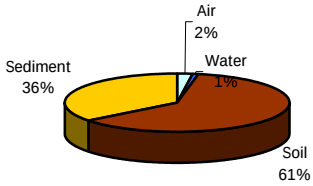
ChemSCORER Beta101 - Level III Model Results

EPA PCB52

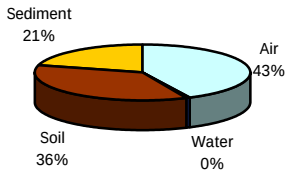
Emission to Air

Emissions to air partition predominantly to soil and sediment.

Steady State Distribution



Reactive Removal



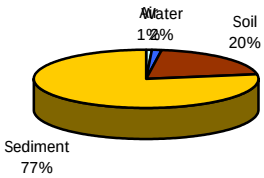
	Persistence
(hours)	46439.1
(days)	1935.0
(years)	5.3

Persistence of air emissions is comparable to that of hexachlorobenzene (2200 days).

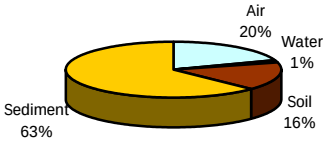
Emission to Water

Emissions to water partition significantly to sediment and may migrate to soil.

Steady State Distribution



Reactive Removal



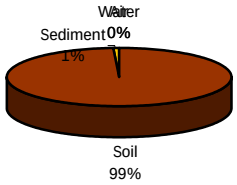
	Persistence
(hours)	64323.0
(days)	2680.1
(years)	7.3

Persistence of water emissions is comparable to that of hexachlorobenzene (2300 days).

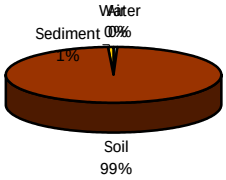
Emission to Soil

Emissions to soil remain predominantly in the soil compartment.

Steady State Distribution



Reactive Removal

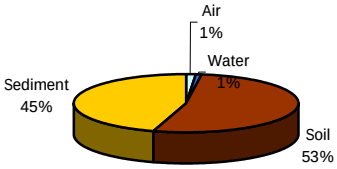


	Persistence
(hours)	79037.8
(days)	3293.2
(years)	9.0

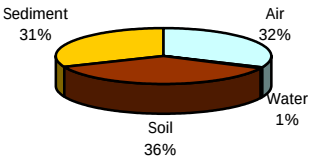
Persistence of soil emissions is comparable to that of hexachlorobenzene (3200 days).

Emission to All 3

Steady State Distribution



Reactive Removal



	Persistence
(hours)	55064.1
(days)	2294.3
(years)	6.3

Persistence under the standard emission scenario is comparable to that of hexachlorobenzene (2300 days).

Details of Level III calculation for: EPA PCB52

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	1.05E+06	3.35E+05	2.85E+07	1.65E+07	4.64E+07
Water	0	1000	0	4.80E+05	1.01E+06	1.30E+07	4.98E+07	6.43E+07
Soil	0	0	1000	1.04E+04	1.21E+04	7.84E+07	5.98E+05	7.90E+07
All 3	600	300	100	7.75E+05	5.05E+05	2.89E+07	2.49E+07	5.51E+07
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	428	4	360	208	1000
Water	0	1000	0	196	13	164	627	1000
Soil	0	0	1000	4	0	988	8	1000
All 3	600	300	100	316	6	364	314	1000

ChemSCORER Beta101 - Transport Model Results

EPA PCB52

TaPL II - Equilibrium distribution Characteristic Travel Distance

Under equilibrium partitioning conditions, this chemical is likely to be transported by both air and water.

TaPL III - Mode of entry assessments

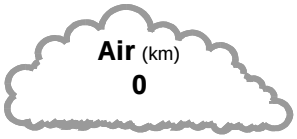
Emission to air - Characteristic Travel Distance in Air

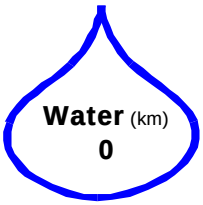
Characteristic Travel Distance in air is high, and is comparable to that of hexachlorinated PCBs (4200 km). This chemical may be subject to long range transport and deposition in the arctic.

Emission to water - Characteristic Travel Distance in Water

Characteristic Travel Distance in water is high, and is comparable to that of toxaphene (9700 km). This chemical may be subject to long range transport in surface and ocean waters.

Emission to soil - Effective Travel Distance





Emissions directly to soil are not expected to partition significantly to air or water, and are not likely to be subject to transport.

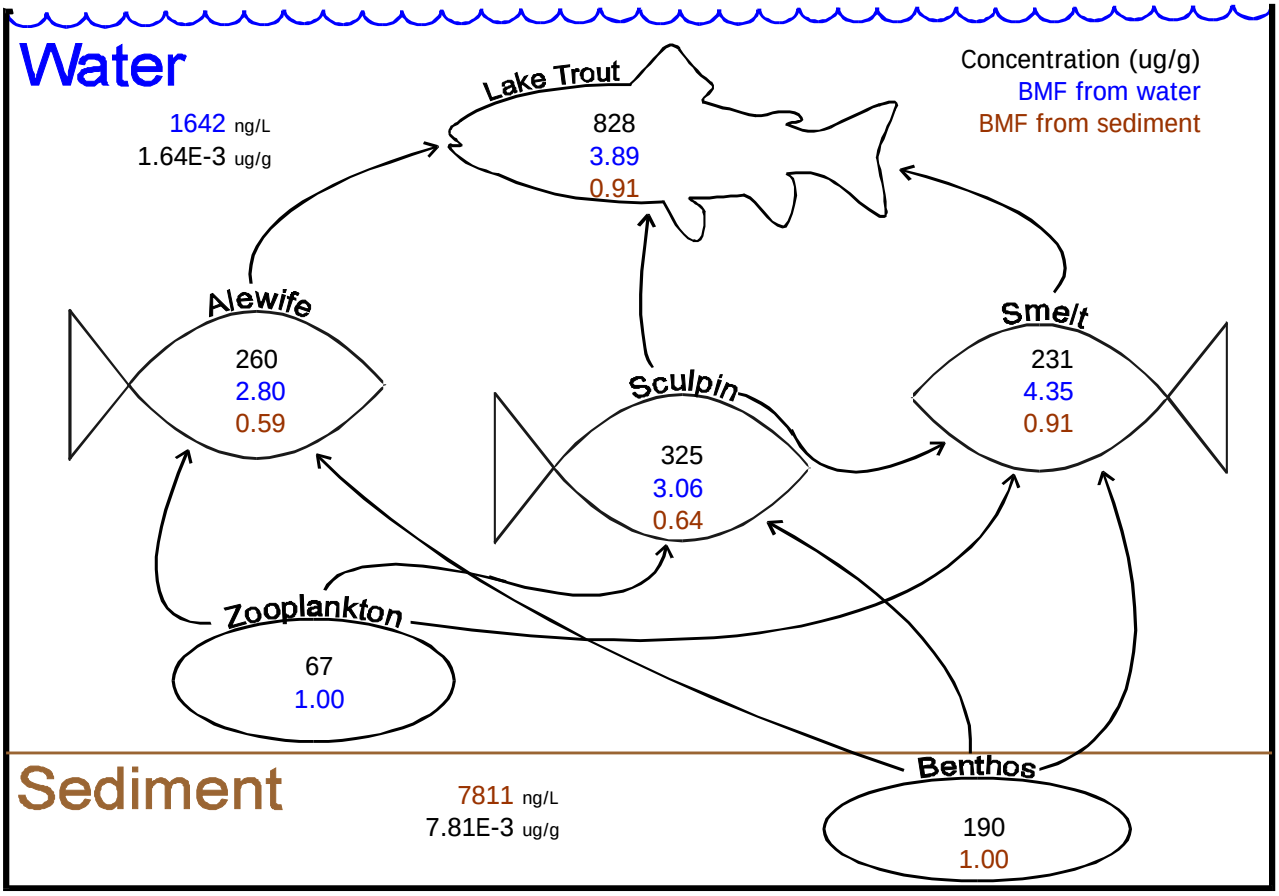
ChemSCORER Beta101 - Toxicity and Bioaccumulation
EPA PCB52

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



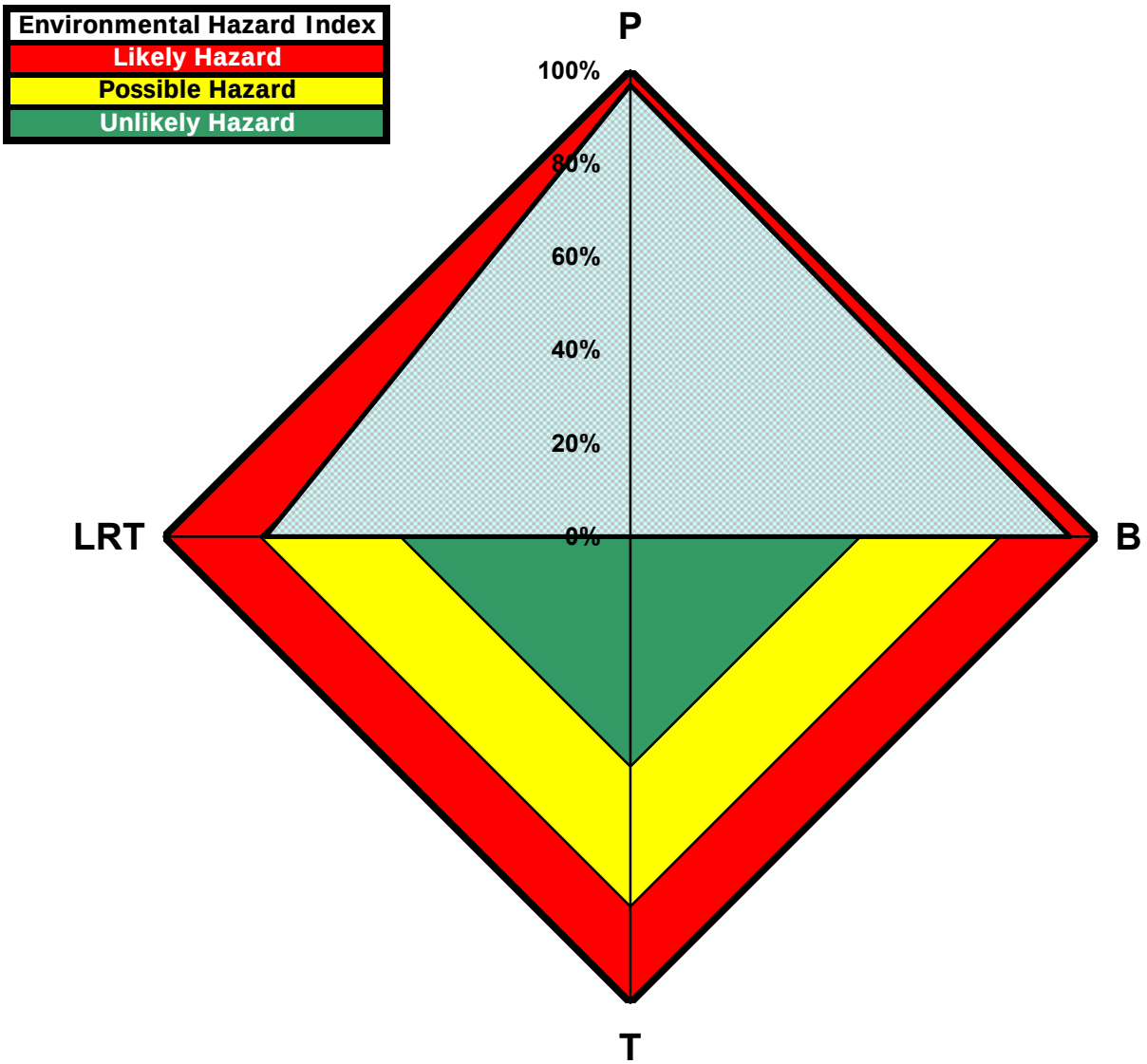
Overall Bioaccumulation Factor, Lake Trout / Water : 504001

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.

ChemSCORER Beta101 Assessment - Summary Ranking

EPA PCB101



Summary Rankings for: EPA PCB101

This chemical ...

is more PERSISTENT (P) than **97 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **94 %** of chemicals in the reference set.

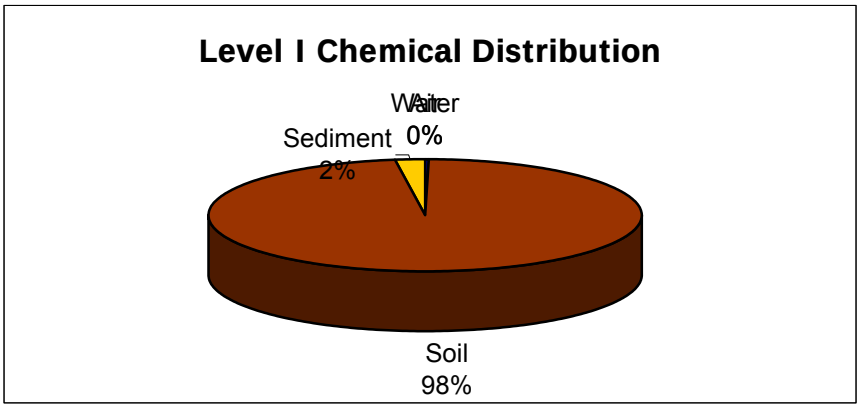
No data on mammalian toxicity was supplied.

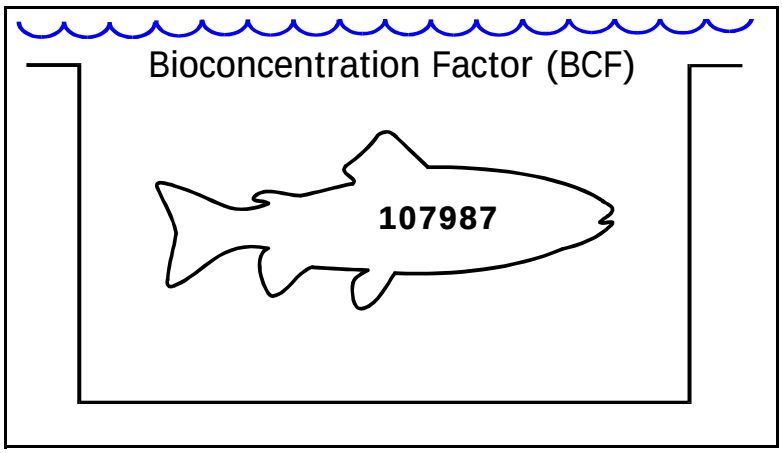
has greater LONG RANGE TRANSPORT (LRT) than **78 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA PCB101

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is substantially greater than the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. In the absence of metabolism by organisms, this substance may bioaccumulate similar to DDT (BCF 63000) or PCBs (BCFs up to 300000).

Details of Level I calculation for: EPA PCB101

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	3.14E-12	1.03E-09	8.66E-07	103	0.103
Water	1.00E-01	7.82E-10	2.55E-07	2.55E-07	51	0.051
Soil	4.26E+03	3.32E-05	1.08E-02	4.52E-03	97604	97.604
Sediment	8.53E+03	6.64E-05	2.17E-02	9.04E-03	2169	2.169
Suspended Sediment	2.66E+04	2.08E-04	6.78E-02	4.52E-02	68	0.068
Biota (Fish)	1.08E+04	8.44E-05	2.76E-02	2.76E-02	6	0.006
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

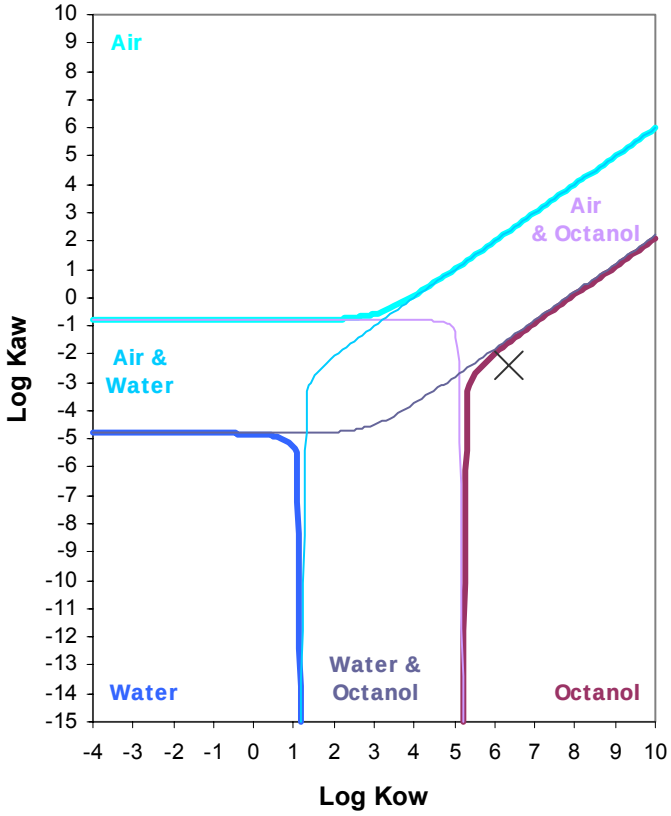
Input Parameters			Partition Coefficients		Three Solubilities	
Molar Mass	326.43	g/mol			(g/m^3)	
Vapor Pressure	1	Pa	Log Kow	6.33	Air	1.32E-01
Aqueous Solubility	32.74501782	g/m^3	Log Kaw	-2.40	Water	3.27E+01
Log Kow	6.3344		Log Koa	8.73	Octanol	7.07E+07
Melting Point	-999	deg C				

ChemSCORER Beta101 - Level II Model Results

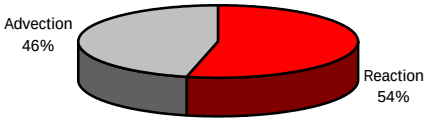
EPA PCB101

Equilibrium Partitioning Persistence Information

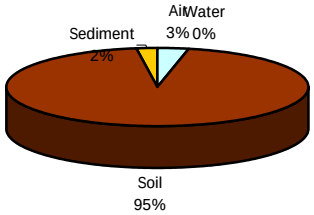
The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.
The equilibrium distribution reaction residence time calculated for this substance is greater than five years, and is comparable to that of hexachlorobenzene (7.6 years). Reactive and advective residence times are comparable, indicating the substance may be subject to long range transport.



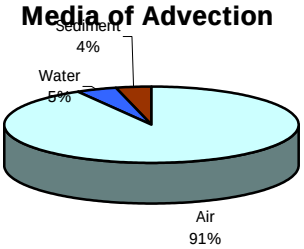
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	1722	days	4.72	years
Reaction Residence Time:	3206	days	8.78	years
Advection Residence Time:	3718	days	10.19	years

Details of Level II calculation for: EPA PCB101

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	1700	1.64E+07	4.03E+08	1.73E+01	4.24E+02	44.128
Water	55000	2.53E+05	2.01E+07	2.66E-01	2.11E+01	2.135
Soil	55000	4.83E+08	0	5.08E+02	0	50.816
Sediment	55000	1.07E+07	1.71E+07	1.13E+01	1.79E+01	2.922
Total		5.11E+08	4.41E+08	5.37E+02	4.63E+02	100.000
Reaction + Advection		9.51E+08		1000		

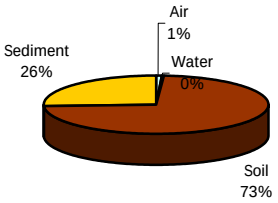
ChemSCORER Beta101 - Level III Model Results

EPA PCB101

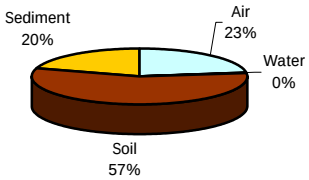
Emission to Air

Emissions to air partition predominantly to soil and sediment.

Steady State Distribution



Reactive Removal



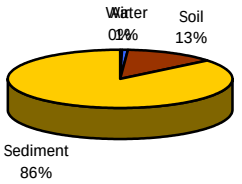
	Persistence
(hours)	61744.9
(days)	2572.7
(years)	7.0

Persistence of air emissions is comparable to that of hexachlorobenzene (2200 days).

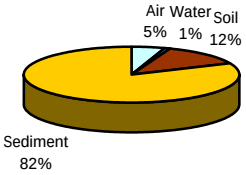
Emission to Water

Emissions to water partition significantly to sediment and may migrate to soil.

Steady State Distribution



Reactive Removal



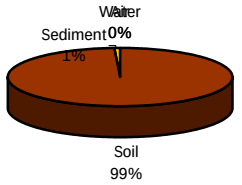
	Persistence
(hours)	75545.0
(days)	3147.7
(years)	8.6

Persistence of water emissions is comparable to that of hexachlorobenzene (2300 days).

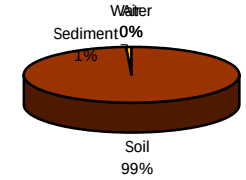
Emission to Soil

Emissions to soil remain predominantly in the soil compartment.

Steady State Distribution



Reactive Removal

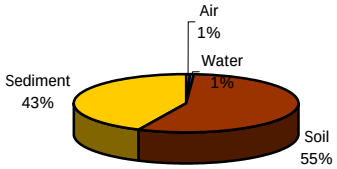


	Persistence
(hours)	79302.2
(days)	3304.3
(years)	9.1

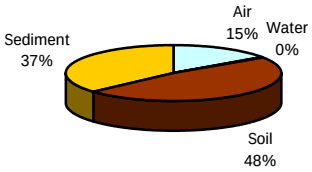
Persistence of soil emissions is comparable to that of hexachlorobenzene (3200 days).

Emission to All 3

Steady State Distribution



Reactive Removal



	Persistence
(hours)	67640.7
(days)	2818.4
(years)	7.7

Persistence under the standard emission scenario is comparable to that of hexachlorobenzene (2300 days).

Details of Level III calculation for: EPA PCB101

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	5.62E+05	1.92E+05	4.50E+07	1.60E+07	6.17E+07
Water	0	1000	0	1.22E+05	7.78E+05	9.75E+06	6.49E+07	7.55E+07
Soil	0	0	1000	2.00E+03	7.15E+03	7.87E+07	5.96E+05	7.93E+07
All 3	600	300	100	3.74E+05	3.49E+05	3.78E+07	2.91E+07	6.76E+07
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	229	2	567	202	1000
Water	0	1000	0	50	10	123	818	1000
Soil	0	0	1000	1	0	992	8	1000
All 3	600	300	100	152	4	476	367	1000

ChemSCORER Beta101 - Transport Model Results

EPA PCB101

TaPL II - Equilibrium distribution Characteristic Travel Distance

Under equilibrium partitioning conditions, this chemical is likely to be transported by both air and water.

TaPL III - Mode of entry assessments

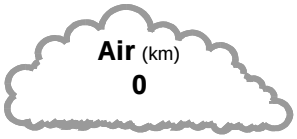
Emission to air - Characteristic Travel Distance in Air

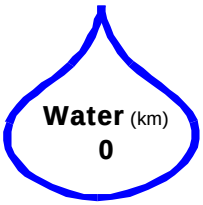
Characteristic Travel Distance in air is high, and is comparable to that of hexachlorinated PCBs (4200 km). This chemical may be subject to long range transport and deposition in the arctic.

Emission to water - Characteristic Travel Distance in Water

Characteristic Travel Distance in water is high, and is comparable to that of toxaphene (9700 km). This chemical may be subject to long range transport in surface and ocean waters.

Emission to soil - Effective Travel Distance





Emissions directly to soil are not expected to partition significantly to air or water, and are not likely to be subject to transport.

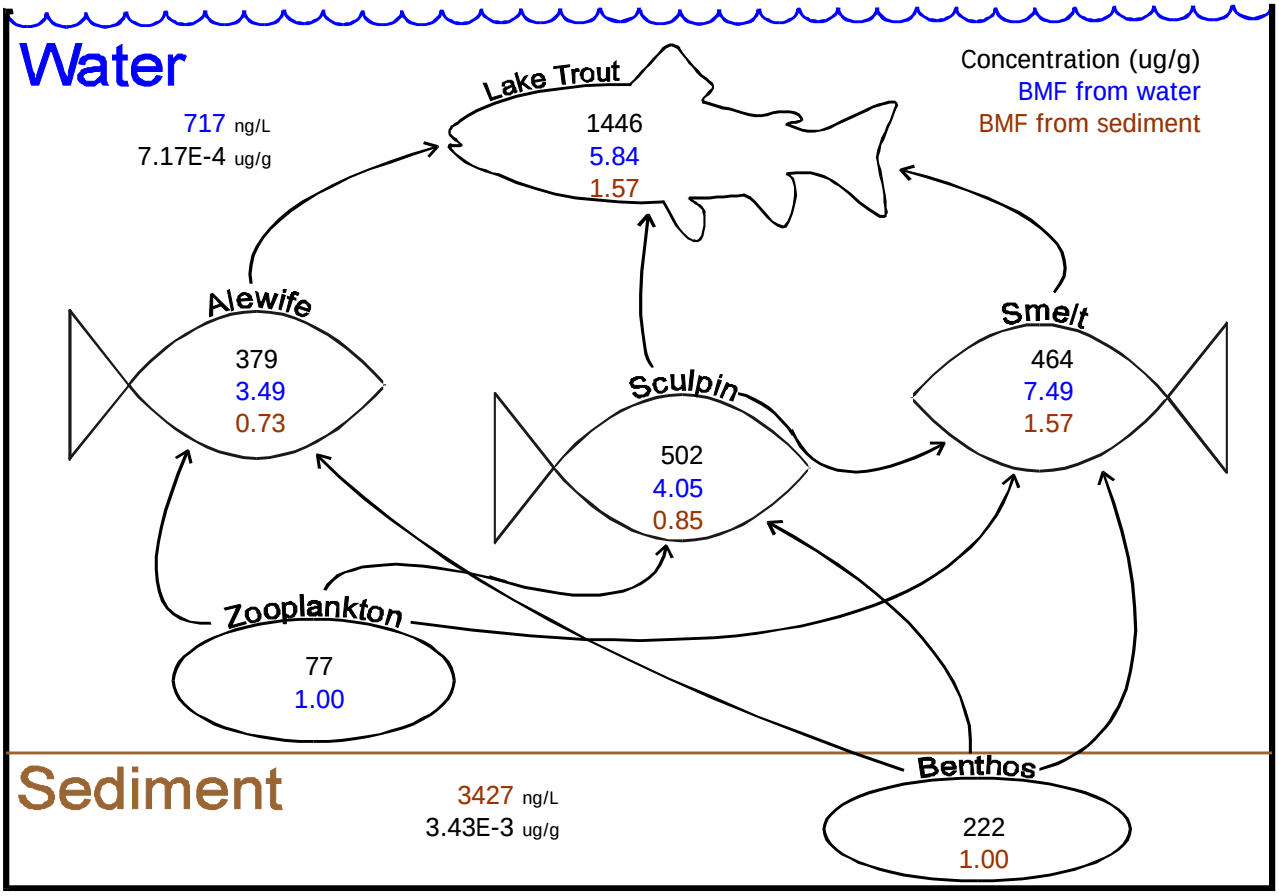
ChemSCORER Beta101 - Toxicity and Bioaccumulation
EPA PCB101

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



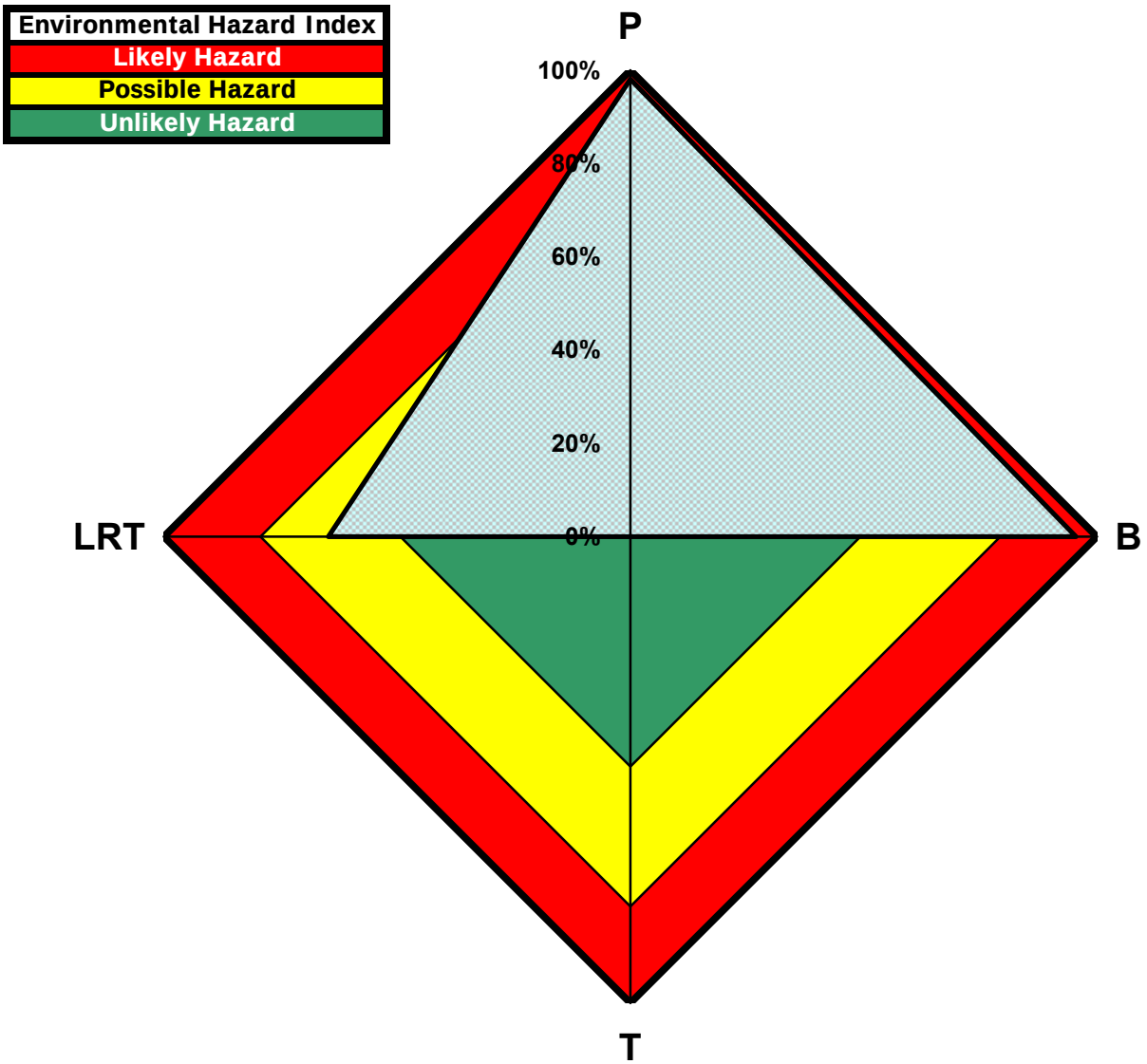
Overall Bioaccumulation Factor, Lake Trout / Water : 2016652

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.

ChemSCORER Beta101 Assessment - Summary Ranking

EPA PCB118



Summary Rankings for: EPA PCB118

This chemical ...

is more PERSISTENT (P) than **98 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **96 %** of chemicals in the reference set.

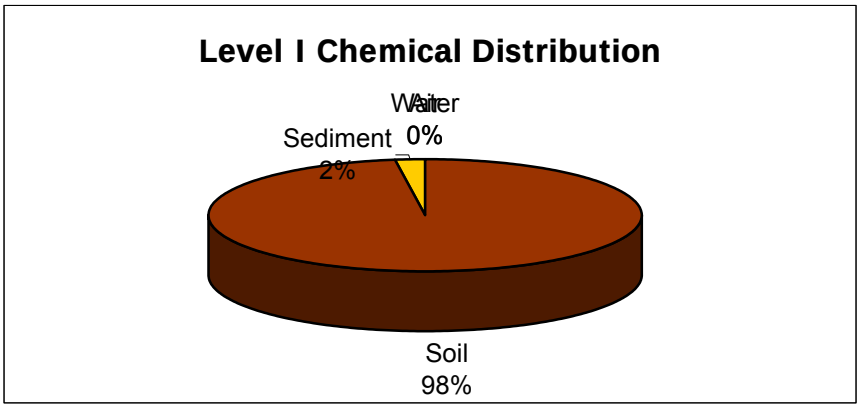
No data on mammalian toxicity was supplied.

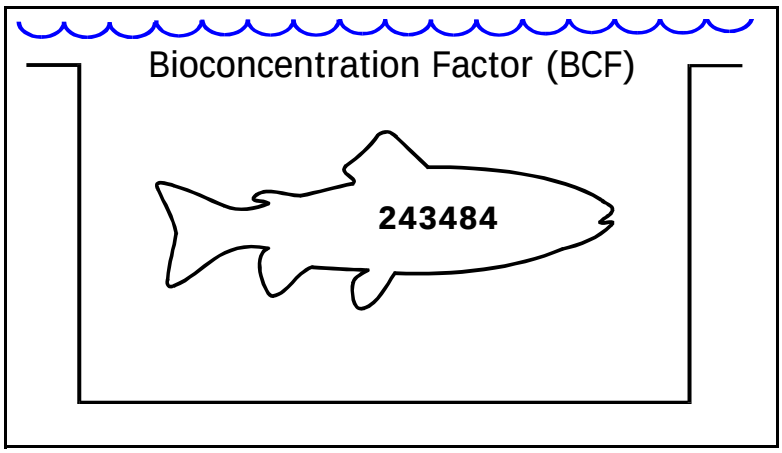
has greater LONG RANGE TRANSPORT (LRT) than **65 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA PCB118

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is substantially greater than the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. In the absence of metabolism by organisms, this substance may bioaccumulate similar to DDT (BCF 63000) or PCBs (BCFs up to 300000).

Details of Level I calculation for: EPA PCB118

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	7.38E-13	2.41E-10	2.03E-07	24	0.024
Water	1.90E-01	3.47E-10	1.13E-07	1.13E-07	23	0.023
Soil	1.82E+04	3.33E-05	1.09E-02	4.52E-03	97709	97.709
Sediment	3.64E+04	6.65E-05	2.17E-02	9.05E-03	2171	2.171
Suspended Sediment	1.14E+05	2.08E-04	6.79E-02	4.52E-02	68	0.068
Biota (Fish)	4.62E+04	8.45E-05	2.76E-02	2.76E-02	6	0.006
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

Input Parameters			Partition Coefficients		Three Solubilities	
					(g/m^3)	
Molar Mass	326.43	g/mol				
Vapor Pressure	1	Pa	Log Kow	6.69	Air	1.32E-01
Aqueous Solubility	61.95055924	g/m^3	Log Kaw	-2.67	Water	6.20E+01
Log Kow	6.6875		Log Koa	9.36	Octanol	3.02E+08
Melting Point	-999	deg C				

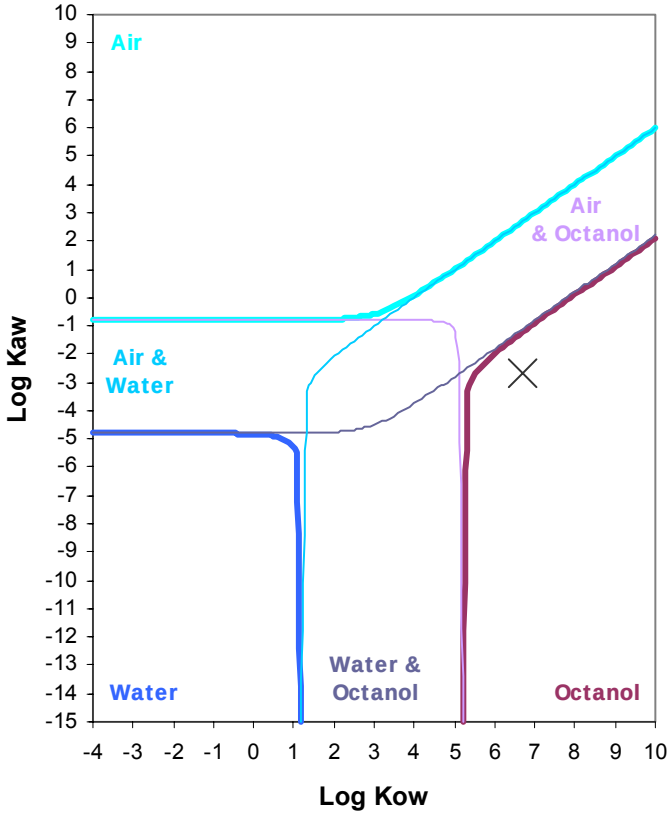
ChemSCORER Beta101 - Level II Model Results

EPA PCB118

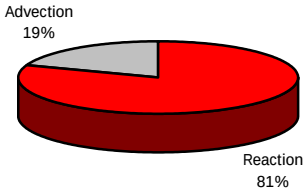
Equilibrium Partitioning Persistence Information

The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.

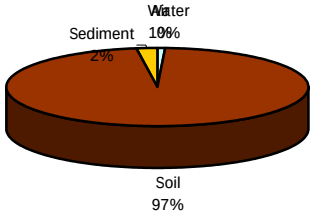
The equilibrium distribution reaction residence time calculated for this substance is greater than five years, and is comparable to that of hexachlorobenzene (7.6 years). Reactive and advective residence times are comparable, indicating the substance may be subject to long range transport.



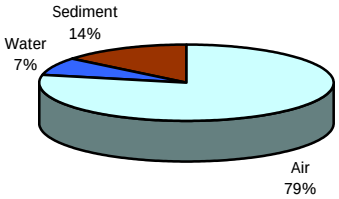
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	2645	days	7.25	years
Reaction Residence Time:	3284	days	9.00	years
Advection Residence Time:	13577	days	37.20	years

Details of Level II calculation for: EPA PCB118

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	1700	1.64E+07	4.03E+08	6.23E+00	1.53E+02	15.908
Water	55000	4.78E+05	3.80E+07	1.81E-01	1.44E+01	1.456
Soil	55000	2.06E+09	0	7.81E+02	0	78.143
Sediment	55000	4.58E+07	7.28E+07	1.74E+01	2.76E+01	4.493
Total		2.13E+09	5.14E+08	8.05E+02	1.95E+02	100.000
Reaction + Advection		2.64E+09		1000		

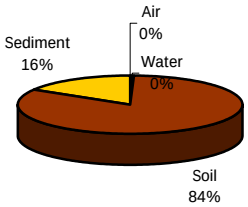
ChemSCORER Beta101 - Level III Model Results

EPA PCB118

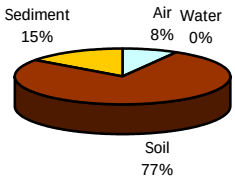
Emission to Air

Emissions to air partition predominantly to soil and sediment.

Steady State Distribution



Reactive Removal



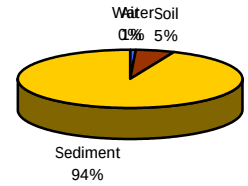
	Persistence
(hours)	72980.4
(days)	3040.9
(years)	8.3

Persistence of air emissions is comparable to that of hexachlorobenzene (2200 days).

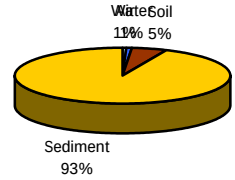
Emission to Water

Emissions to water partition significantly to sediment and may migrate to soil.

Steady State Distribution



Reactive Removal



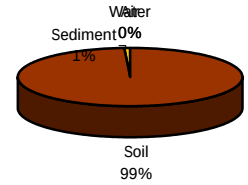
	Persistence
(hours)	78918.9
(days)	3288.3
(years)	9.0

Persistence of water emissions is comparable to that of hexachlorobenzene (2300 days).

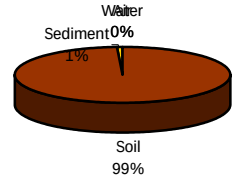
Emission to Soil

Emissions to soil remain predominantly in the soil compartment.

Steady State Distribution



Reactive Removal

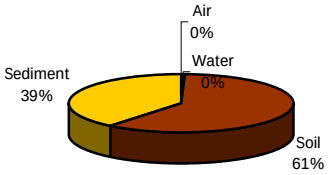


	Persistence
(hours)	79358.6
(days)	3306.6
(years)	9.1

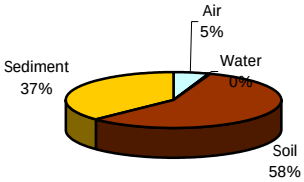
Persistence of soil emissions is comparable to that of hexachlorobenzene (3200 days).

Emission to All 3

Steady State Distribution



Reactive Removal



	Persistence
(hours)	75399.8
(days)	3141.7
(years)	8.6

Persistence under the standard emission scenario is comparable to that of hexachlorobenzene (2300 days).

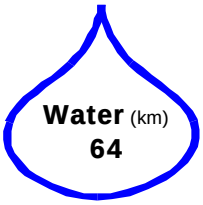
Details of Level III calculation for: EPA PCB118

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	2.04E+05	1.11E+05	6.07E+07	1.20E+07	7.30E+07
Water	0	1000	0	1.42E+04	6.83E+05	4.24E+06	7.40E+07	7.89E+07
Soil	0	0	1000	2.05E+02	5.71E+03	7.87E+07	6.18E+05	7.94E+07
All 3	600	300	100	1.26E+05	2.72E+05	4.55E+07	2.95E+07	7.54E+07
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	83	1	764	151	1000
Water	0	1000	0	6	9	53	932	1000
Soil	0	0	1000	0	0	992	8	1000
All 3	600	300	100	52	3	574	371	1000

ChemSCORER Beta101 - Transport Model Results

EPA PCB118

TaPL II - Equilibrium distribution Characteristic Travel Distance



Under equilibrium partitioning conditions, this chemical is likely to be transported by both air and water.

TaPL III - Mode of entry assessments

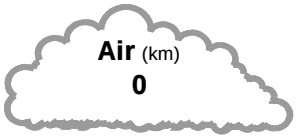
Emission to air - Characteristic Travel Distance in Air

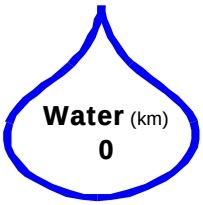
Characteristic Travel Distance in air is high, and is comparable to that of hexachlorinated PCBs (4200 km). This chemical may be subject to long range transport and deposition in the arctic.

Emission to water - Characteristic Travel Distance in Water

Characteristic Travel Distance in water is high, and is comparable to that of toxaphene (9700 km). This chemical may be subject to long range transport in surface and ocean waters.

Emission to soil - Effective Travel Distance





Emissions directly to soil are not expected to partition significantly to air or water, and are not likely to be subject to transport.

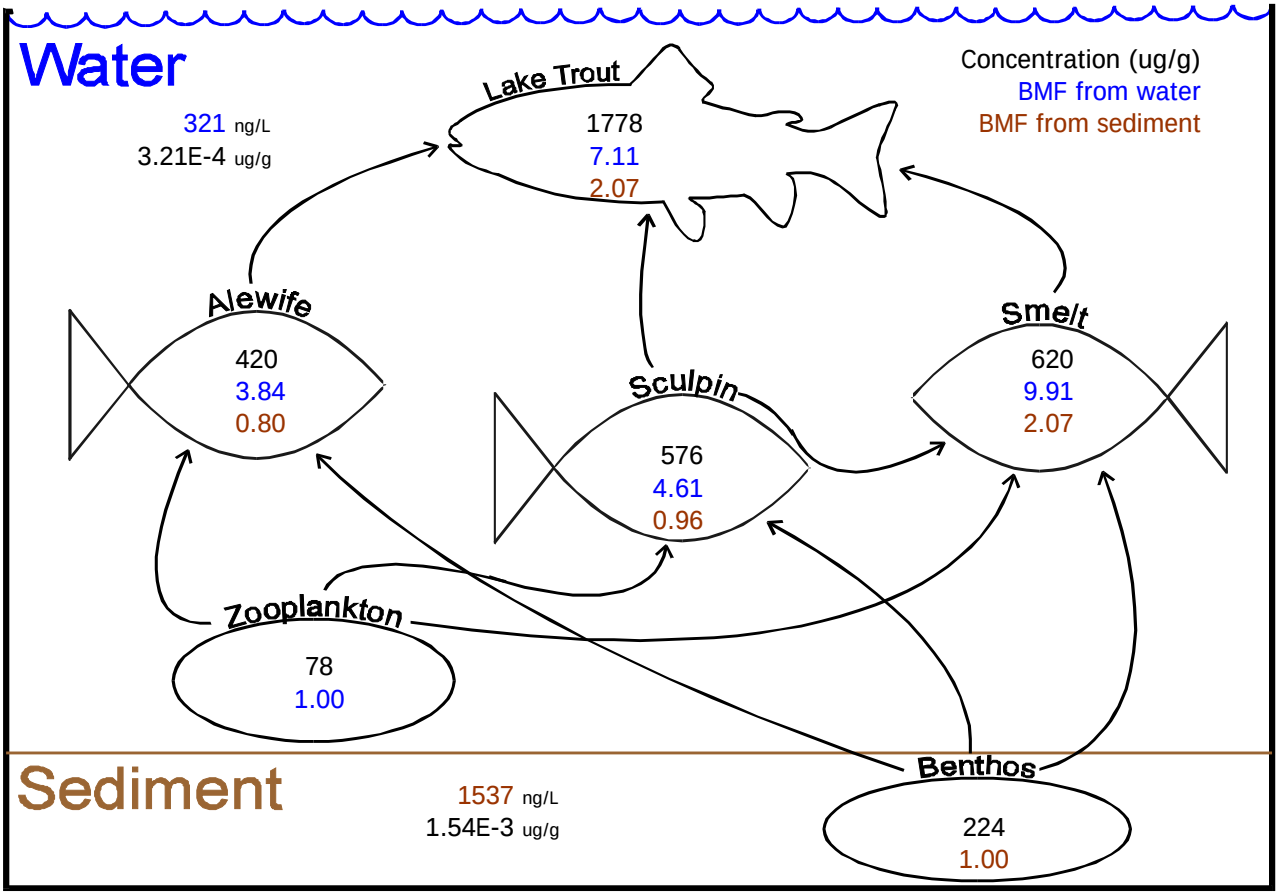
ChemSCORER Beta101 - Toxicity and Bioaccumulation
EPA PCB118

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



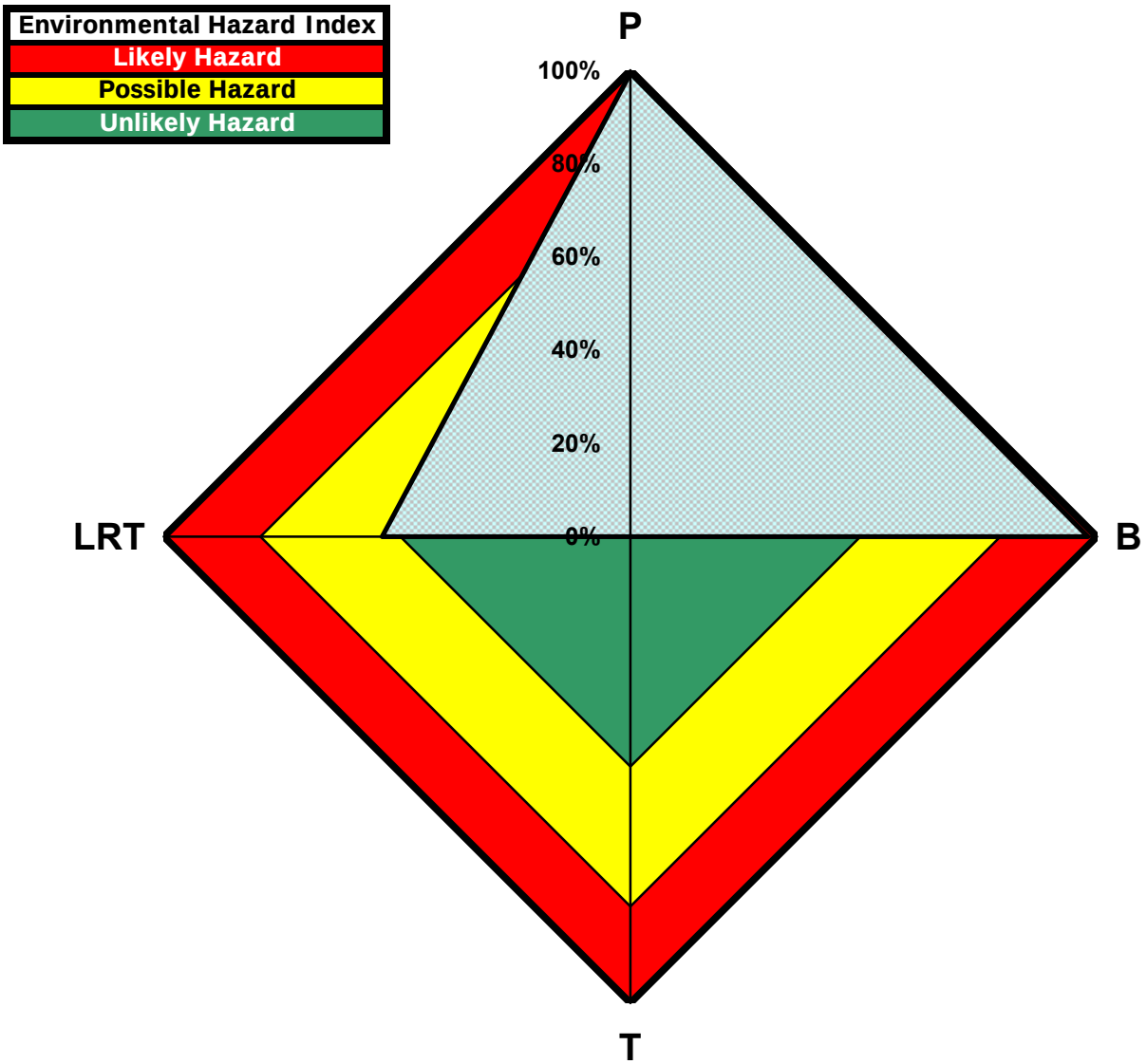
Overall Bioaccumulation Factor, Lake Trout / Water : 5537523

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.

ChemSCORER Beta101 Assessment - Summary Ranking

EPA PCB138



Summary Rankings for: EPA PCB138

This chemical ...

is more PERSISTENT (P) than **99 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **98 %** of chemicals in the reference set.

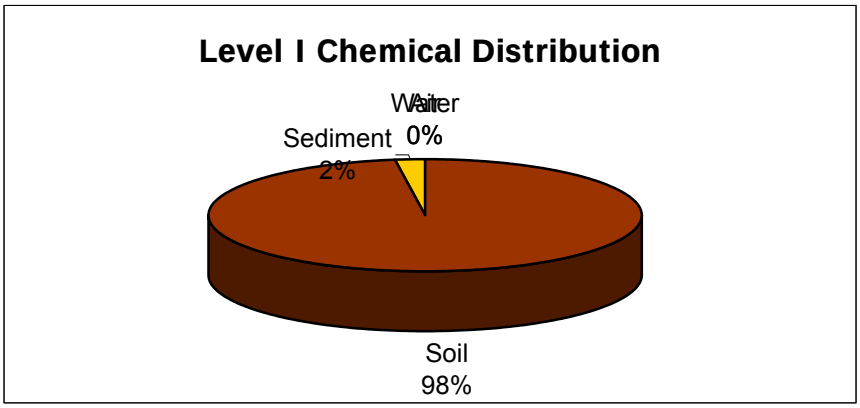
No data on mammalian toxicity was supplied.

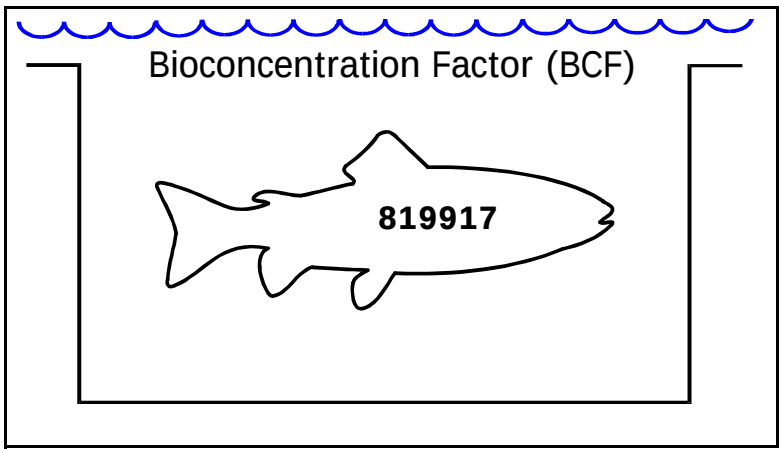
has greater LONG RANGE TRANSPORT (LRT) than **53 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA PCB138

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is substantially greater than the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. In the absence of metabolism by organisms, this substance may bioaccumulate similar to DDT (BCF 63000) or PCBs (BCFs up to 300000).

Details of Level I calculation for: EPA PCB138

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	3.35E-13	1.21E-10	1.02E-07	12	0.012
Water	1.12E-01	9.32E-11	3.37E-08	3.37E-08	7	0.007
Soil	3.63E+04	3.01E-05	1.09E-02	4.52E-03	97736	97.736
Sediment	7.26E+04	6.02E-05	2.17E-02	9.05E-03	2172	2.172
Suspended Sediment	2.27E+05	1.88E-04	6.79E-02	4.52E-02	68	0.068
Biota (Fish)	9.22E+04	7.65E-05	2.76E-02	2.76E-02	6	0.006
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

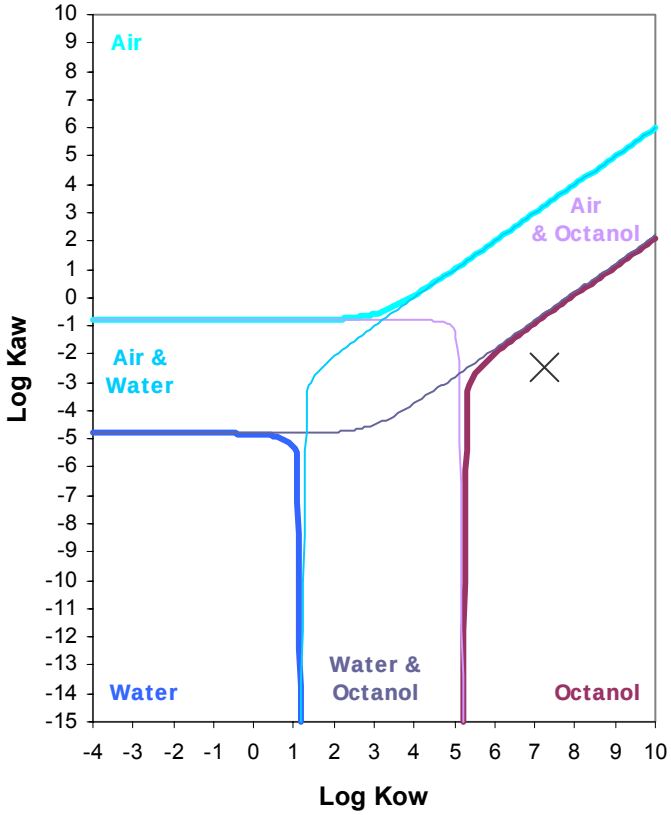
Input Parameters			Partition Coefficients		Three Solubilities	
					(g/m^3)	
Molar Mass	360.88	g/mol				
Vapor Pressure	1	Pa	Log Kow	7.21	Air	1.46E-01
Aqueous Solubility	40.5805548	g/m^3	Log Kaw	-2.44	Water	4.06E+01
Log Kow	7.2148		Log Koa	9.66	Octanol	6.65E+08
Melting Point	-999	deg C				

ChemSCORER Beta101 - Level II Model Results

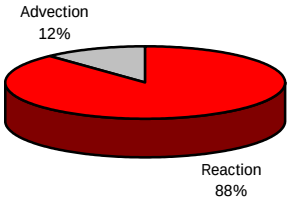
EPA PCB138

Equilibrium Partitioning Persistence Information

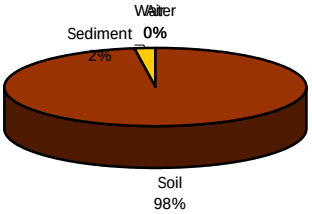
The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.
The equilibrium distribution reaction residence time calculated for this substance is greater than five years, and is comparable to that of hexachlorobenzene (7.6 years). Reactive and advective residence times are comparable, indicating the substance may be subject to long range transport.



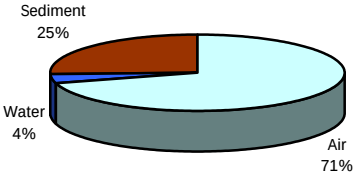
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	2911	days	7.98	years
Reaction Residence Time:	3306	days	9.06	years
Advection Residence Time:	24382	days	66.80	years

Details of Level II calculation for: EPA PCB138

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	5500	5.08E+06	4.03E+08	1.06E+00	8.43E+01	8.541
Water	55000	2.83E+05	2.25E+07	5.92E-02	4.70E+00	0.476
Soil	55000	4.12E+09	0	8.60E+02	0	86.037
Sediment	55000	9.14E+07	1.45E+08	1.91E+01	3.03E+01	4.947
Total		4.21E+09	5.71E+08	8.81E+02	1.19E+02	100.000
Reaction + Advection		4.78E+09		1000		

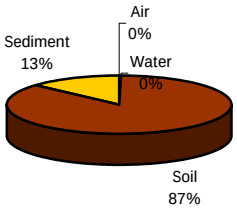
ChemSCORER Beta101 - Level III Model Results

EPA PCB138

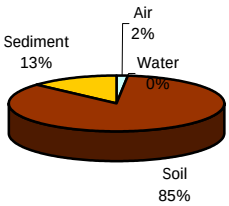
Emission to Air

Emissions to air partition predominantly to soil and sediment.

Steady State Distribution



Reactive Removal



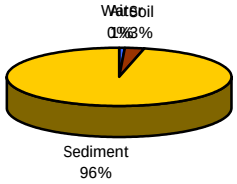
	Persistence
(hours)	78192.8
(days)	3258.0
(years)	8.9

Persistence of air emissions is comparable to that of hexachlorobenzene (2200 days).

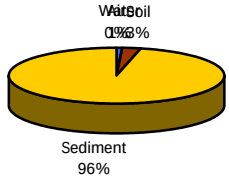
Emission to Water

Emissions to water partition significantly to sediment and may migrate to soil.

Steady State Distribution



Reactive Removal



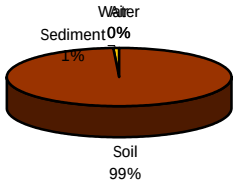
	Persistence
(hours)	79326.9
(days)	3305.3
(years)	9.1

Persistence of water emissions is comparable to that of hexachlorobenzene (2300 days).

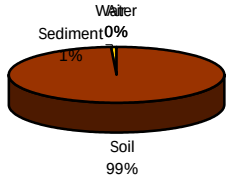
Emission to Soil

Emissions to soil remain predominantly in the soil compartment.

Steady State Distribution



Reactive Removal

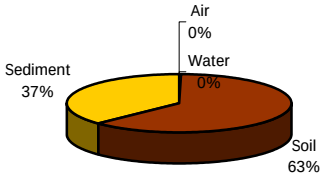


	Persistence
(hours)	79364.5
(days)	3306.9
(years)	9.1

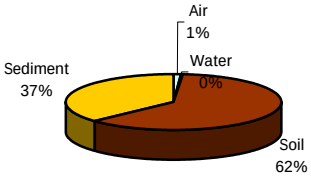
Persistence of soil emissions is comparable to that of hexachlorobenzene (3200 days).

Emission to All 3

Steady State Distribution



Reactive Removal



	Persistence
(hours)	78650.2
(days)	3277.1
(years)	9.0

Persistence under the standard emission scenario is comparable to that of hexachlorobenzene (2300 days).

Details of Level III calculation for: EPA PCB138

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	1.30E+05	8.11E+04	6.75E+07	1.05E+07	7.82E+07
Water	0	1000	0	4.24E+03	5.89E+05	2.19E+06	7.65E+07	7.93E+07
Soil	0	0	1000	5.97E+01	4.73E+03	7.87E+07	6.14E+05	7.94E+07
All 3	600	300	100	7.94E+04	2.26E+05	4.90E+07	2.93E+07	7.87E+07
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	16	1	850	133	1000
Water	0	1000	0	1	7	28	964	1000
Soil	0	0	1000	0	0	992	8	1000
All 3	600	300	100	10	3	617	370	1000

ChemSCORER Beta101 - Transport Model Results

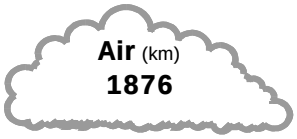
EPA PCB138

TaPL II - Equilibrium distribution Characteristic Travel Distance

Under equilibrium partitioning conditions, this chemical is likely to be transported by both air and water.

TaPL III - Mode of entry assessments

Emission to air - Characteristic Travel Distance in Air



Characteristic Travel Distance in air is moderate, and is comparable to that of DDT (830 km). This chemical may be found in remote areas, but is not necessarily transported over very long distances.

Emission to water - Characteristic Travel Distance in Water

Characteristic Travel Distance in water is high, and is comparable to that of toxaphene (9700 km). This chemical may be subject to long range transport in surface and ocean waters.

Emission to soil - Effective Travel Distance

Emissions directly to soil are not expected to partition significantly to air or water, and are not likely to be subject to transport.

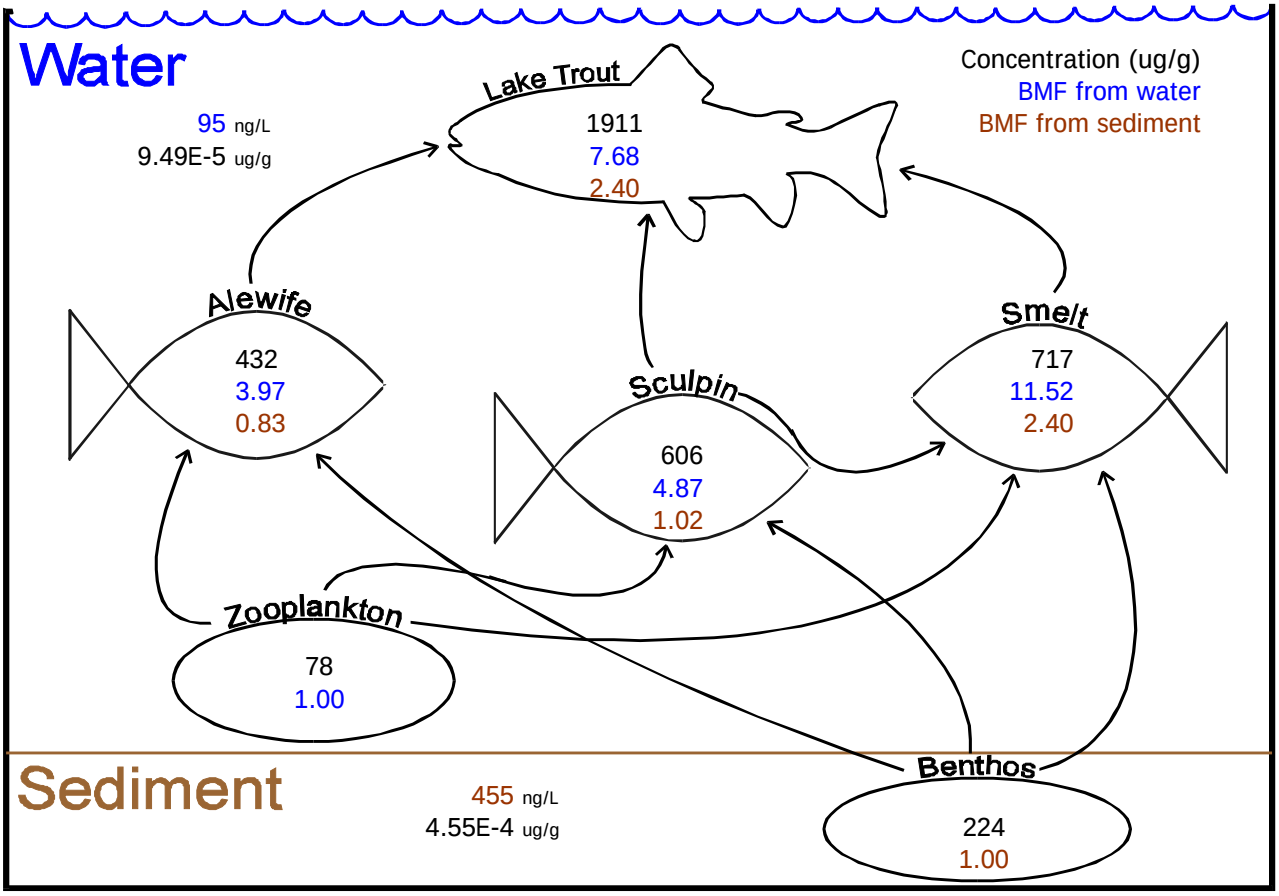
ChemSCORER Beta101 - Toxicity and Bioaccumulation
EPA PCB138

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



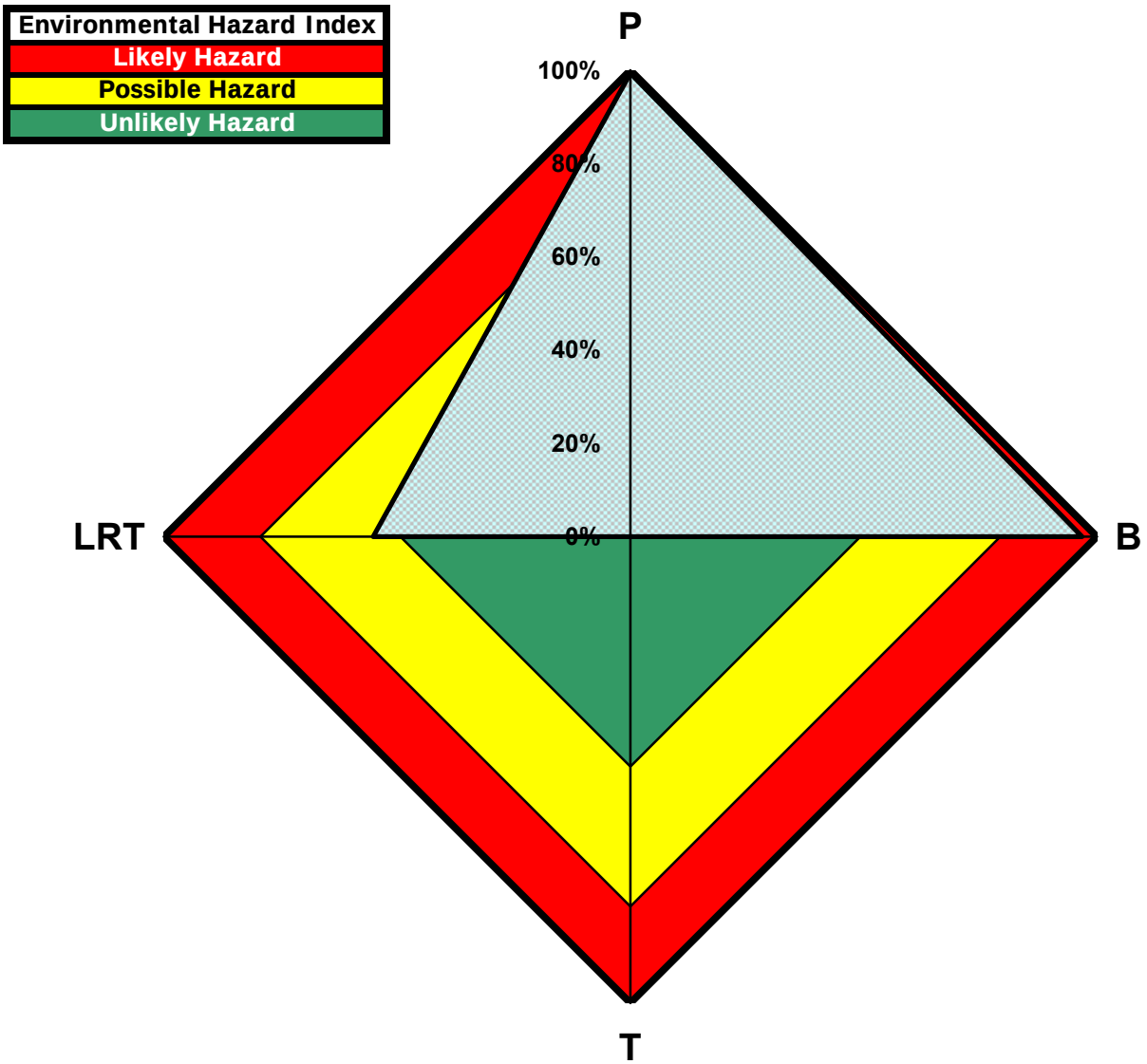
Overall Bioaccumulation Factor, Lake Trout / Water : 20147458

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.

ChemSCORER Beta101 Assessment - Summary Ranking

EPA PCB153



Summary Rankings for: EPA PCB153

This chemical ...

is more PERSISTENT (P) than **99 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **97 %** of chemicals in the reference set.

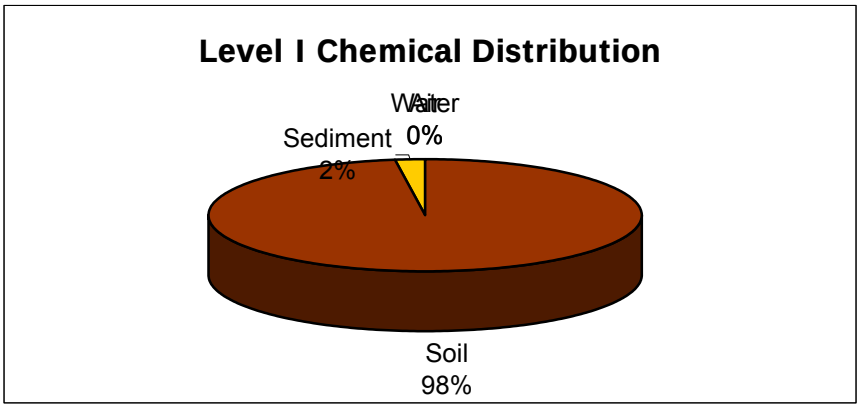
No data on mammalian toxicity was supplied.

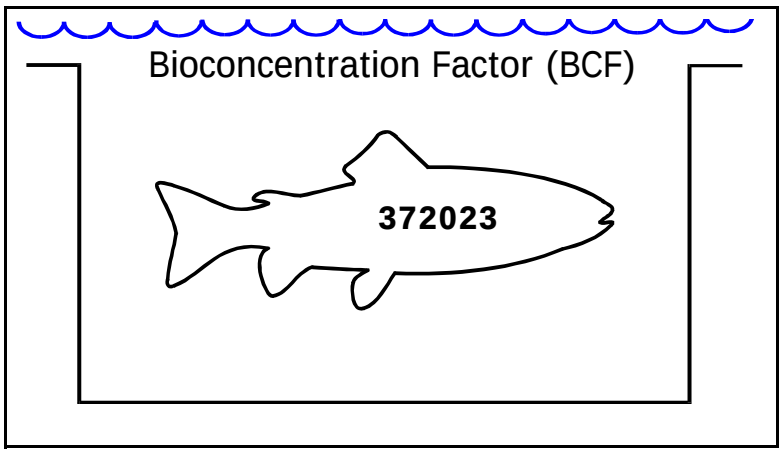
has greater LONG RANGE TRANSPORT (LRT) than **55 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA PCB153

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is substantially greater than the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. In the absence of metabolism by organisms, this substance may bioaccumulate similar to DDT (BCF 63000) or PCBs (BCFs up to 300000).

Details of Level I calculation for: EPA PCB153

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	5.55E-13	2.00E-10	1.69E-07	20	0.020
Water	1.49E-01	2.05E-10	7.42E-08	7.42E-08	15	0.015
Soil	2.19E+04	3.01E-05	1.09E-02	4.52E-03	97720	97.720
Sediment	4.37E+04	6.02E-05	2.17E-02	9.05E-03	2172	2.172
Suspended Sediment	1.37E+05	1.88E-04	6.79E-02	4.52E-02	68	0.068
Biota (Fish)	5.56E+04	7.64E-05	2.76E-02	2.76E-02	6	0.006
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

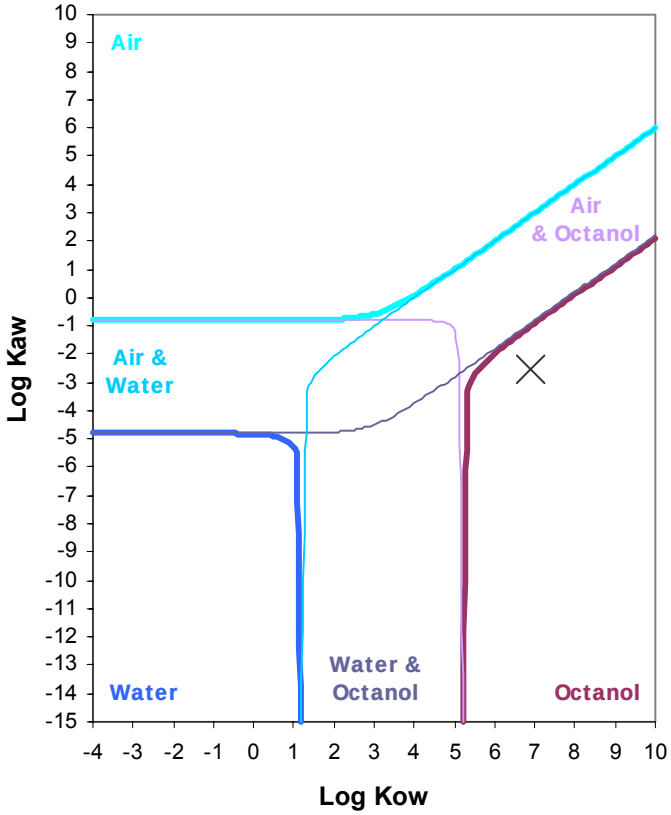
Input Parameters			Partition Coefficients		Three Solubilities	
					(g/m^3)	
Molar Mass	360.88	g/mol				
Vapor Pressure	1	Pa	Log Kow	6.87	Air	1.46E-01
Aqueous Solubility	53.89121564	g/m^3	Log Kaw	-2.57	Water	5.39E+01
Log Kow	6.8716		Log Koa	9.44	Octanol	4.01E+08
Melting Point	-999	deg C				

ChemSCORER Beta101 - Level II Model Results

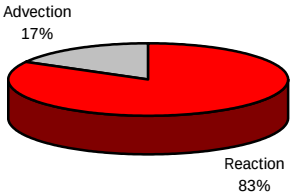
EPA PCB153

Equilibrium Partitioning Persistence Information

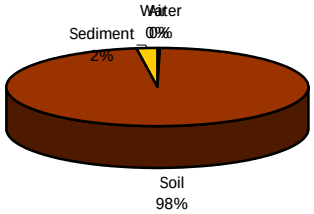
The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.
The equilibrium distribution reaction residence time calculated for this substance is greater than five years, and is comparable to that of hexachlorobenzene (7.6 years). Reactive and advective residence times are comparable, indicating the substance may be subject to long range transport.



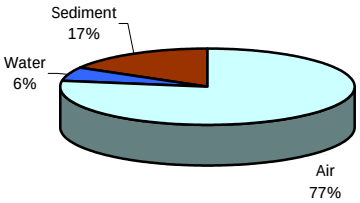
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	2741	days	7.51	years
Reaction Residence Time:	3303	days	9.05	years
Advection Residence Time:	16114	days	44.15	years

Details of Level II calculation for: EPA PCB153

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	5500	5.08E+06	4.03E+08	1.66E+00	1.32E+02	13.345
Water	55000	3.76E+05	2.99E+07	1.23E-01	9.76E+00	0.988
Soil	55000	2.48E+09	0	8.10E+02	0	81.009
Sediment	55000	5.51E+07	8.75E+07	1.80E+01	2.86E+01	4.658
Total		2.54E+09	5.21E+08	8.30E+02	1.70E+02	100.000
Reaction + Advection		3.06E+09		1000		

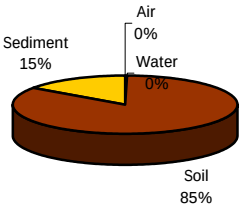
ChemSCORER Beta101 - Level III Model Results

EPA PCB153

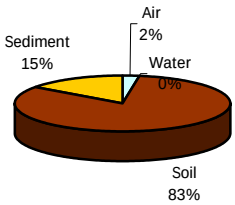
Emission to Air

Emissions to air partition predominantly to soil and sediment.

Steady State Distribution



Reactive Removal



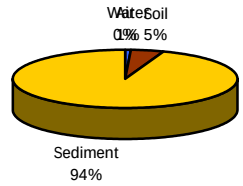
	Persistence
(hours)	77668.3
(days)	3236.2
(years)	8.9

Persistence of air emissions is comparable to that of hexachlorobenzene (2200 days).

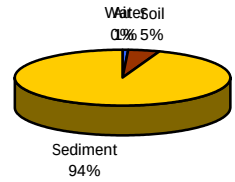
Emission to Water

Emissions to water partition significantly to sediment and may migrate to soil.

Steady State Distribution



Reactive Removal



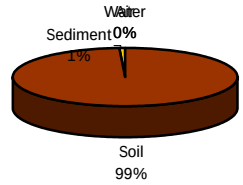
	Persistence
(hours)	79269.5
(days)	3302.9
(years)	9.0

Persistence of water emissions is comparable to that of hexachlorobenzene (2300 days).

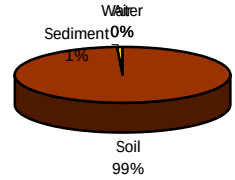
Emission to Soil

Emissions to soil remain predominantly in the soil compartment.

Steady State Distribution



Reactive Removal

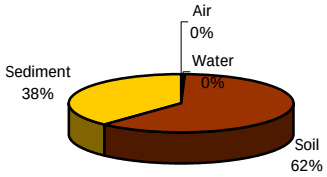


	Persistence
(hours)	79363.7
(days)	3306.8
(years)	9.1

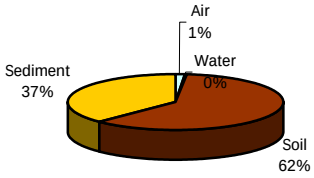
Persistence of soil emissions is comparable to that of hexachlorobenzene (3200 days).

Emission to All 3

Steady State Distribution



Reactive Removal



	Persistence
(hours)	78318.2
(days)	3263.3
(years)	8.9

Persistence under the standard emission scenario is comparable to that of hexachlorobenzene (2300 days).

Details of Level III calculation for: EPA PCB153

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	1.89E+05	1.01E+05	6.54E+07	1.20E+07	7.77E+07
Water	0	1000	0	1.06E+04	6.36E+05	3.68E+06	7.49E+07	7.93E+07
Soil	0	0	1000	1.51E+02	5.21E+03	7.87E+07	6.14E+05	7.94E+07
All 3	600	300	100	1.16E+05	2.52E+05	4.82E+07	2.97E+07	7.83E+07
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	24	1	824	151	1000
Water	0	1000	0	1	8	46	944	1000
Soil	0	0	1000	0	0	992	8	1000
All 3	600	300	100	15	3	608	374	1000

ChemSCORER Beta101 - Transport Model Results

EPA PCB153

TaPL II - Equilibrium distribution Characteristic Travel Distance

Under equilibrium partitioning conditions, this chemical is likely to be transported by both air and water.

TaPL III - Mode of entry assessments

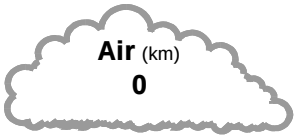
Emission to air - Characteristic Travel Distance in Air

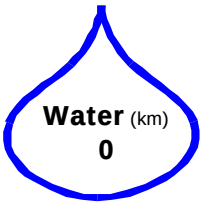
Characteristic Travel Distance in air is high, and is comparable to that of hexachlorinated PCBs (4200 km). This chemical may be subject to long range transport and deposition in the arctic.

Emission to water - Characteristic Travel Distance in Water

Characteristic Travel Distance in water is high, and is comparable to that of toxaphene (9700 km). This chemical may be subject to long range transport in surface and ocean waters.

Emission to soil - Effective Travel Distance





Emissions directly to soil are not expected to partition significantly to air or water, and are not likely to be subject to transport.

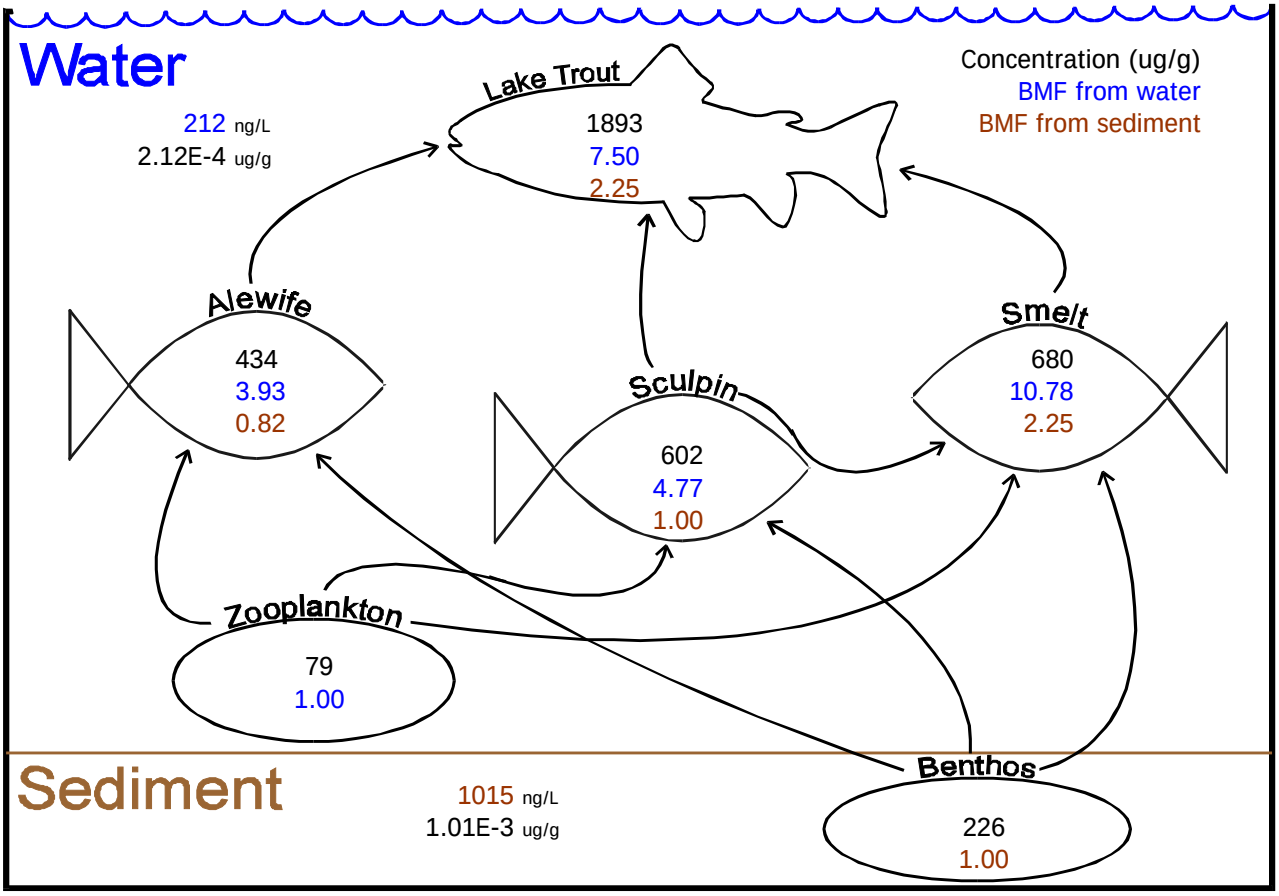
ChemSCORER Beta101 - Toxicity and Bioaccumulation
EPA PCB153

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



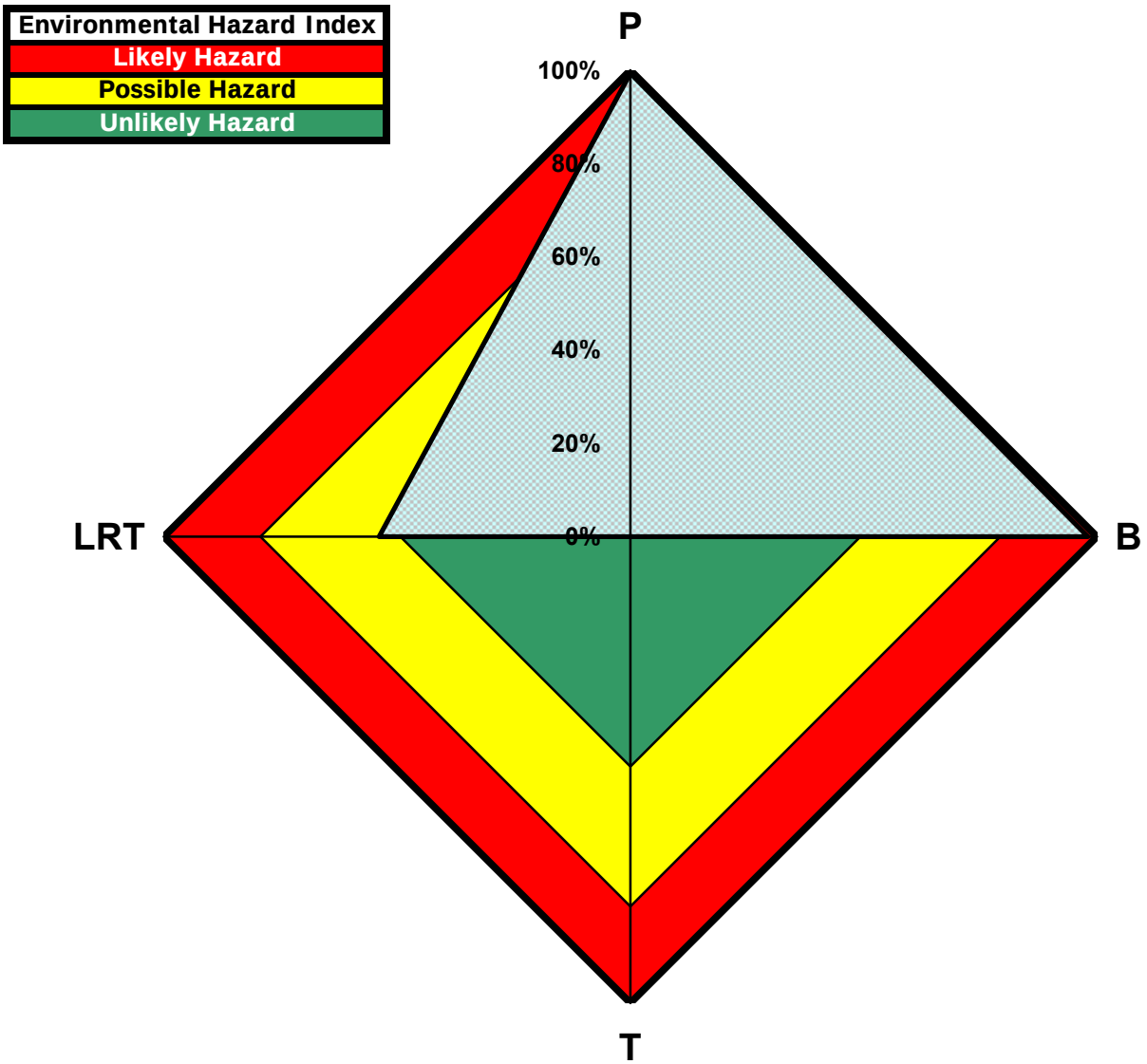
Overall Bioaccumulation Factor, Lake Trout / Water : 8933519

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.

ChemSCORER Beta101 Assessment - Summary Ranking

EPA PCB180



Summary Rankings for: EPA PCB180

This chemical ...

is more PERSISTENT (P) than **99 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **98 %** of chemicals in the reference set.

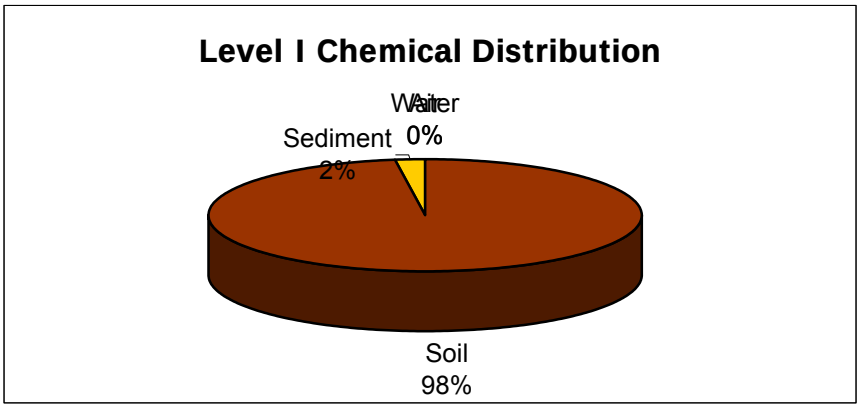
No data on mammalian toxicity was supplied.

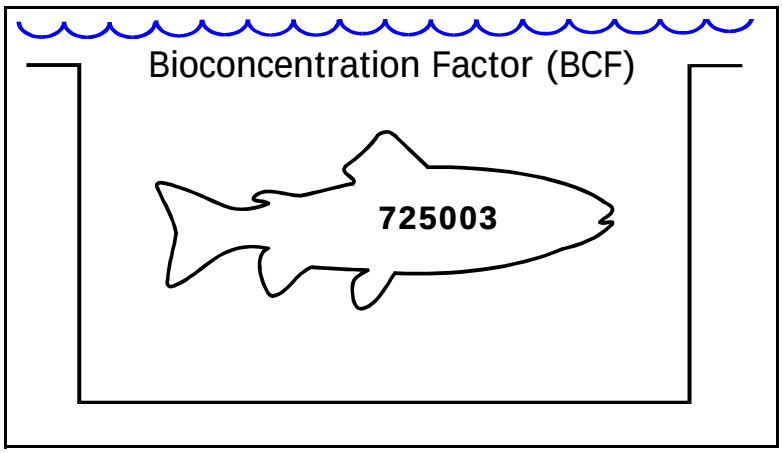
has greater LONG RANGE TRANSPORT (LRT) than **54 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA PCB180

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is substantially greater than the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. In the absence of metabolism by organisms, this substance may bioaccumulate similar to DDT (BCF 63000) or PCBs (BCFs up to 300000).

Details of Level I calculation for: EPA PCB180

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	8.81E-14	3.48E-11	2.94E-08	3	0.003
Water	4.41E-01	9.63E-11	3.81E-08	3.81E-08	8	0.008
Soil	1.26E+05	2.75E-05	1.09E-02	4.53E-03	97743	97.743
Sediment	2.52E+05	5.49E-05	2.17E-02	9.05E-03	2172	2.172
Suspended Sediment	7.86E+05	1.72E-04	6.79E-02	4.53E-02	68	0.068
Biota (Fish)	3.20E+05	6.98E-05	2.76E-02	2.76E-02	6	0.006
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

Input Parameters			Partition Coefficients		Three Solubilities	
					(g/m^3)	
Molar Mass	395.32	g/mol				
Vapor Pressure	1	Pa	Log Kow	7.16	Air	1.60E-01
Aqueous Solubility	174.3146759	g/m^3	Log Kaw	-3.04	Water	1.74E+02
Log Kow	7.16137		Log Koa	10.20	Octanol	2.53E+09
Melting Point	-999	deg C				

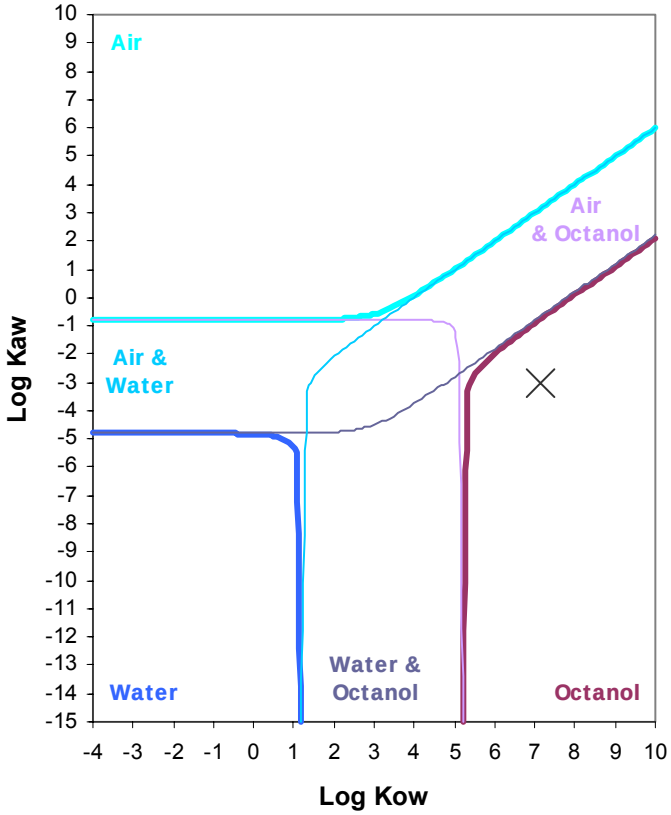
ChemSCORER Beta101 - Level II Model Results

EPA PCB180

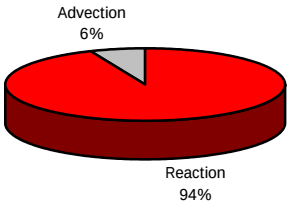
Equilibrium Partitioning Persistence Information

The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.

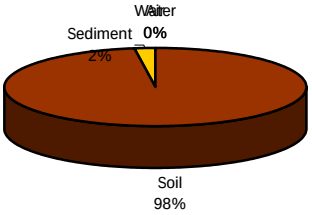
The equilibrium distribution reaction residence time calculated for this substance is greater than five years, and is comparable to that of hexachlorobenzene (7.6 years). Reactive residence time is more than 10 times shorter than advective residence time, indicating potential for long range transport is low.



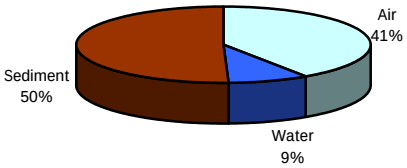
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	3097	days	8.49	years
Reaction Residence Time:	3308	days	9.06	years
Advection Residence Time:	48522	days	132.94	years
Details of Level II calculation for:	EPA PCB180			

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	5500	5.08E+06	4.03E+08	3.26E-01	2.59E+01	2.621
Water	55000	1.11E+06	8.82E+07	7.13E-02	5.66E+00	0.573
Soil	55000	1.43E+10	0	9.15E+02	0	91.543
Sediment	55000	3.17E+08	5.03E+08	2.03E+01	3.23E+01	5.263
Total		1.46E+10	9.95E+08	9.36E+02	6.38E+01	100.000
Reaction + Advection		1.56E+10		1000		

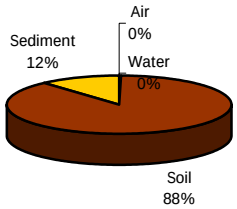
ChemSCORER Beta101 - Level III Model Results

EPA PCB180

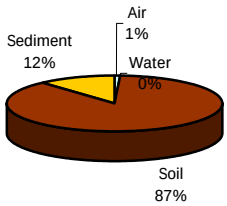
Emission to Air

Emissions to air partition predominantly to soil and sediment.

Steady State Distribution



Reactive Removal



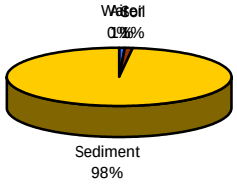
	Persistence
(hours)	78808.2
(days)	3283.7
(years)	9.0

Persistence of air emissions is comparable to that of hexachlorobenzene (2200 days).

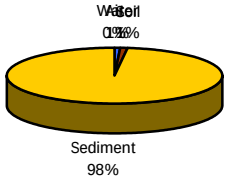
Emission to Water

Emissions to water partition significantly to sediment and may migrate to soil.

Steady State Distribution



Reactive Removal



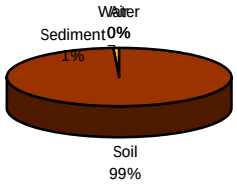
	Persistence
(hours)	79358.4
(days)	3306.6
(years)	9.1

Persistence of water emissions is comparable to that of hexachlorobenzene (2300 days).

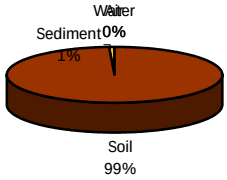
Emission to Soil

Emissions to soil remain predominantly in the soil compartment.

Steady State Distribution



Reactive Removal

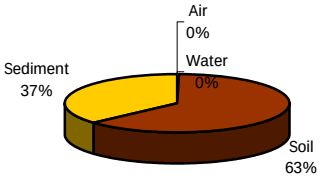


	Persistence
(hours)	79365.0
(days)	3306.9
(years)	9.1

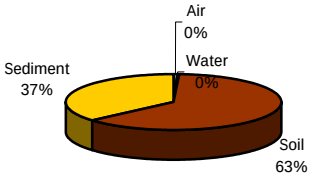
Persistence of soil emissions is comparable to that of hexachlorobenzene (3200 days).

Emission to All 3

Steady State Distribution



Reactive Removal



	Persistence
(hours)	79029.0
(days)	3292.9
(years)	9.0

Persistence under the standard emission scenario is comparable to that of hexachlorobenzene (2300 days).

Details of Level III calculation for: EPA PCB180

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	6.19E+04	7.17E+04	6.95E+07	9.22E+06	7.88E+07
Water	0	1000	0	7.38E+02	6.07E+05	8.28E+05	7.79E+07	7.94E+07
Soil	0	0	1000	1.07E+01	4.86E+03	7.87E+07	6.25E+05	7.94E+07
All 3	600	300	100	3.73E+04	2.26E+05	4.98E+07	2.90E+07	7.90E+07
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	8	1	875	116	1000
Water	0	1000	0	0	8	10	982	1000
Soil	0	0	1000	0	0	992	8	1000
All 3	600	300	100	5	3	627	365	1000

ChemSCORER Beta101 - Transport Model Results

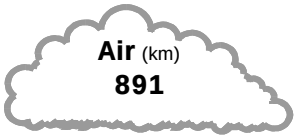
EPA PCB180

TaPL II - Equilibrium distribution Characteristic Travel Distance

Under equilibrium partitioning conditions, this chemical is likely to be transported by both air and water.

TaPL III - Mode of entry assessments

Emission to air - Characteristic Travel Distance in Air

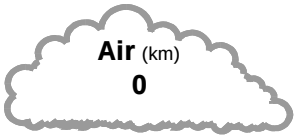


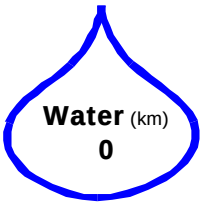
Characteristic Travel Distance in air is moderate, and is comparable to that of DDT (830 km). This chemical may be found in remote areas, but is not necessarily transported over very long distances.

Emission to water - Characteristic Travel Distance in Water

Characteristic Travel Distance in water is high, and is comparable to that of toxaphene (9700 km). This chemical may be subject to long range transport in surface and ocean waters.

Emission to soil - Effective Travel Distance





Emissions directly to soil are not expected to partition significantly to air or water, and are not likely to be subject to transport.

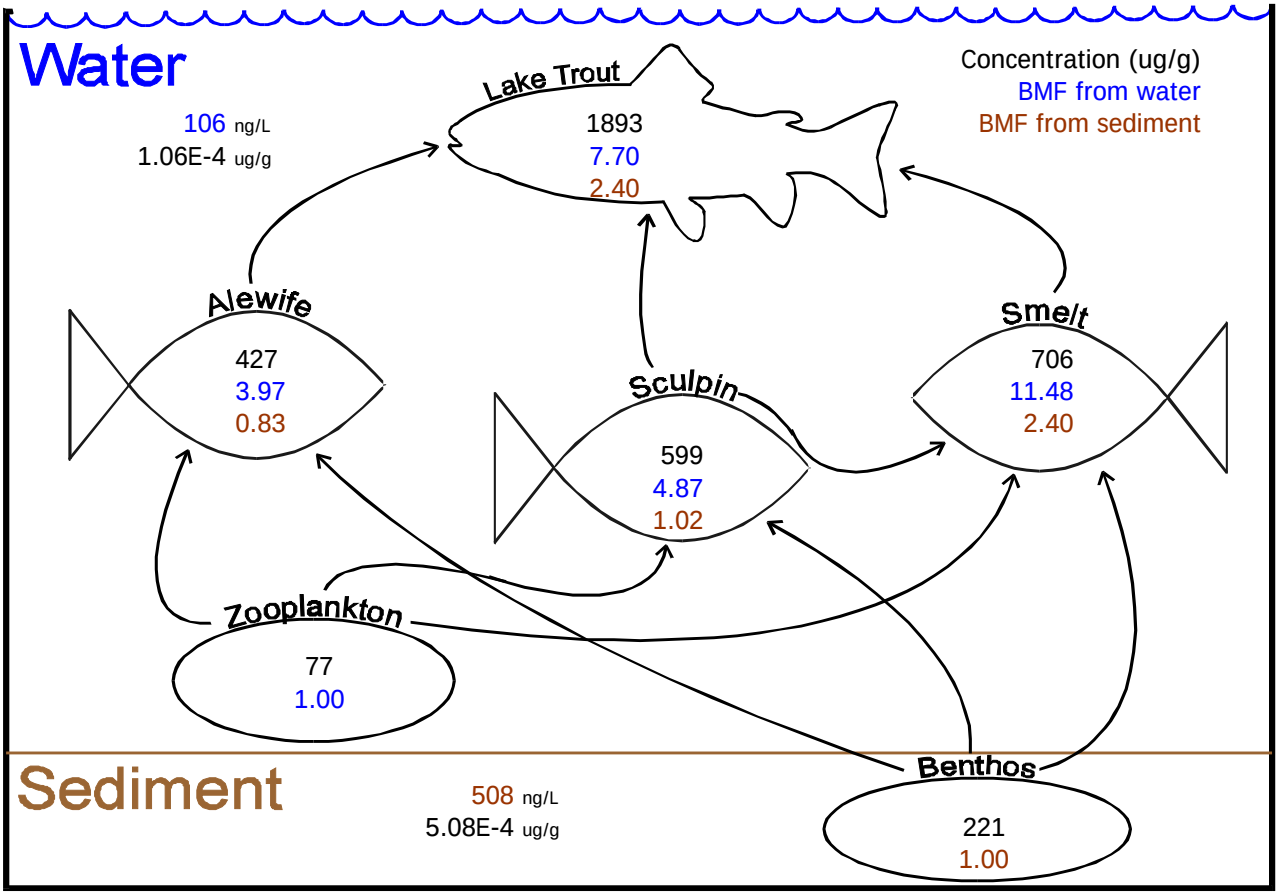
ChemSCORER Beta101 - Toxicity and Bioaccumulation
EPA PCB180

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



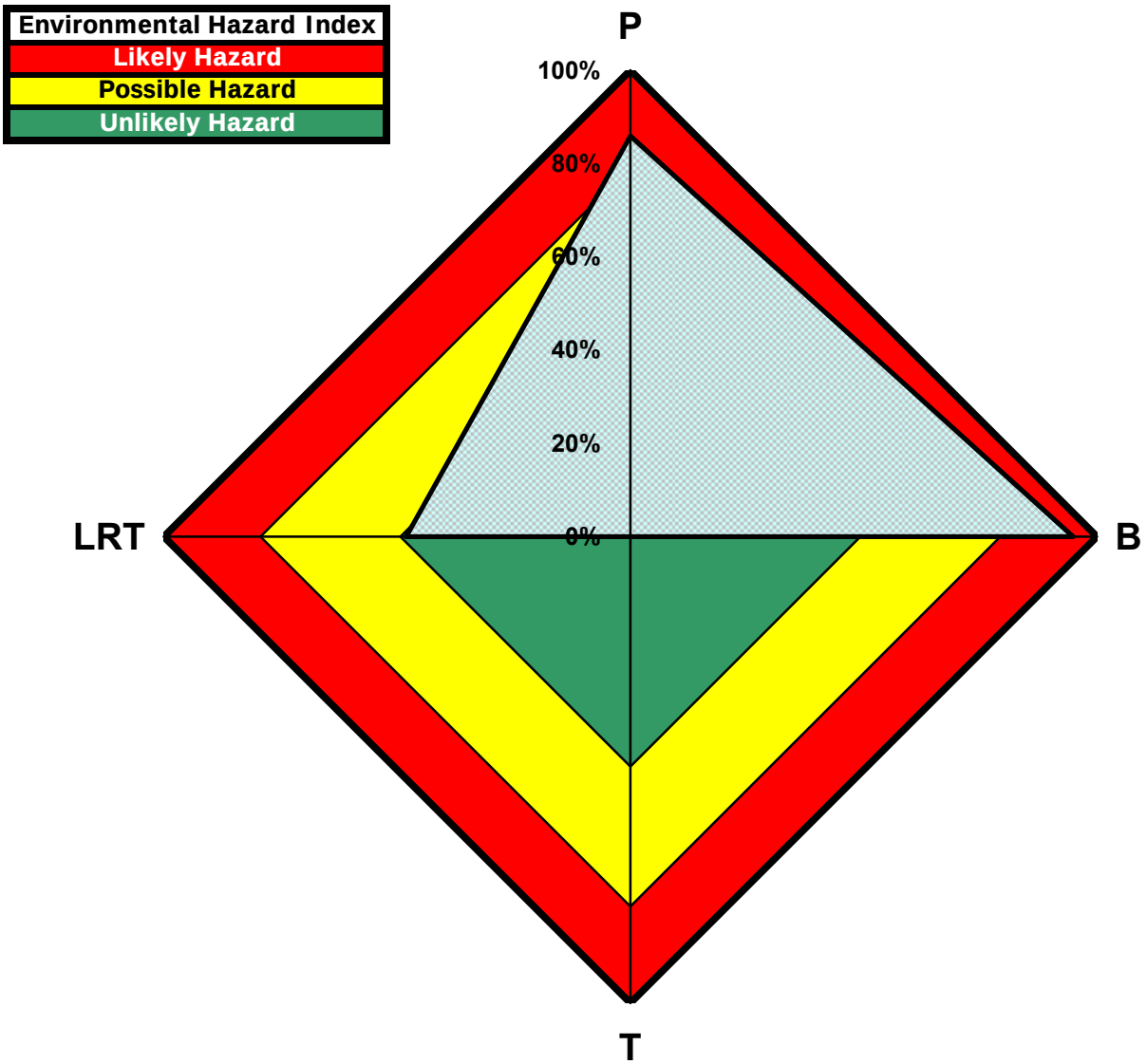
Overall Bioaccumulation Factor, Lake Trout / Water : 17867941

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.

ChemSCORER Beta101 Assessment - Summary Ranking

EPA Dieldrin



Summary Rankings for: EPA Dieldrin

This chemical ...

is more PERSISTENT (P) than **86 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **95 %** of chemicals in the reference set.

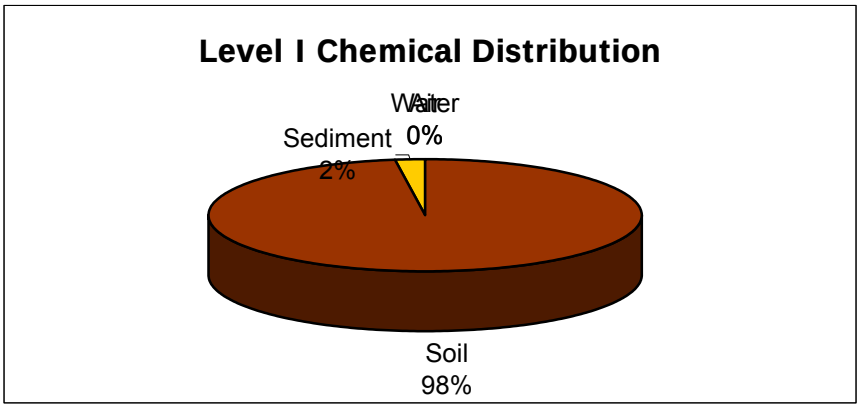
No data on mammalian toxicity was supplied.

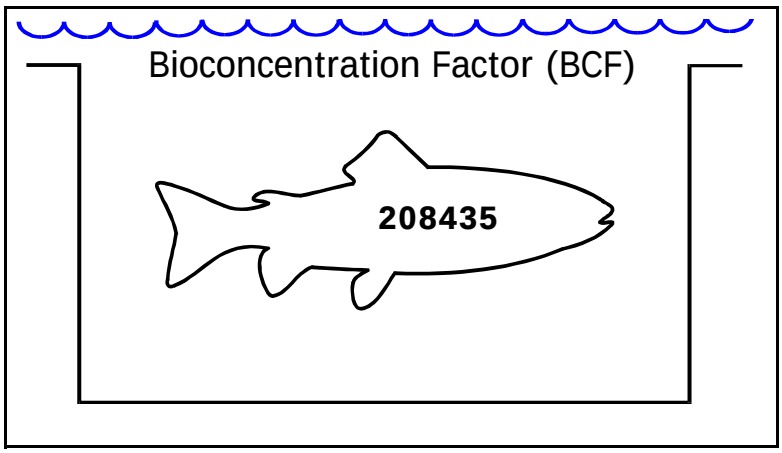
has greater LONG RANGE TRANSPORT (LRT) than **48 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA Dieldrin

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is substantially greater than the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. In the absence of metabolism by organisms, this substance may bioaccumulate similar to DDT (BCF 63000) or PCBs (BCFs up to 300000).

Details of Level I calculation for: EPA Dieldrin

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	8.76E-14	3.34E-11	2.81E-08	3	0.003
Water	1.60E+00	3.47E-10	1.32E-07	1.32E-07	26	0.026
Soil	1.31E+05	2.85E-05	1.09E-02	4.52E-03	97725	97.725
Sediment	2.63E+05	5.70E-05	2.17E-02	9.05E-03	2172	2.172
Suspended Sediment	8.21E+05	1.78E-04	6.79E-02	4.52E-02	68	0.068
Biota (Fish)	3.34E+05	7.24E-05	2.76E-02	2.76E-02	6	0.006
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

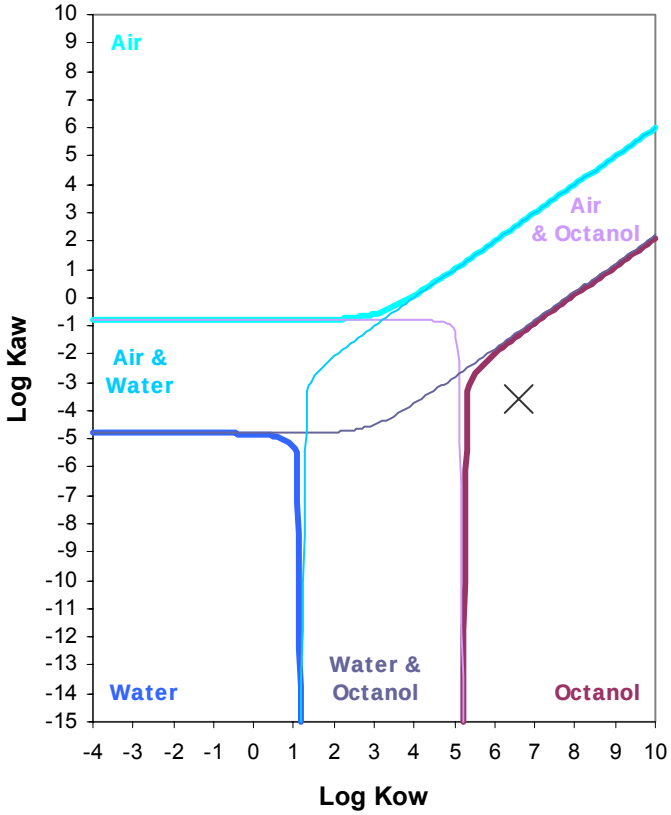
Input Parameters			Partition Coefficients		Three Solubilities	
					(g/m^3)	
Molar Mass	380.93	g/mol				
Vapor Pressure	1	Pa	Log Kow	6.62	Air	1.54E-01
Aqueous Solubility	609.570253	g/m^3	Log Kaw	-3.60	Water	6.10E+02
Log Kow	6.62		Log Koa	10.22	Octanol	2.54E+09
Melting Point	-999	deg C				

ChemSCORER Beta101 - Level II Model Results

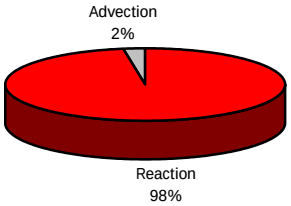
EPA Dieldrin

Equilibrium Partitioning Persistence Information

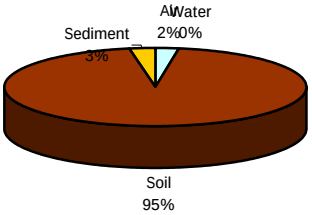
The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.
The equilibrium distribution reaction residence time calculated for this substance can be measured in years, and is comparable to that of pentachlorobenzene (2 years). Reactive residence time is more than 10 times shorter than advective residence time, indicating potential for transport to other regions is low.



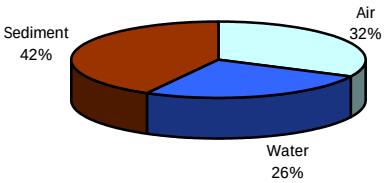
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	954	days	2.61	years
Reaction Residence Time:	977	days	2.68	years
Advection Residence Time:	40347	days	110.54	years

Details of Level II calculation for: EPA Dieldrin

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	22.25	1.26E+09	4.03E+08	2.38E+01	7.64E+00	3.143
Water	15240	1.46E+07	3.20E+08	2.76E-01	6.06E+00	0.634
Soil	16744	4.89E+10	0	9.26E+02	0	92.608
Sediment	13152	1.38E+09	5.25E+08	2.62E+01	9.94E+00	3.614
Total		5.16E+10	1.25E+09	9.76E+02	2.36E+01	100.000
Reaction + Advection		5.28E+10		1000		

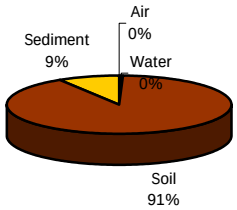
ChemSCORER Beta101 - Level III Model Results

EPA Dieldrin

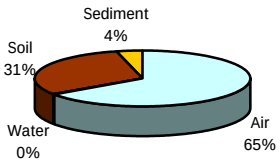
Emission to Air

Emissions to air partition predominantly to soil and sediment.

Steady State Distribution



Reactive Removal



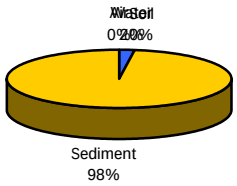
	Persistence
(hours)	8191.5
(days)	341.3
(years)	0.9

Persistence of air emissions is comparable to that of the tetrachlorobenzenes (110 days).

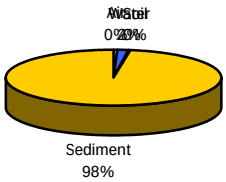
Emission to Water

Emissions to water partition significantly to sediment and may migrate to soil.

Steady State Distribution



Reactive Removal



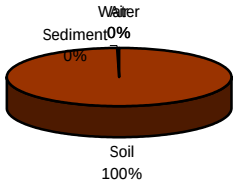
	Persistence
(hours)	18963.0
(days)	790.1
(years)	2.2

Persistence of water emissions is comparable to that of hexachlorobenzene (2300 days).

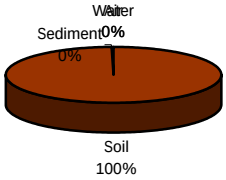
Emission to Soil

Emissions to soil remain predominantly in the soil compartment.

Steady State Distribution



Reactive Removal

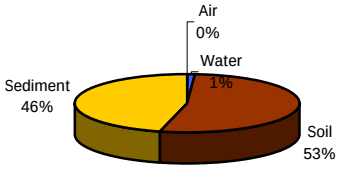


	Persistence
(hours)	24147.6
(days)	1006.2
(years)	2.8

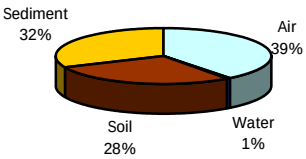
Persistence of soil emissions is comparable to that of hexachlorobenzene (3200 days).

Emission to All 3

Steady State Distribution



Reactive Removal



	Persistence
(hours)	13018.6
(days)	542.4
(years)	1.5

Persistence under the standard emission scenario is comparable to that of hexachlorobenzene (2300 days).

Details of Level III calculation for: EPA Dieldrin

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	2.10E+04	1.57E+04	7.42E+06	7.35E+05	8.19E+06
Water	0	1000	0	1.35E+02	3.96E+05	4.79E+04	1.85E+07	1.90E+07
Soil	0	0	1000	1.26E+00	1.01E+03	2.41E+07	4.74E+04	2.41E+07
All 3	600	300	100	1.26E+04	1.28E+05	6.88E+06	6.00E+06	1.30E+07
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	653	1	307	39	1000
Water	0	1000	0	4	18	2	976	1000
Soil	0	0	1000	0	0	997	2	1000
All 3	600	300	100	393	6	285	316	1000

ChemSCORER Beta101 - Transport Model Results

EPA Dieldrin

TaPL II - Equilibrium distribution Characteristic Travel Distance

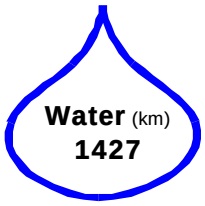
Under equilibrium partitioning conditions, this chemical is likely to be transported by both air and water.

TaPL III - Mode of entry assessments

Emission to air - Characteristic Travel Distance in Air

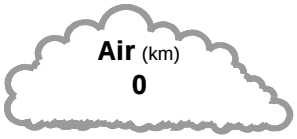
Characteristic Travel Distance in air is low. This chemical is not likely to be transported a significant distance in the atmosphere.

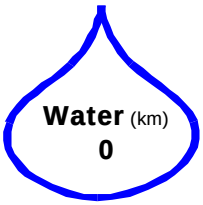
Emission to water - Characteristic Travel Distance in Water



Characteristic Travel Distance in water is moderate, and is comparable to that of chlorobenzene (1300 km). This chemical may be subject to transport in surface and near-shore marine waters.

Emission to soil - Effective Travel Distance





Emissions directly to soil are not expected to partition significantly to air or water, and are not likely to be subject to transport.

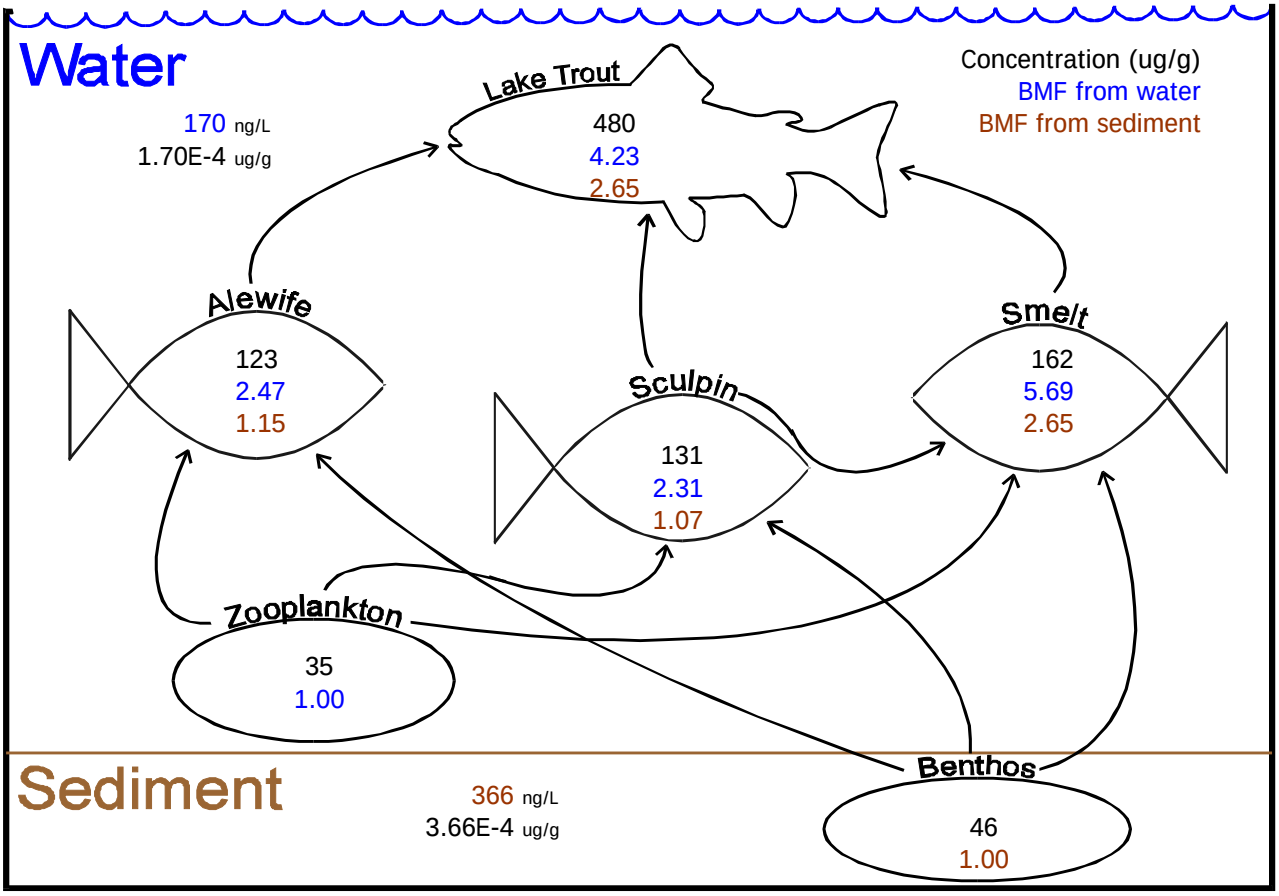
ChemSCORER Beta101 - Toxicity and Bioaccumulation
EPA Dieldrin

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



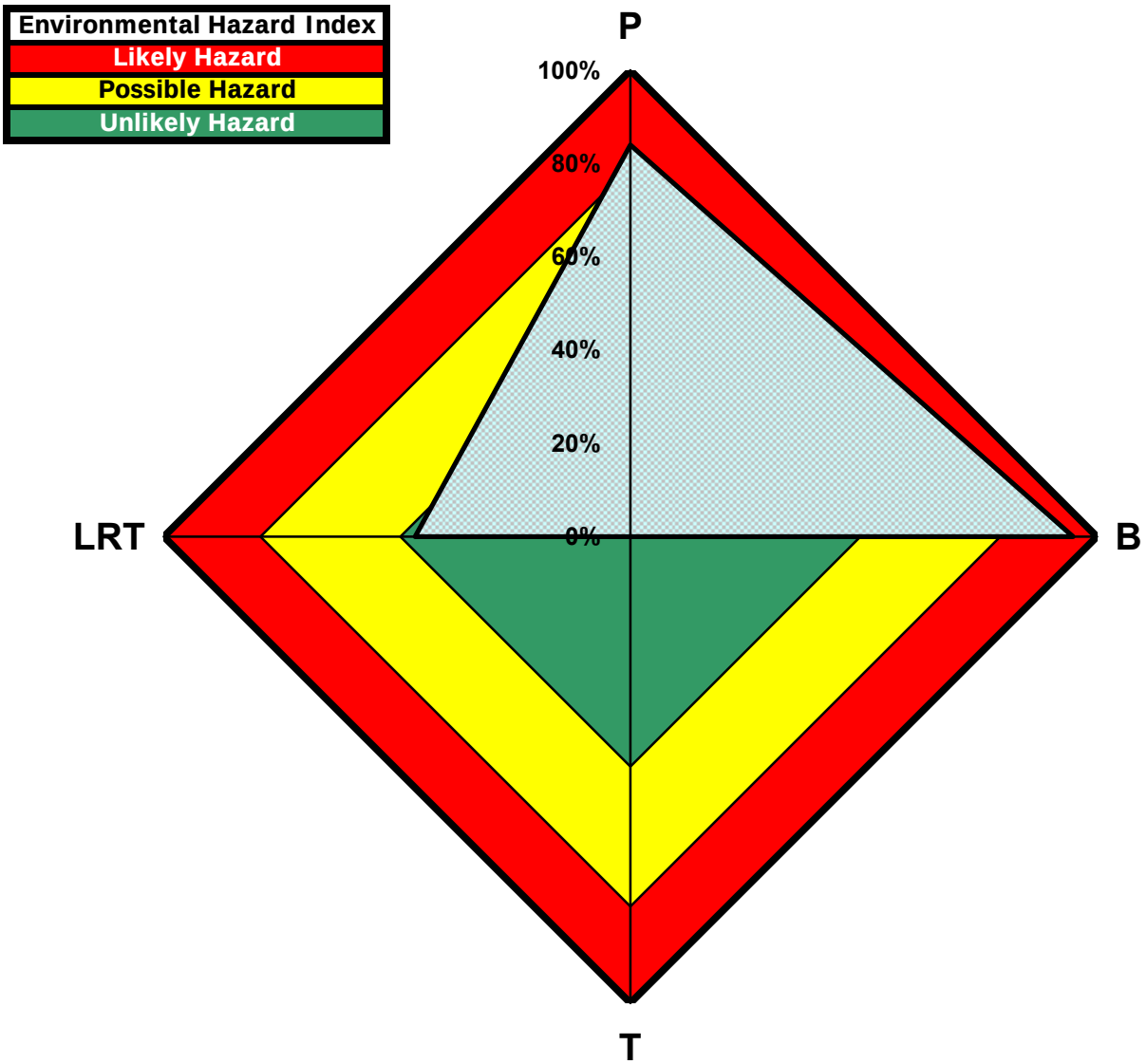
Overall Bioaccumulation Factor, Lake Trout / Water : 2821351

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.

ChemSCORER Beta101 Assessment - Summary Ranking

EPA Aldrin



Summary Rankings for: EPA Aldrin

This chemical ...

is more PERSISTENT (P) than **84 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **95 %** of chemicals in the reference set.

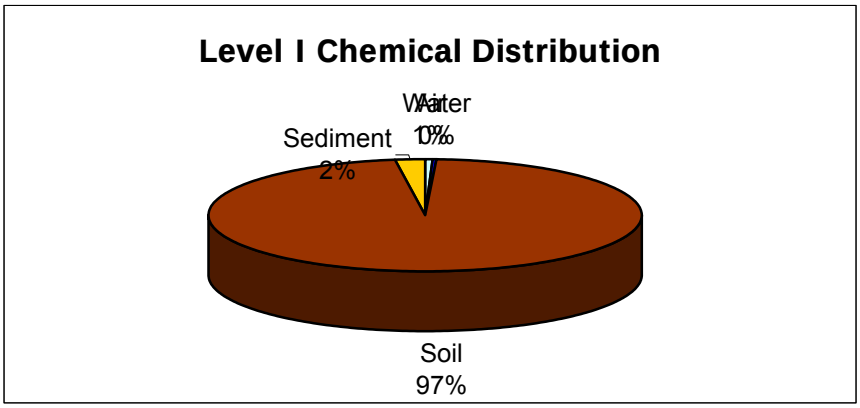
No data on mammalian toxicity was supplied.

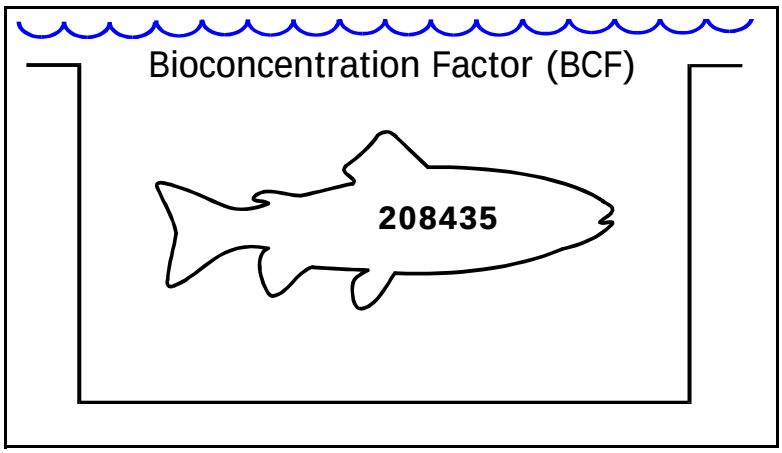
has greater LONG RANGE TRANSPORT (LRT) than **46 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA Aldrin

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is substantially greater than the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. In the absence of metabolism by organisms, this substance may bioaccumulate similar to DDT (BCF 63000) or PCBs (BCFs up to 300000).

Details of Level I calculation for: EPA Aldrin

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	1.65E-11	6.01E-09	5.07E-06	601	0.601
Water	8.83E-03	3.61E-10	1.32E-07	1.32E-07	26	0.026
Soil	7.24E+02	2.96E-05	1.08E-02	4.50E-03	97141	97.141
Sediment	1.45E+03	5.92E-05	2.16E-02	8.99E-03	2159	2.159
Suspended Sediment	4.53E+03	1.85E-04	6.75E-02	4.50E-02	67	0.067
Biota (Fish)	1.84E+03	7.51E-05	2.74E-02	2.74E-02	5	0.005
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

Input Parameters			Partition Coefficients		Three Solubilities	
					(g/m^3)	
Molar Mass	364.93	g/mol				
Vapor Pressure	1	Pa	Log Kow	6.62	Air	1.47E-01
Aqueous Solubility	3.220807236	g/m^3	Log Kaw	-1.34	Water	3.22E+00
Log Kow	6.62		Log Koa	7.96	Octanol	1.34E+07
Melting Point	-999	deg C				

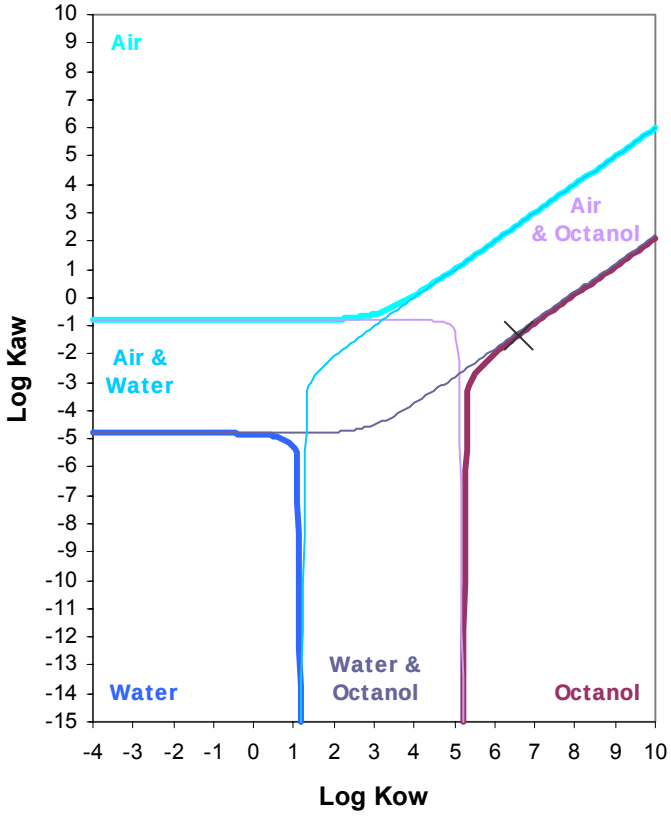
ChemSCORER Beta101 - Level II Model Results

EPA Aldrin

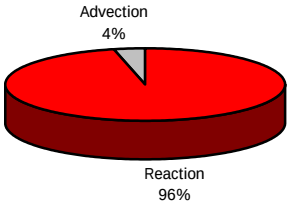
Equilibrium Partitioning Persistence Information

The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.

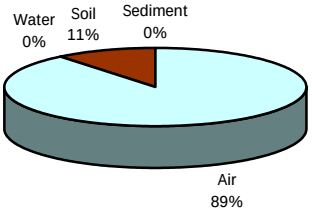
The equilibrium distribution reaction residence time calculated for this substance can be measured in months, and is comparable to that of the tetrachlorobenzenes (120 days). Reactive residence time is more than 10 times shorter than advective residence time, indicating potential for transport to other regions is low.



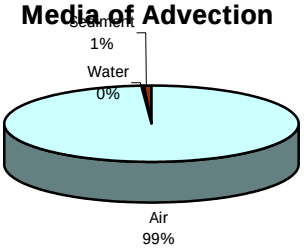
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	590	hours	24.59	days
Reaction Residence Time:	612	hours	25.51	days
Advection Residence Time:	16439	hours	684.96	days

Details of Level II calculation for: EPA Aldrin

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	2.86	9.78E+09	4.03E+08	8.60E+02	3.55E+01	89.548
Water	2670	4.58E+05	1.77E+06	4.03E-02	1.55E-01	0.020
Soil	3830	1.18E+09	0	1.04E+02	0	10.374
Sediment	26700	3.76E+06	2.90E+06	3.31E-01	2.55E-01	0.059
Total		1.10E+10	4.08E+08	9.64E+02	3.59E+01	100.000
Reaction + Advection		1.14E+10		1000		

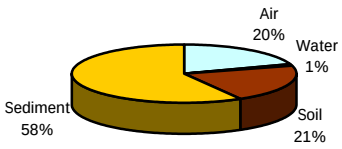
ChemSCORER Beta101 - Level III Model Results

EPA Aldrin

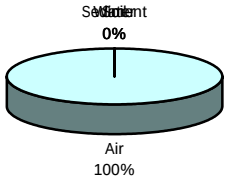
Emission to Air

Emissions to air partition significantly to soil and sediment.

Steady State Distribution



Reactive Removal



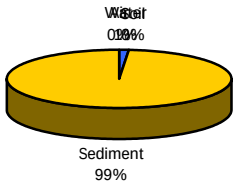
	Persistence
(hours)	20.79
(days)	0.87
(years)	0.00

Persistence of air emissions is comparable to that of benzene (25 hours).

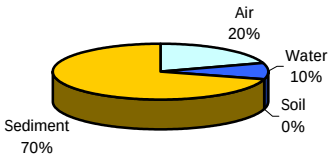
Emission to Water

Emissions to water partition significantly to sediment and may migrate to soil.

Steady State Distribution



Reactive Removal



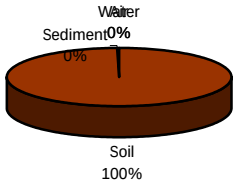
	Persistence
(hours)	27524.39
(days)	1146.85
(years)	3.14

Persistence of water emissions is comparable to that of hexachlorobenzene (2300 days).

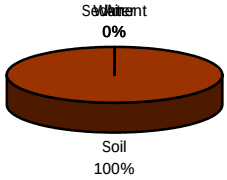
Emission to Soil

Emissions to soil remain predominantly in the soil compartment.

Steady State Distribution



Reactive Removal

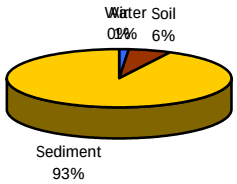


	Persistence
(hours)	5536.17
(days)	230.67
(years)	0.63

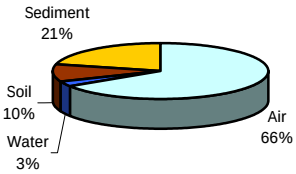
Persistence of soil emissions is comparable to that of the tetrachlorobenzenes (250 days).

Emission to All 3

Steady State Distribution



Reactive Removal



	Persistence
(hours)	8823.41
(days)	367.64
(years)	1.01

Persistence under the standard emission scenario is comparable to that of the tetrachlorobenzenes (130 days).

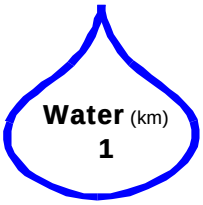
Details of Level III calculation for: EPA Aldrin

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	4.12E+03	1.64E+02	4.35E+03	1.21E+04	2.08E+04
Water	0	1000	0	8.24E+02	3.68E+05	8.70E+02	2.72E+07	2.75E+07
Soil	0	0	1000	3.04E+00	2.15E+02	5.52E+06	1.59E+04	5.54E+06
All 3	600	300	100	2.72E+03	1.10E+05	5.55E+05	8.16E+06	8.82E+06
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	999	0	1	0	1000
Water	0	1000	0	200	95	0	705	1000
Soil	0	0	1000	1	0	999	0	1000
All 3	600	300	100	659	29	100	212	1000

ChemSCORER Beta101 - Transport Model Results

EPA Aldrin

TaPL II - Equilibrium distribution Characteristic Travel Distance



Under equilibrium partitioning conditions, this chemical is likely to be transported most effectively in air.

TaPL III - Mode of entry assessments

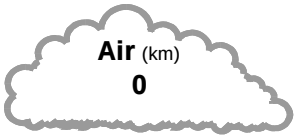
Emission to air - Characteristic Travel Distance in Air

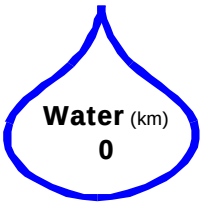
Characteristic Travel Distance in air is low. This chemical is not likely to be transported a significant distance in the atmosphere.

Emission to water - Characteristic Travel Distance in Water

Characteristic Travel Distance in water is moderate, and is comparable to that of chlorobenzene (1300 km). This chemical may be subject to transport in surface and near-shore marine waters.

Emission to soil - Effective Travel Distance





Emissions directly to soil are not expected to partition significantly to air or water, and are not likely to be subject to transport.

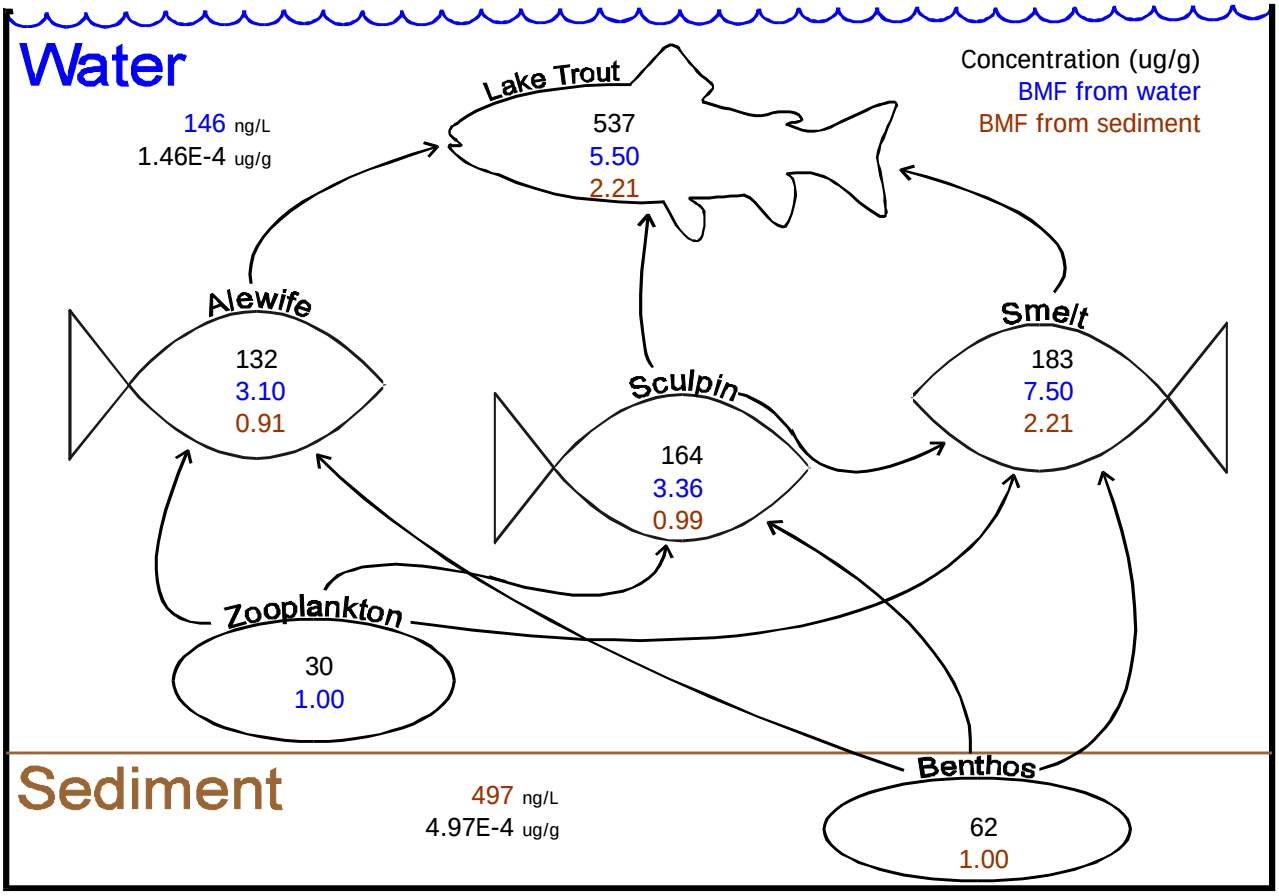
ChemSCORER Beta101 - Toxicity and Bioaccumulation
EPA Aldrin

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



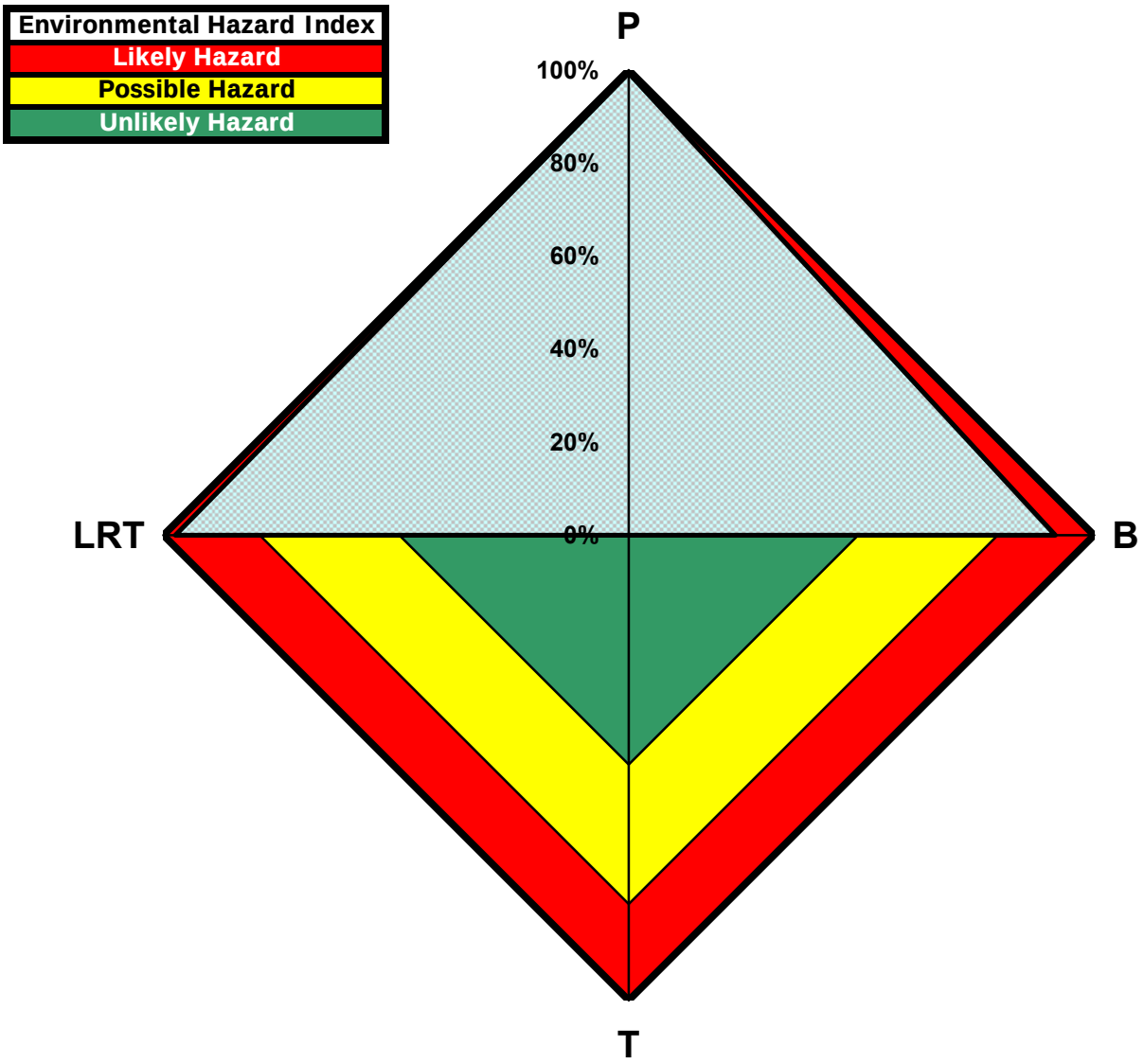
Overall Bioaccumulation Factor, Lake Trout / Water : 3668028

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.

ChemSCORER Beta101 Assessment - Summary Ranking

EPA Hexachlorobenzene



Summary Rankings for: EPA Hexachlorobenzene

This chemical ...

is more PERSISTENT (P) than **99 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **92 %** of chemicals in the reference set.

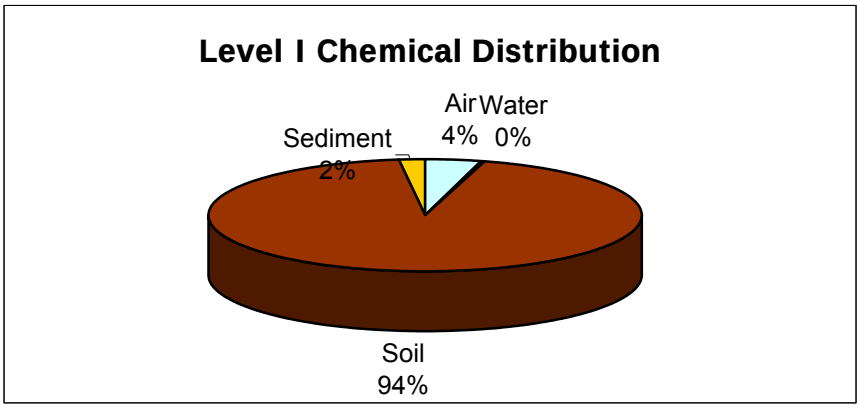
No data on mammalian toxicity was supplied.

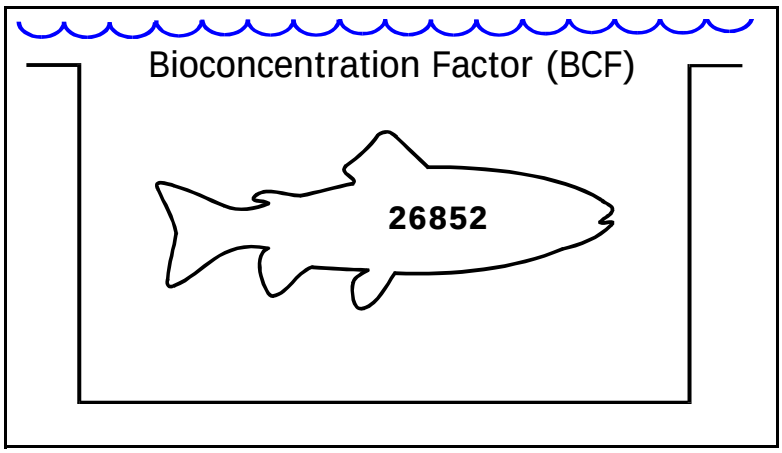
has greater LONG RANGE TRANSPORT (LRT) than **97 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA Hexachlorobenzene

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is greater than the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. In the absence of rapid metabolism by organisms, this substance is expected to bioaccumulate.

Details of Level I calculation for: EPA Hexachlorobenzene

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	1.44E-10	4.10E-08	3.46E-05	4100	4.100
Water	9.68E-03	3.45E-09	9.84E-07	9.84E-07	197	0.197
Soil	1.02E+02	3.65E-05	1.04E-02	4.33E-03	93554	93.554
Sediment	2.05E+02	7.30E-05	2.08E-02	8.66E-03	2079	2.079
Suspended Sediment	6.39E+02	2.28E-04	6.50E-02	4.33E-02	65	0.065
Biota (Fish)	2.60E+02	9.27E-05	2.64E-02	2.64E-02	5	0.005
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

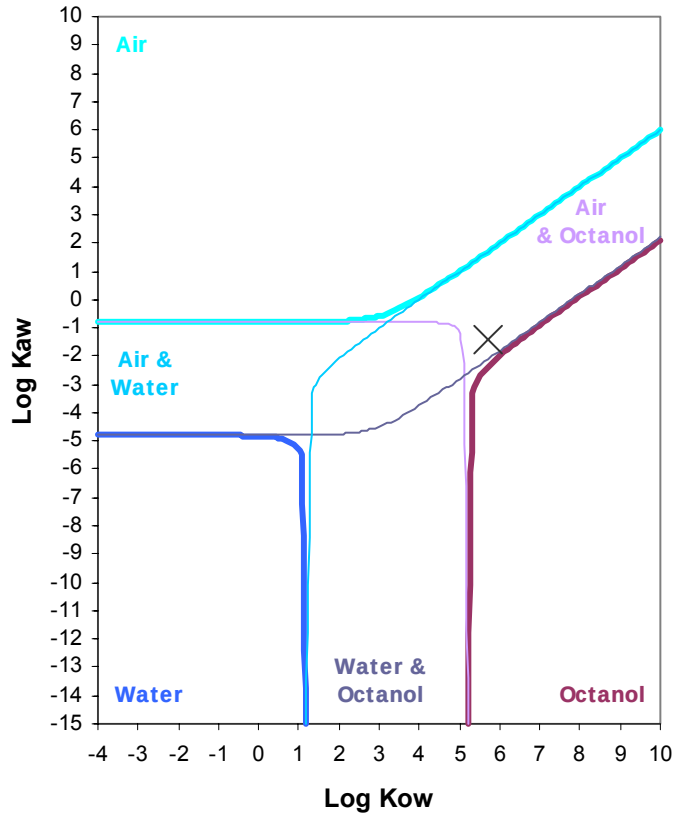
Input Parameters			Partition Coefficients		Three Solubilities	
Molar Mass	284.79	g/mol			(g/m^3)	
Vapor Pressure	1	Pa	Log Kow	5.73	Air	1.15E-01
Aqueous Solubility	2.756004369	g/m^3	Log Kaw	-1.38	Water	2.76E+00
Log Kow	5.73		Log Koa	7.11	Octanol	1.48E+06
Melting Point	230	deg C				

ChemSCORER Beta101 - Level II Model Results

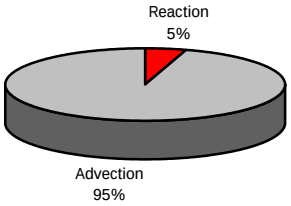
EPA Hexachlorobenzene

Equilibrium Partitioning Persistence Information

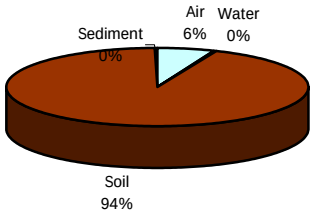
The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.
The equilibrium distribution reaction residence time calculated for this substance can be measured in years, and is comparable to that of pentachlorobenzene (2 years). Advective residence time is more than 10 times shorter than reactive residence time, indicating the substance may be transported to other regions.



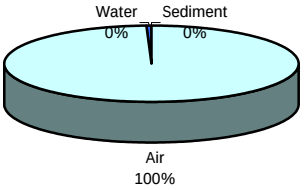
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	96	days	0.26	years
Reaction Residence Time:	2047	days	5.61	years
Advection Residence Time:	101	days	0.28	years

Details of Level II calculation for: EPA Hexachlorobenzene

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	22600	1.24E+06	4.03E+08	2.91E+00	9.47E+02	95.037
Water	34100	3.93E+04	1.94E+06	9.24E-02	4.55E+00	0.464
Soil	34100	1.87E+07	0	4.39E+01	0	4.393
Sediment	341000	4.16E+04	4.09E+05	9.76E-02	9.61E-01	0.106
Total		2.00E+07	4.06E+08	4.70E+01	9.53E+02	100.000
Reaction + Advection		4.26E+08		1000		

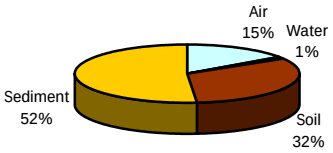
ChemSCORER Beta101 - Level III Model Results

EPA Hexachlorobenzene

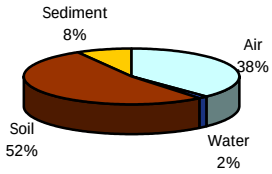
Emission to Air

Emissions to air partition significantly to soil and sediment.

Steady State Distribution



Reactive Removal



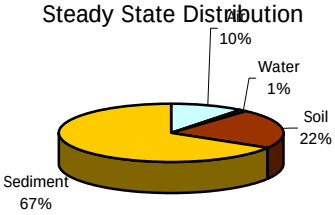
	Persistence
(hours)	80036.0
(days)	3334.8
(years)	9.1

Persistence of air emissions is comparable to that of hexachlorobenzene (2200 days).

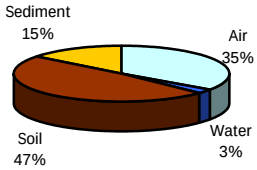
Emission to Water

Emissions to water partition significantly to sediment and may migrate to soil.

Steady State Distribution



Reactive Removal



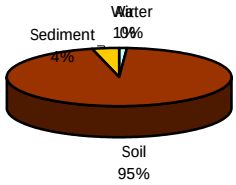
	Persistence
(hours)	107748.9
(days)	4489.5
(years)	12.3

Persistence of water emissions is comparable to that of the PCBs (up to 80 years).

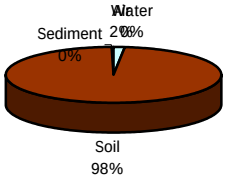
Emission to Soil

Emissions to soil partition significantly to other media.

Steady State Distribution



Reactive Removal

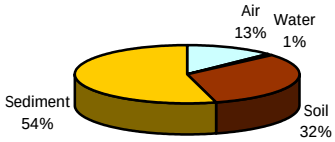


	Persistence
(hours)	50764.5
(days)	2115.2
(years)	5.8

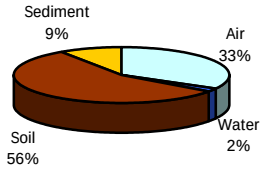
Persistence of soil emissions is comparable to that of hexachlorobenzene (3200 days).

Emission to All 3

Steady State Distribution



Reactive Removal



	Persistence
(hours)	85422.7
(days)	3559.3
(years)	9.8

Persistence under the standard emission scenario is comparable to that of hexachlorobenzene (2300 days).

Details of Level III calculation for: EPA Hexachlorobenzene

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	1.23E+07	7.60E+05	2.58E+07	4.12E+07	8.00E+07
Water	0	1000	0	1.13E+07	1.32E+06	2.37E+07	7.14E+07	1.08E+08
Soil	0	0	1000	5.38E+05	3.75E+04	4.82E+07	2.04E+06	5.08E+07
All 3	600	300	100	1.08E+07	8.55E+05	2.74E+07	4.64E+07	8.54E+07
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	377	15	524	84	1000
Water	0	1000	0	346	27	482	145	1000
Soil	0	0	1000	16	1	979	4	1000
All 3	600	300	100	332	17	557	94	1000

ChemSCORER Beta101 - Transport Model Results

EPA Hexachlorobenzene

TaPL II - Equilibrium distribution Characteristic Travel Distance

Under equilibrium partitioning conditions, this chemical is likely to be transported most effectively in air.

TaPL III - Mode of entry assessments

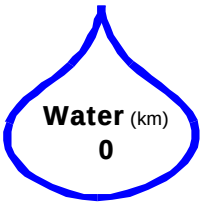
Emission to air - Characteristic Travel Distance in Air

Characteristic Travel Distance in air is extremely high, and is comparable to that of hexachlorobenzene (110 000 km). This chemical is likely subject to long range transport and deposition in the arctic.

Emission to water - Characteristic Travel Distance in Water

Characteristic Travel Distance in water is high, and is comparable to that of toxaphene (9700 km). This chemical may be subject to long range transport in surface and ocean waters.

Emission to soil - Effective Travel Distance



Emissions directly to soil may partition to air and be subject to transport in the atmosphere.

ChemSCORER Beta101 - Toxicity and Bioaccumulation

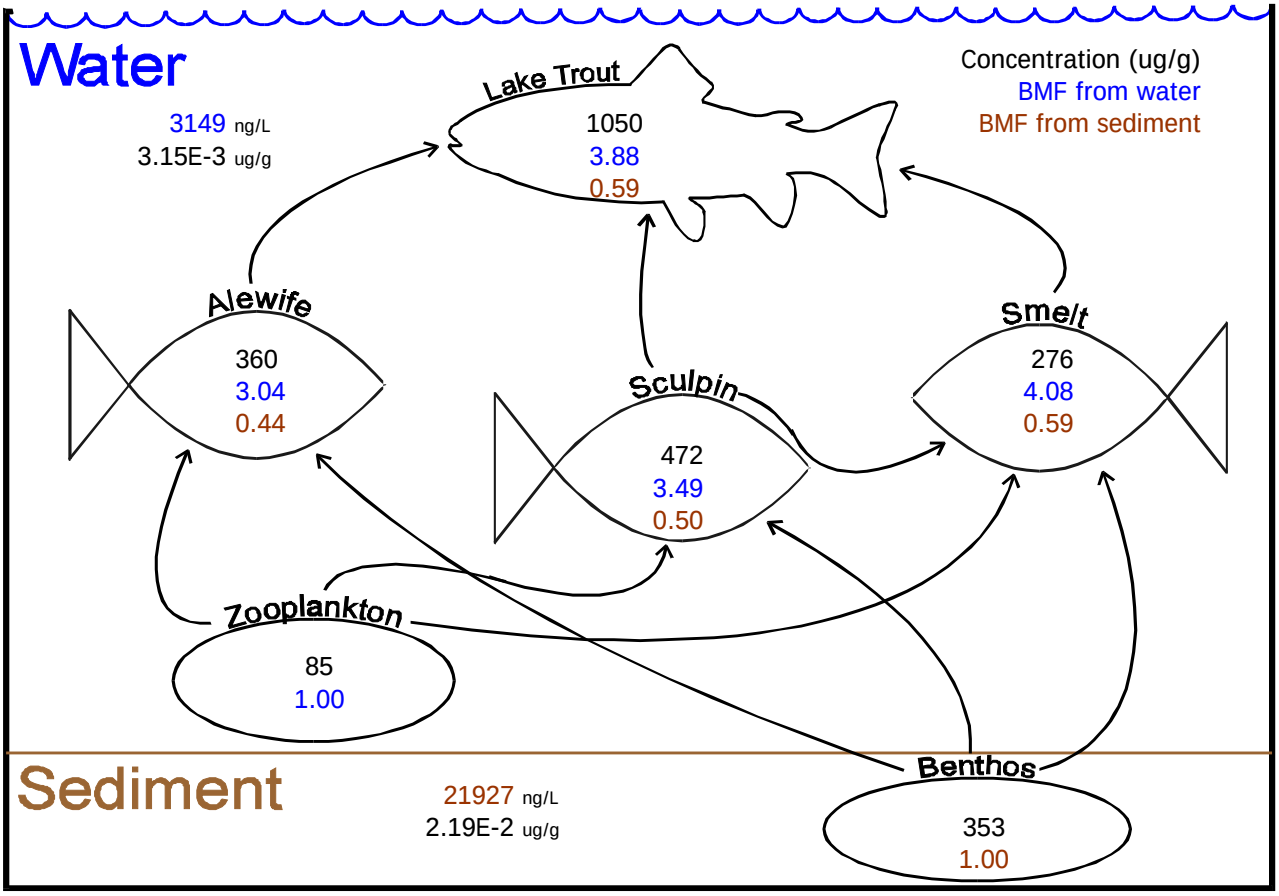
EPA Hexachlorobenzene

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



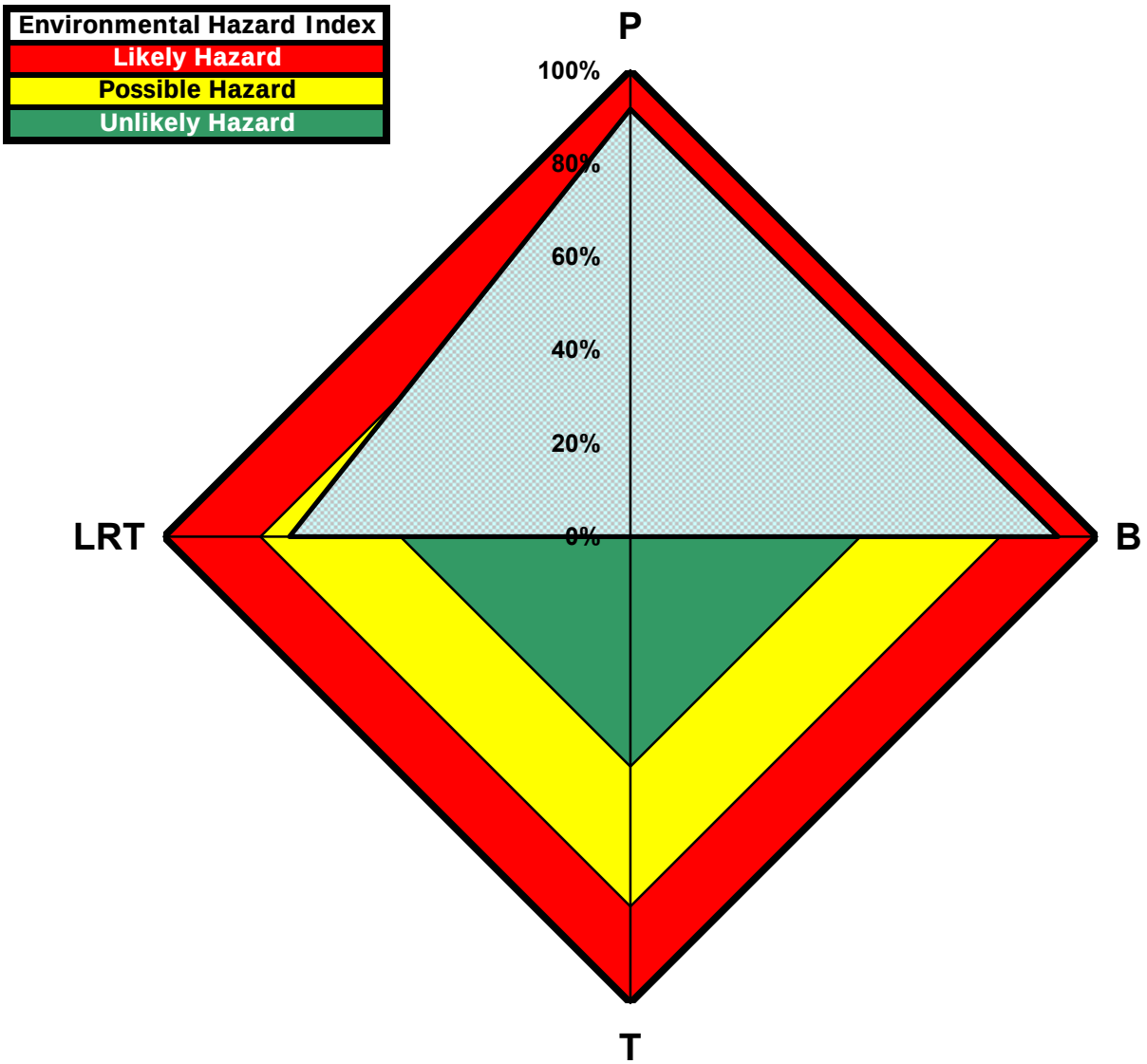
Overall Bioaccumulation Factor, Lake Trout / Water : 333618

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.

ChemSCORER Beta101 Assessment - Summary Ranking

EPA Total Chlordanes



Summary Rankings for: EPA Total Chlordanes

This chemical ...

is more PERSISTENT (P) than **92 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **92 %** of chemicals in the reference set.

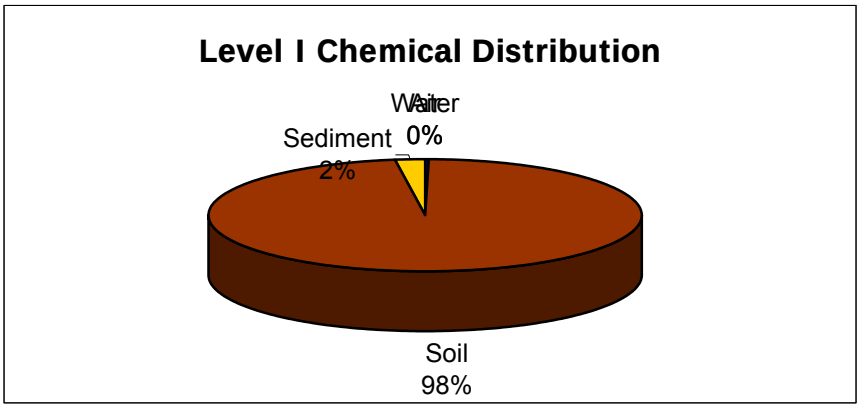
No data on mammalian toxicity was supplied.

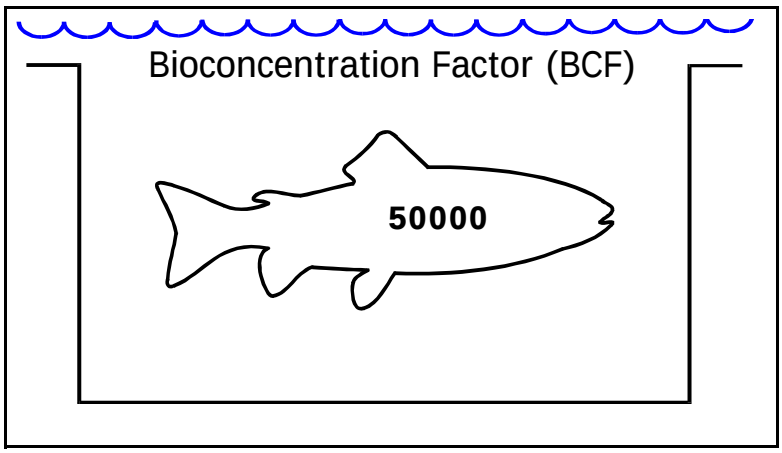
has greater LONG RANGE TRANSPORT (LRT) than **73 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA Total Chlordanes

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is substantially greater than the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. In the absence of metabolism by organisms, this substance may bioaccumulate similar to DDT (BCF 63000) or PCBs (BCFs up to 300000).

Details of Level I calculation for: EPA Total Chlordanes

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	1.79E-12	7.32E-10	6.17E-07	73	0.073
Water	3.04E-01	1.34E-09	5.51E-07	5.51E-07	110	0.110
Soil	5.98E+03	2.65E-05	1.08E-02	4.52E-03	97575	97.575
Sediment	1.20E+04	5.29E-05	2.17E-02	9.03E-03	2168	2.168
Suspended Sediment	3.74E+04	1.65E-04	6.78E-02	4.52E-02	68	0.068
Biota (Fish)	1.52E+04	6.72E-05	2.75E-02	2.75E-02	6	0.006
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

Input Parameters			Partition Coefficients		Three Solubilities	
Molar Mass	409.8	g/mol			(g/m^3)	
Vapor Pressure	0.00045	Pa	Log Kow	6.00	Air	7.44E-05
Aqueous Solubility	0.056	g/m^3	Log Kaw	-2.88	Water	5.60E-02
Log Kow	6		Log Koa	8.88	Octanol	5.60E+04
Melting Point	103	deg C				

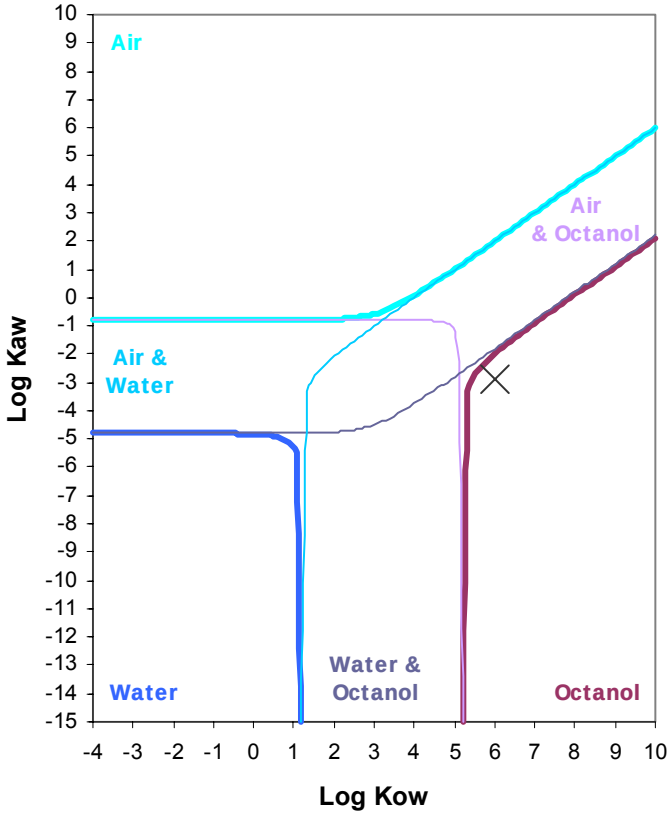
ChemSCORER Beta101 - Level II Model Results

EPA Total Chlordanes

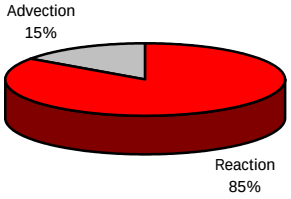
Equilibrium Partitioning Persistence Information

The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.

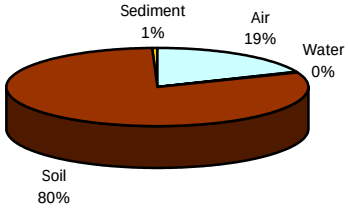
The equilibrium distribution reaction residence time calculated for this substance can be measured in years, and is comparable to that of pentachlorobenzene (2 years). Reactive and advective residence times are comparable, indicating the substance may be mobile to other regions.



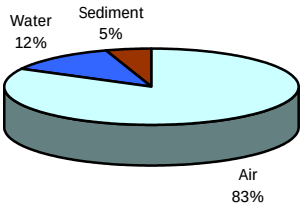
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	716	days	1.96	years
Reaction Residence Time:	845	days	2.31	years
Advection Residence Time:	4706	days	12.89	years

Details of Level II calculation for: EPA Total Chlordanes

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	55	5.08E+08	4.03E+08	1.59E+02	1.26E+02	28.434
Water	17000	2.48E+06	6.07E+07	7.72E-01	1.89E+01	1.971
Soil	17000	2.19E+09	0	6.84E+02	0	68.380
Sediment	55000	1.51E+07	2.39E+07	4.70E+00	7.46E+00	1.215
Total		2.72E+09	4.88E+08	8.48E+02	1.52E+02	100.000
Reaction + Advection		3.21E+09		1000		

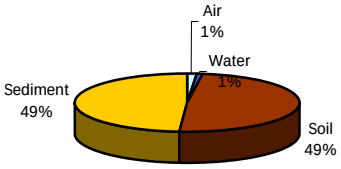
ChemSCORER Beta101 - Level III Model Results

EPA Total Chlordanes

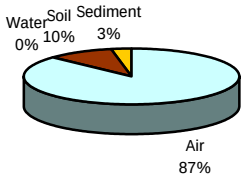
Emission to Air

Emissions to air partition predominantly to soil and sediment.

Steady State Distribution



Reactive Removal



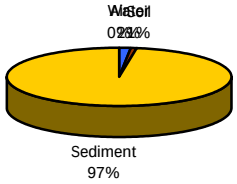
	Persistence
(hours)	4972.6
(days)	207.2
(years)	0.6

Persistence of air emissions is comparable to that of the tetrachlorobenzenes (110 days).

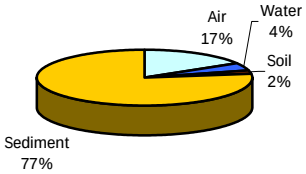
Emission to Water

Emissions to water partition significantly to sediment and may migrate to soil.

Steady State Distribution



Reactive Removal



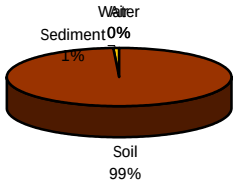
	Persistence
(hours)	62811.4
(days)	2617.1
(years)	7.2

Persistence of water emissions is comparable to that of hexachlorobenzene (2300 days).

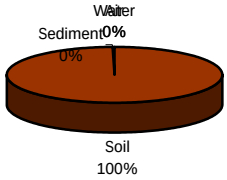
Emission to Soil

Emissions to soil remain predominantly in the soil compartment.

Steady State Distribution



Reactive Removal

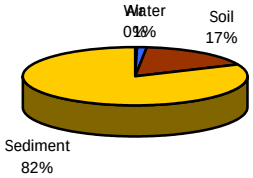


	Persistence
(hours)	24639.5
(days)	1026.6
(years)	2.8

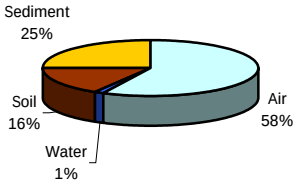
Persistence of soil emissions is comparable to that of hexachlorobenzene (3200 days).

Emission to All 3

Steady State Distribution



Reactive Removal



	Persistence
(hours)	24290.9
(days)	1012.1
(years)	2.8

Persistence under the standard emission scenario is comparable to that of hexachlorobenzene (2300 days).

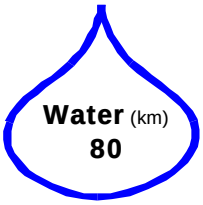
Details of Level III calculation for: EPA Total Chlordanes

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	6.89E+04	4.32E+04	2.43E+06	2.43E+06	4.97E+06
Water	0	1000	0	1.31E+04	1.09E+06	4.61E+05	6.12E+07	6.28E+07
Soil	0	0	1000	7.13E+01	3.35E+03	2.44E+07	1.89E+05	2.46E+07
All 3	600	300	100	4.53E+04	3.53E+05	4.04E+06	1.99E+07	2.43E+07
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	869	2	99	31	1000
Water	0	1000	0	165	44	19	772	1000
Soil	0	0	1000	1	0	997	2	1000
All 3	600	300	100	571	14	165	250	1000

ChemSCORER Beta101 - Transport Model Results

EPA Total Chlordanes

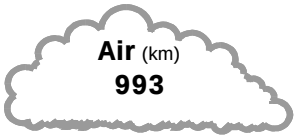
TaPL II - Equilibrium distribution Characteristic Travel Distance



Under equilibrium partitioning conditions, this chemical is likely to be transported by both air and water.

TaPL III - Mode of entry assessments

Emission to air - Characteristic Travel Distance in Air

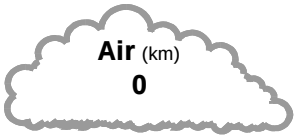


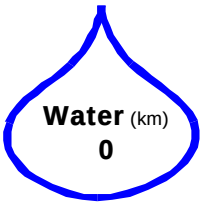
Characteristic Travel Distance in air is moderate, and is comparable to that of DDT (830 km). This chemical may be found in remote areas, but is not necessarily transported over very long distances.

Emission to water - Characteristic Travel Distance in Water

Characteristic Travel Distance in water is high, and is comparable to that of toxaphene (9700 km). This chemical may be subject to long range transport in surface and ocean waters.

Emission to soil - Effective Travel Distance





Emissions directly to soil are not expected to partition significantly to air or water, and are not likely to be subject to transport.

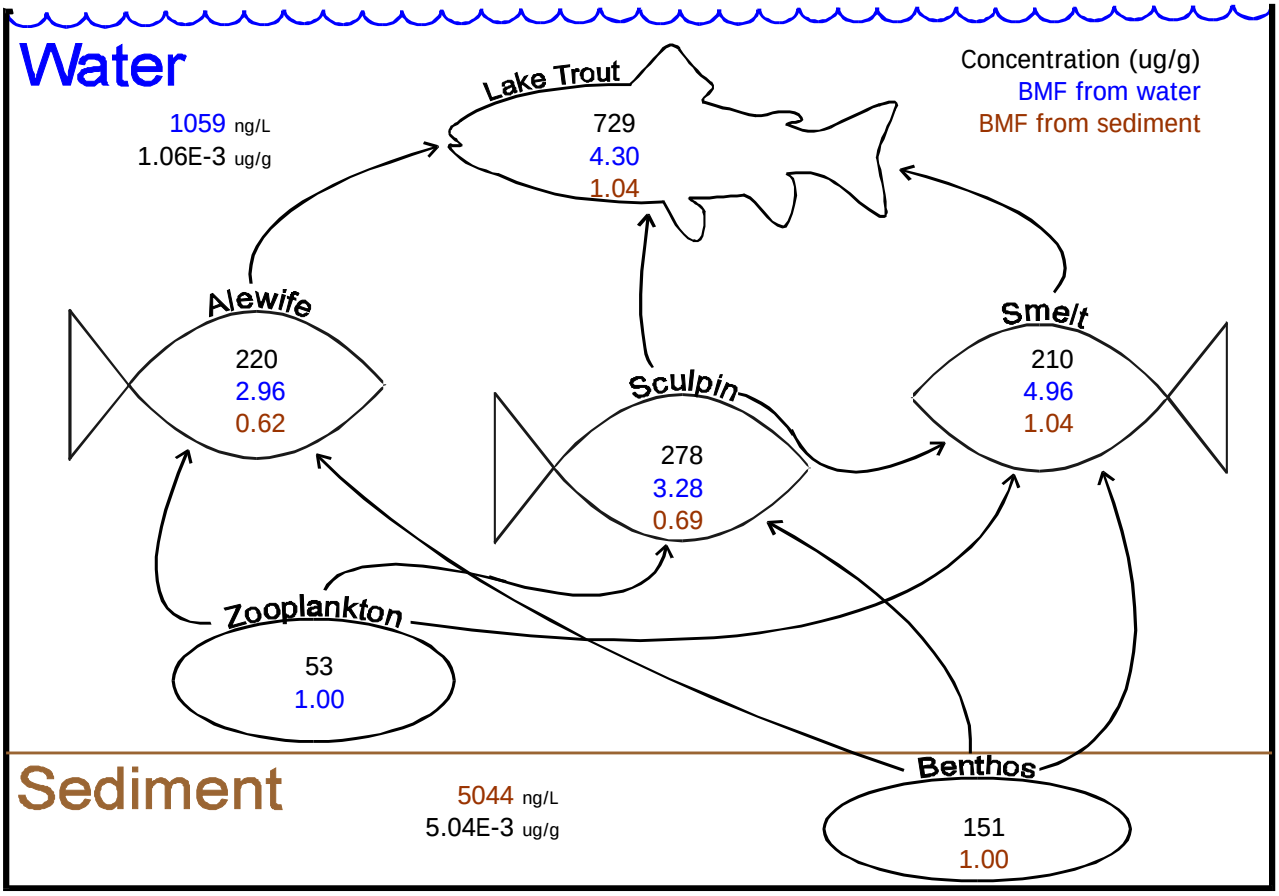
ChemSCORER Beta101 - Toxicity and Bioaccumulation
EPA Total Chlordanes

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



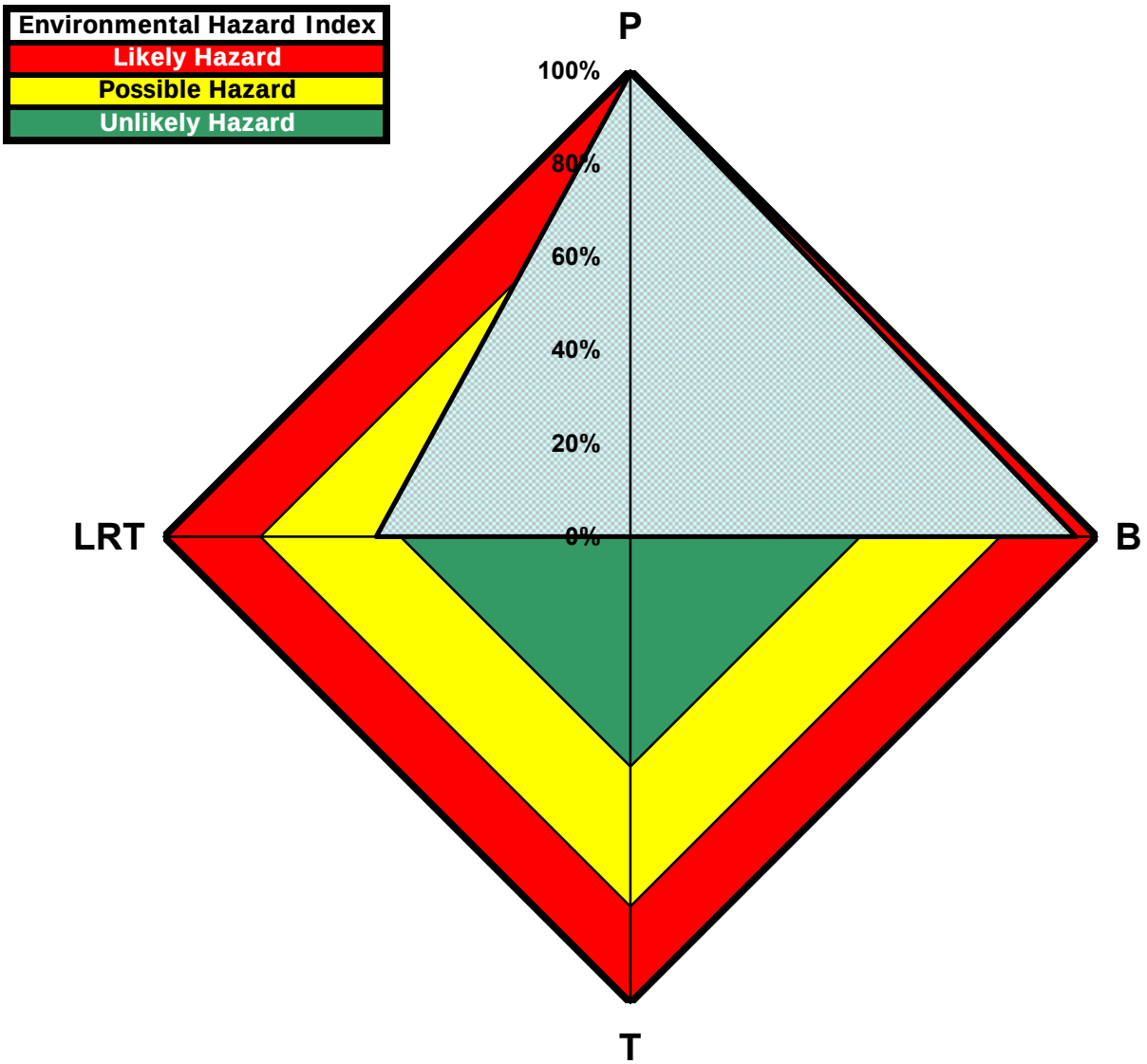
Overall Bioaccumulation Factor, Lake Trout / Water : 688249

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.

ChemSCORER Beta101 Assessment - Summary Ranking

EPA 2,3,7,8-TCDD



Summary Rankings for: EPA 2,3,7,8-TCDD

This chemical ...

is more PERSISTENT (P) than **99 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **96 %** of chemicals in the reference set.

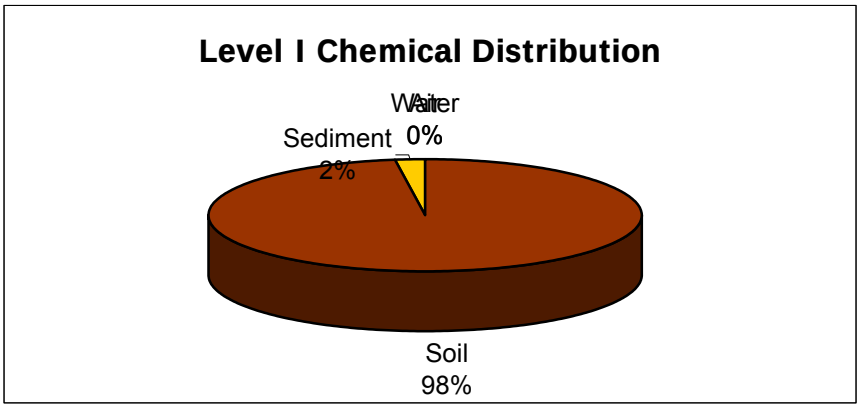
No data on mammalian toxicity was supplied.

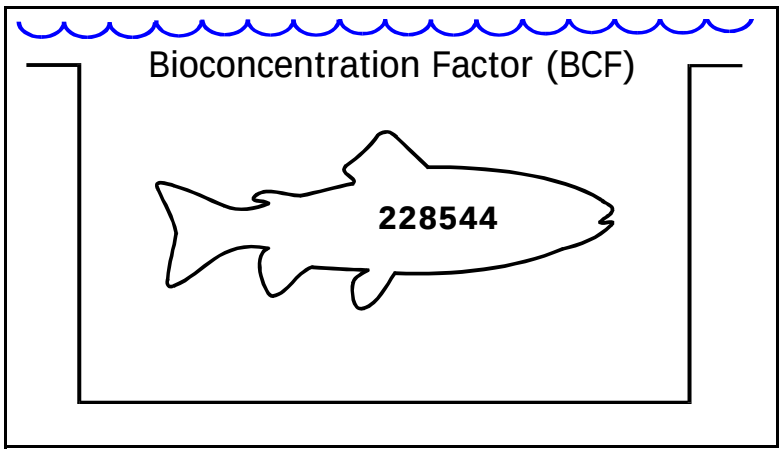
has greater LONG RANGE TRANSPORT (LRT) than **54 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA 2,3,7,8-TCDD

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is substantially greater than the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. In the absence of metabolism by organisms, this substance may bioaccumulate similar to DDT (BCF 63000) or PCBs (BCFs up to 300000).

Details of Level I calculation for: EPA 2,3,7,8-TCDD

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	4.67E-13	1.51E-10	1.27E-07	15	0.015
Water	3.23E-01	3.75E-10	1.21E-07	1.21E-07	24	0.024
Soil	2.91E+04	3.37E-05	1.09E-02	4.52E-03	97716	97.716
Sediment	5.82E+04	6.74E-05	2.17E-02	9.05E-03	2171	2.171
Suspended Sediment	1.82E+05	2.11E-04	6.79E-02	4.52E-02	68	0.068
Biota (Fish)	7.39E+04	8.57E-05	2.76E-02	2.76E-02	6	0.006
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

Input Parameters			Partition Coefficients		Three Solubilities	
					(g/m^3)	
Molar Mass	321.98	g/mol				
Vapor Pressure	1	Pa	Log Kow	6.66	Air	1.30E-01
Aqueous Solubility	104.1531518	g/m^3	Log Kaw	-2.90	Water	1.04E+02
Log Kow	6.66		Log Koa	9.56	Octanol	4.76E+08
Melting Point	-999	deg C				

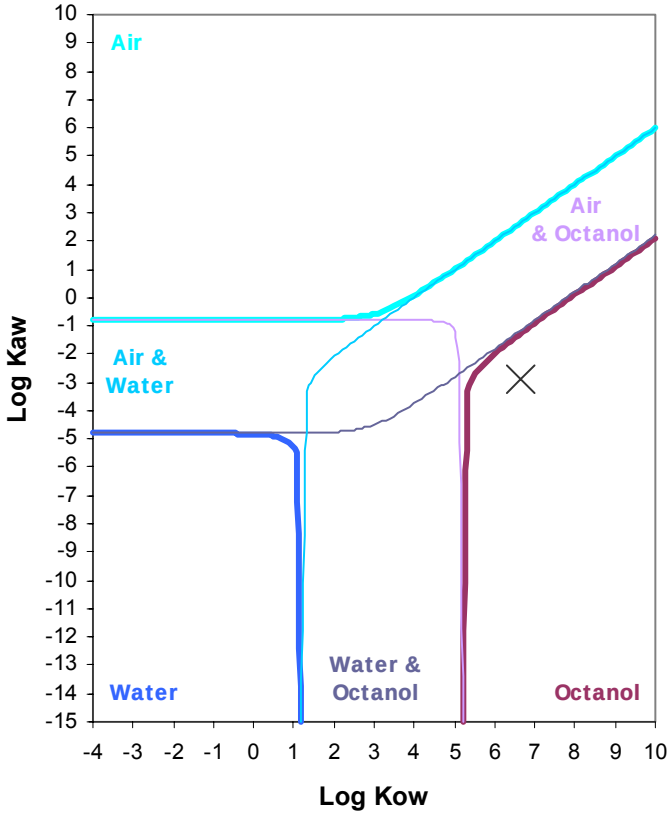
ChemSCORER Beta101 - Level II Model Results

EPA 2,3,7,8-TCDD

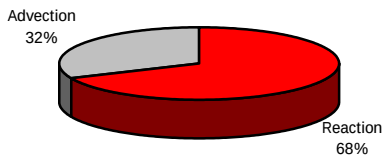
Equilibrium Partitioning Persistence Information

The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.

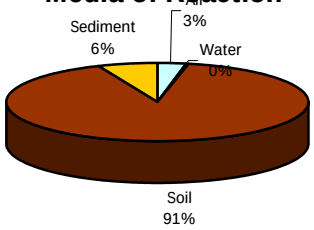
The equilibrium distribution reaction residence time calculated for this substance is greater than ten years, and is comparable to that of Total PCBs (77 years). Reactive and advective residence times are comparable, indicating the substance is likely to be subject to long range transport.



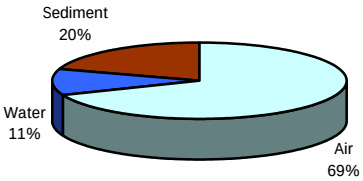
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	6057	days	16.59	years
Reaction Residence Time:	8869	days	24.30	years
Advection Residence Time:	19105	days	52.34	years

Details of Level II calculation for: EPA 2,3,7,8-TCDD

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	720	3.88E+07	4.03E+08	2.11E+01	2.19E+02	23.988
Water	10300	4.35E+06	6.47E+07	2.36E+00	3.51E+01	3.745
Soil	160000	1.13E+09	0	6.15E+02	0	61.525
Sediment	49400	8.16E+07	1.16E+08	4.43E+01	6.31E+01	10.742
Total		1.26E+09	5.85E+08	6.83E+02	3.17E+02	100.000
Reaction + Advection		1.84E+09		1000		

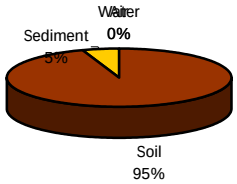
ChemSCORER Beta101 - Level III Model Results

EPA 2,3,7,8-TCDD

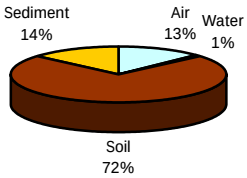
Emission to Air

Emissions to air partition predominantly to soil and sediment.

Steady State Distribution



Reactive Removal



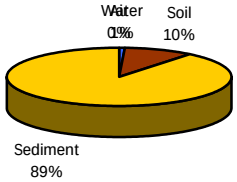
	Persistence
(hours)	178335
(days)	7431
(years)	20

Persistence of air emissions is comparable to that of the PCBs (up to 80 years).

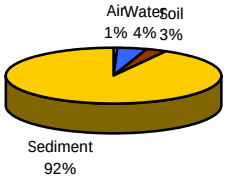
Emission to Water

Emissions to water partition significantly to sediment and may migrate to soil.

Steady State Distribution



Reactive Removal



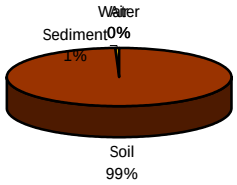
	Persistence
(hours)	73548
(days)	3064
(years)	8

Persistence of water emissions is comparable to that of hexachlorobenzene (2300 days).

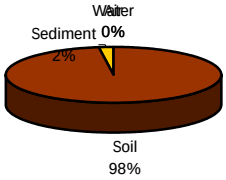
Emission to Soil

Emissions to soil remain predominantly in the soil compartment.

Steady State Distribution



Reactive Removal

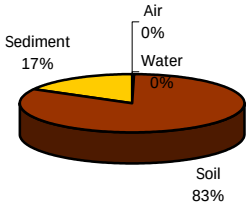


	Persistence
(hours)	227095
(days)	9462
(years)	26

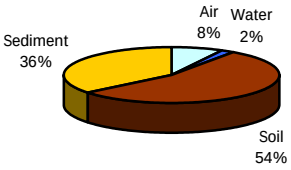
Persistence of soil emissions is comparable to that of the PCBs (up to 80 years).

Emission to All 3

Steady State Distribution



Reactive Removal



	Persistence
(hours)	151775
(days)	6324
(years)	17

Persistence under the standard emission scenario is comparable to that of the PCBs (up to 80 years).

Details of Level III calculation for: EPA 2,3,7,8-TCDD

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	1.34E+05	9.43E+04	1.68E+08	9.63E+06	1.78E+08
Water	0	1000	0	5.86E+03	6.42E+05	7.37E+06	6.55E+07	7.35E+07
Soil	0	0	1000	2.56E+02	1.53E+04	2.26E+08	1.57E+06	2.27E+08
All 3	600	300	100	8.21E+04	2.51E+05	1.26E+08	2.56E+07	1.52E+08
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	129	6	730	135	1000
Water	0	1000	0	6	43	32	919	1000
Soil	0	0	1000	0	1	977	22	1000
All 3	600	300	100	79	17	545	359	1000

ChemSCORER Beta101 - Transport Model Results

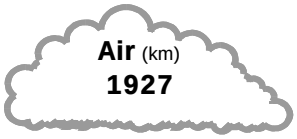
EPA 2,3,7,8-TCDD

TaPL II - Equilibrium distribution Characteristic Travel Distance

Under equilibrium partitioning conditions, this chemical is likely to be transported by both air and water.

TaPL III - Mode of entry assessments

Emission to air - Characteristic Travel Distance in Air



Characteristic Travel Distance in air is moderate, and is comparable to that of DDT (830 km). This chemical may be found in remote areas, but is not necessarily transported over very long distances.

Emission to water - Characteristic Travel Distance in Water

Characteristic Travel Distance in water is high, and is comparable to that of toxaphene (9700 km). This chemical may be subject to long range transport in surface and ocean waters.

Emission to soil - Effective Travel Distance

Emissions directly to soil are not expected to partition significantly to air or water, and are not likely to be subject to transport.

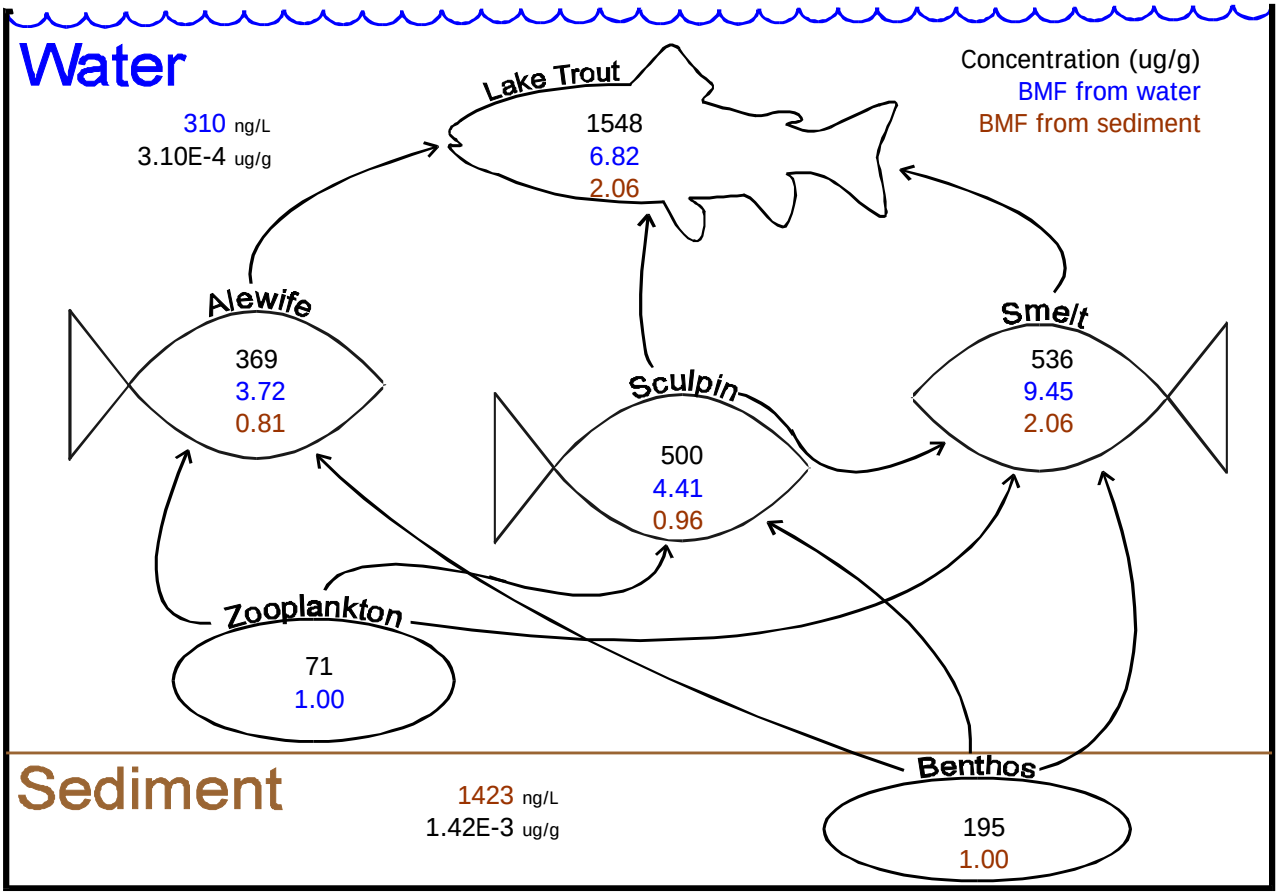
ChemSCORER Beta101 - Toxicity and Bioaccumulation
EPA 2,3,7,8-TCDD

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



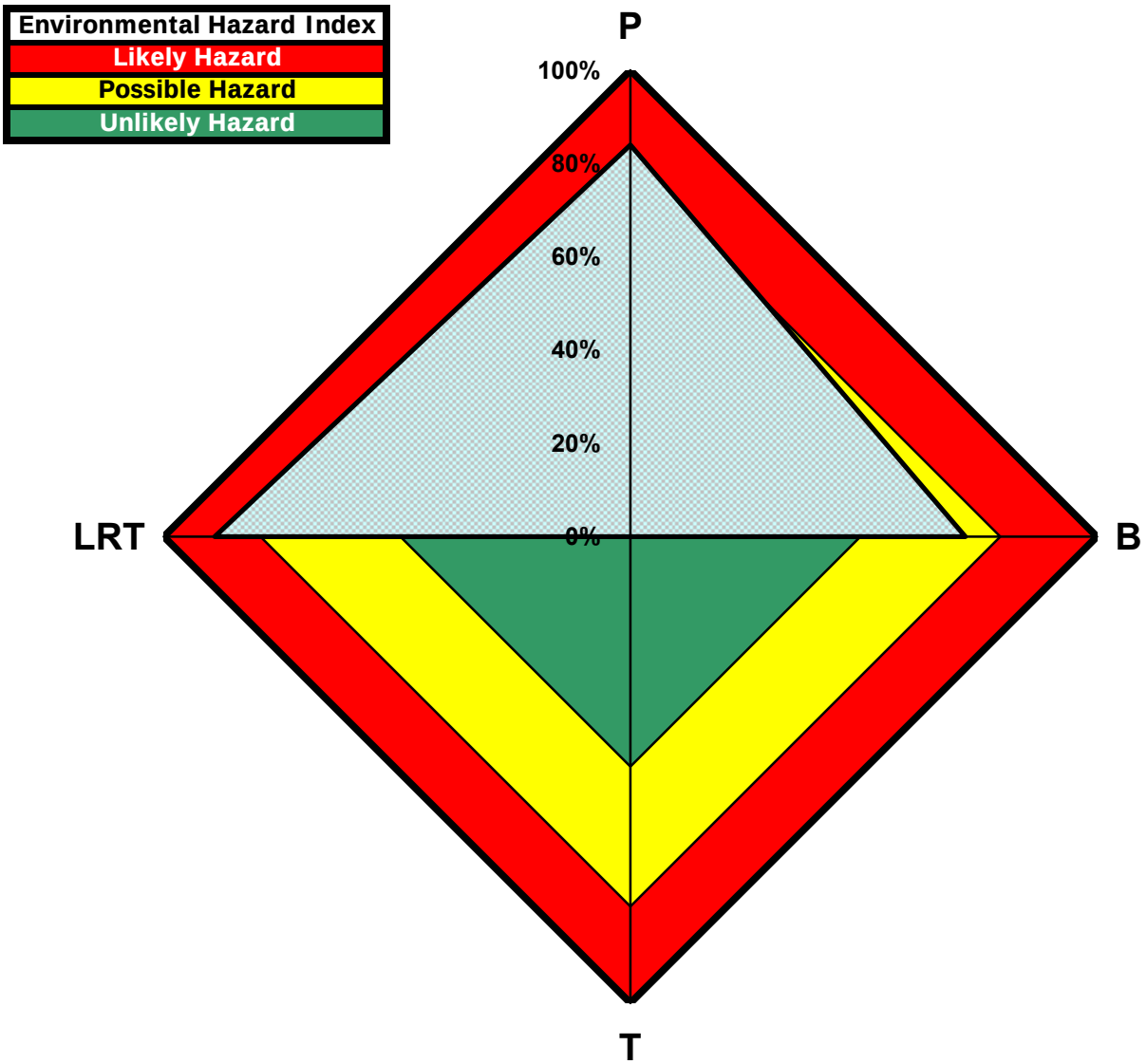
Overall Bioaccumulation Factor, Lake Trout / Water : 4989267

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.

ChemSCORER Beta101 Assessment - Summary Ranking

EPA alpha-HCH



Summary Rankings for: EPA alpha-HCH

This chemical ...

is more PERSISTENT (P) than **84 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **72 %** of chemicals in the reference set.

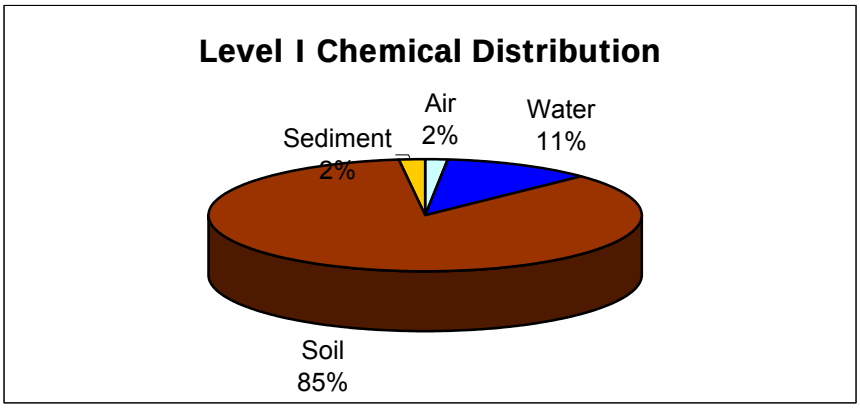
No data on mammalian toxicity was supplied.

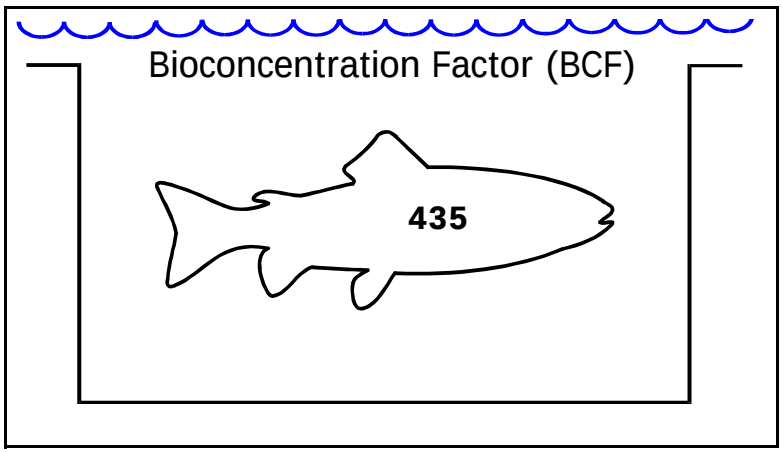
has greater LONG RANGE TRANSPORT (LRT) than **89 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA alpha-HCH

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is below the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. This substance is not expected to bioaccumulate to a significant degree.

Details of Level I calculation for: EPA alpha-HCH

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	5.61E-11	1.63E-08	1.38E-05	1633	1.633
Water	1.37E+00	1.90E-07	5.53E-05	5.53E-05	11064	11.064
Soil	2.34E+02	3.26E-05	9.48E-03	3.95E-03	85342	85.342
Sediment	4.69E+02	6.52E-05	1.90E-02	7.90E-03	1896	1.896
Suspended Sediment	1.46E+03	2.04E-04	5.93E-02	3.95E-02	59	0.059
Biota (Fish)	5.95E+02	8.28E-05	2.41E-02	2.41E-02	5	0.005
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

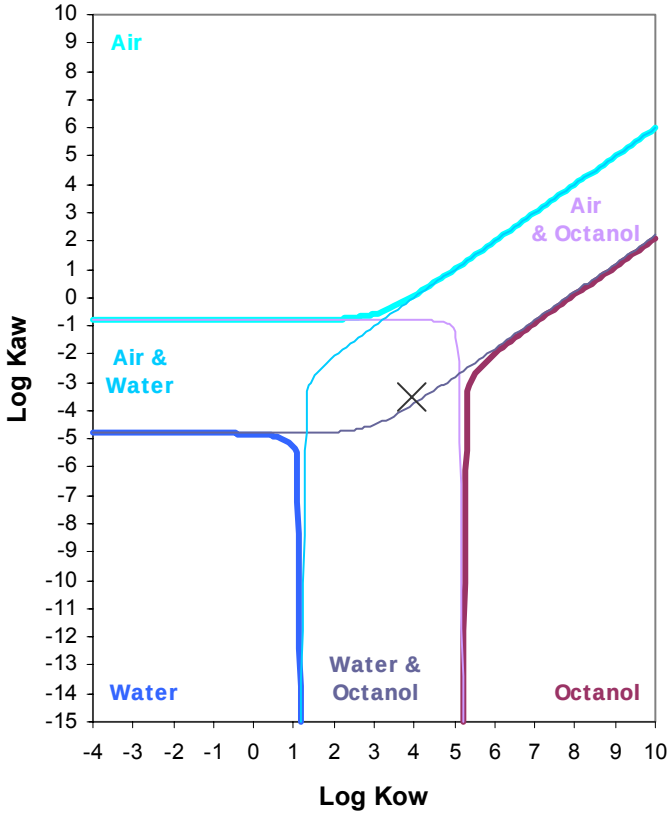
Input Parameters			Partition Coefficients		Three Solubilities	
					(g/m^3)	
Molar Mass	290.85	g/mol				
Vapor Pressure	1	Pa	Log Kow	3.94	Air	1.17E-01
Aqueous Solubility	397.5797299	g/m^3	Log Kaw	-3.53	Water	3.98E+02
Log Kow	3.94		Log Koa	7.47	Octanol	3.46E+06
Melting Point	-999	deg C				

ChemSCORER Beta101 - Level II Model Results

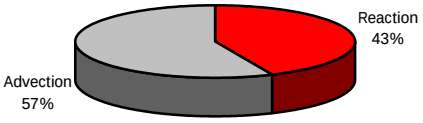
EPA alpha-HCH

Equilibrium Partitioning Persistence Information

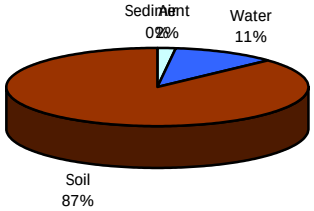
The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.
The equilibrium distribution reaction residence time calculated for this substance can be measured in months, and is comparable to that of the tetrachlorobenzenes (120 days). Reactive and advective residence times are comparable, indicating the substance may be mobile to other regions.



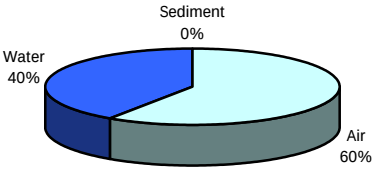
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	2063	hours	85.97	days
Reaction Residence Time:	4754	hours	198.06	days
Advection Residence Time:	3646	hours	151.91	days

Details of Level II calculation for: EPA alpha-HCH

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	2880	9.71E+06	4.03E+08	8.11E+00	3.37E+02	34.497
Water	3240	5.85E+07	2.73E+08	4.88E+01	2.28E+02	27.712
Soil	3240	4.51E+08	0	3.77E+02	0	37.663
Sediment	55000	5.90E+05	9.37E+05	4.93E-01	7.83E-01	0.128
Total		5.20E+08	6.78E+08	4.34E+02	5.66E+02	100.000
Reaction + Advection		1.20E+09		1000		

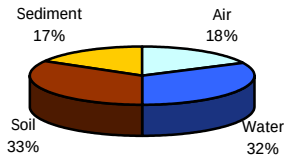
ChemSCORER Beta101 - Level III Model Results

EPA alpha-HCH

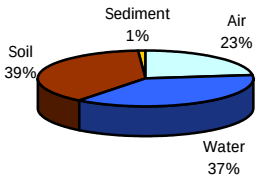
Emission to Air

Emissions to air partition significantly to other media.

Steady State Distribution



Reactive Removal



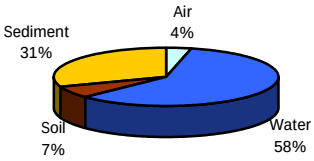
	Persistence
(hours)	5403.30
(days)	225.14
(years)	0.62

Persistence of air emissions is comparable to that of the tetrachlorobenzenes (110 days).

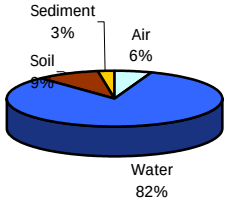
Emission to Water

Emissions to water partition significantly to other media.

Steady State Distribution



Reactive Removal



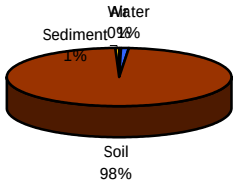
	Persistence
(hours)	6519.17
(days)	271.63
(years)	0.74

Persistence of water emissions is comparable to that of the tetrachlorobenzenes (140 days).

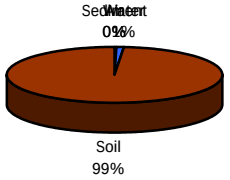
Emission to Soil

Emissions to soil remain predominantly in the soil compartment.

Steady State Distribution



Reactive Removal

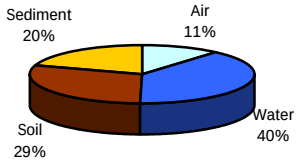


	Persistence
(hours)	4703.83
(days)	195.99
(years)	0.54

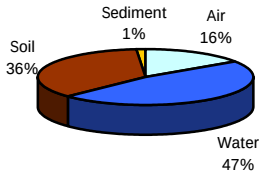
Persistence of soil emissions is comparable to that of the tetrachlorobenzenes (250 days).

Emission to All 3

Steady State Distribution



Reactive Removal



	Persistence
(hours)	5668.11
(days)	236.17
(years)	0.65

Persistence under the standard emission scenario is comparable to that of the tetrachlorobenzenes (130 days).

Details of Level III calculation for: EPA alpha-HCH

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	9.60E+05	1.75E+06	1.80E+06	9.01E+05	5.40E+06
Water	0	1000	0	2.34E+05	3.86E+06	4.39E+05	1.99E+06	6.52E+06
Soil	0	0	1000	7.27E+03	6.05E+04	4.60E+06	3.13E+04	4.70E+06
All 3	600	300	100	6.47E+05	2.21E+06	1.67E+06	1.14E+06	5.67E+06
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	231	373	384	11	1000
Water	0	1000	0	56	825	94	25	1000
Soil	0	0	1000	2	13	985	0	1000
All 3	600	300	100	156	473	357	14	1000

ChemSCORER Beta101 - Transport Model Results

EPA alpha-HCH

TaPL II - Equilibrium distribution Characteristic Travel Distance

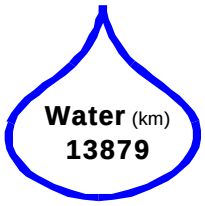
Under equilibrium partitioning conditions, this chemical is likely to be transported by both air and water.

TaPL III - Mode of entry assessments

Emission to air - Characteristic Travel Distance in Air

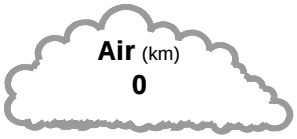
Characteristic Travel Distance in air is high, and is comparable to that of hexachlorinated PCBs (4200 km). This chemical may be subject to long range transport and deposition in the arctic.

Emission to water - Characteristic Travel Distance in Water



Characteristic Travel Distance in water is high, and is comparable to that of toxaphene (9700 km). This chemical may be subject to long range transport in surface and ocean waters.

Emission to soil - Effective Travel Distance



Emissions directly to soil may run-off to water and be subject to transport in surface water and oceans.

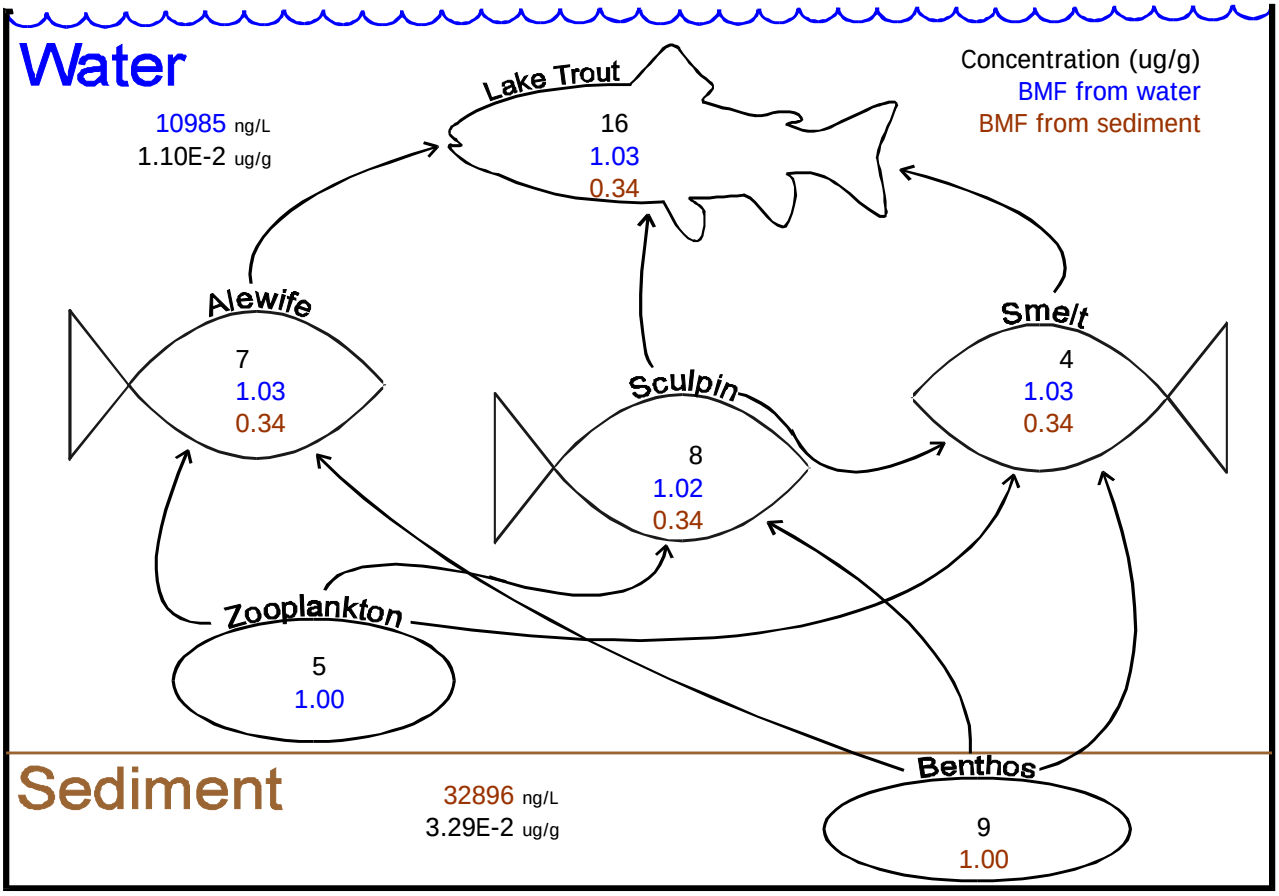
ChemSCORER Beta101 - Toxicity and Bioaccumulation
EPA alpha-HCH

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



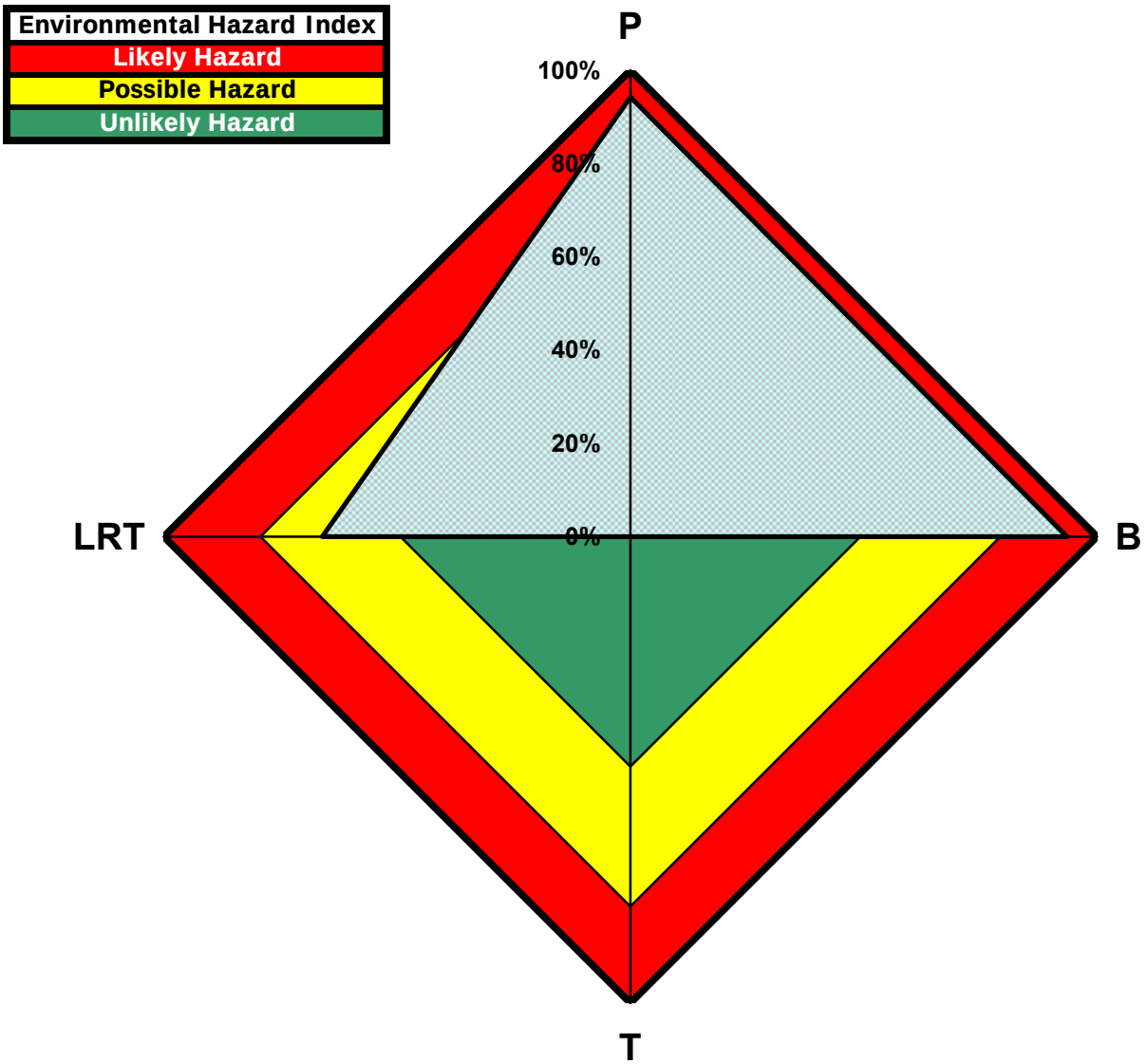
Overall Bioaccumulation Factor, Lake Trout / Water : 1432

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.

ChemSCORER Beta101 Assessment - Summary Ranking

EPA p,p'-DDT



Summary Rankings for: EPA p,p'-DDT

This chemical ...

is more PERSISTENT (P) than **94 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **94 %** of chemicals in the reference set.

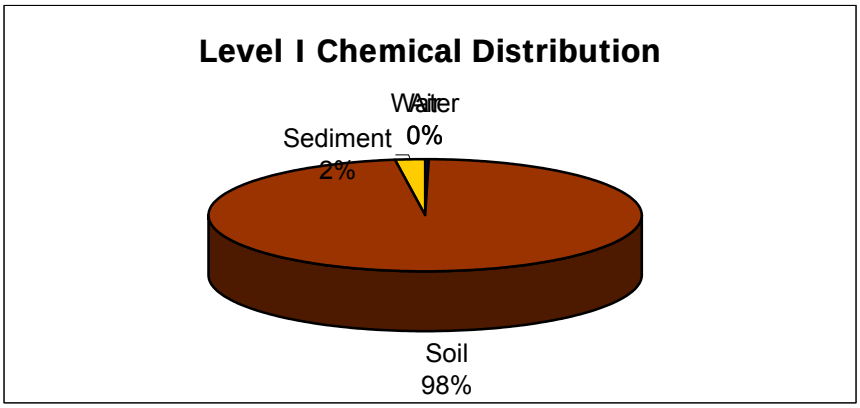
No data on mammalian toxicity was supplied.

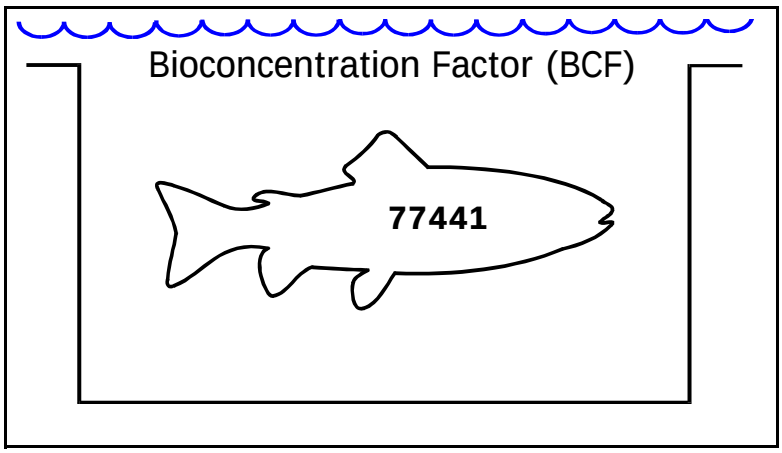
has greater LONG RANGE TRANSPORT (LRT) than **66 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA p,p'-DDT

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is substantially greater than the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. In the absence of metabolism by organisms, this substance may bioaccumulate similar to DDT (BCF 63000) or PCBs (BCFs up to 300000).

Details of Level I calculation for: EPA p,p'-DDT

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	5.22E-13	1.85E-10	1.56E-07	19	0.019
Water	7.76E-01	1.00E-09	3.56E-07	3.56E-07	71	0.071
Soil	2.36E+04	3.06E-05	1.09E-02	4.52E-03	97667	97.667
Sediment	4.73E+04	6.12E-05	2.17E-02	9.04E-03	2170	2.170
Suspended Sediment	1.48E+05	1.91E-04	6.78E-02	4.52E-02	68	0.068
Biota (Fish)	6.01E+04	7.78E-05	2.76E-02	2.76E-02	6	0.006
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

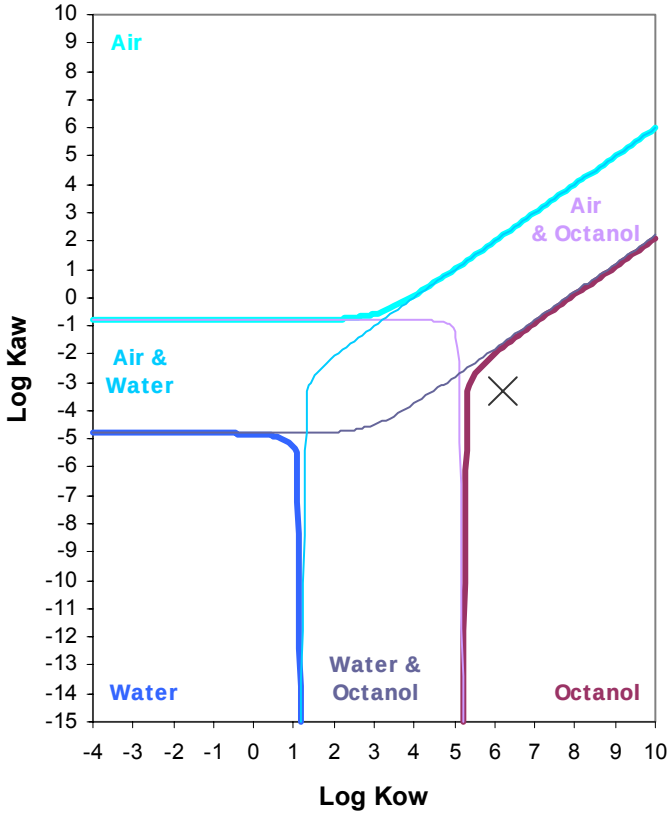
Input Parameters			Partition Coefficients		Three Solubilities	
Molar Mass	354.5	g/mol			(g/m^3)	
Vapor Pressure	0.00002	Pa	Log Kow	6.19	Air	2.86E-06
Aqueous Solubility	0.0055	g/m^3	Log Kaw	-3.28	Water	5.50E-03
Log Kow	6.19		Log Koa	9.47	Octanol	8.52E+03
Melting Point	108.5	deg C				

ChemSCORER Beta101 - Level II Model Results

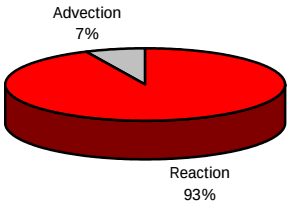
EPA p,p'-DDT

Equilibrium Partitioning Persistence Information

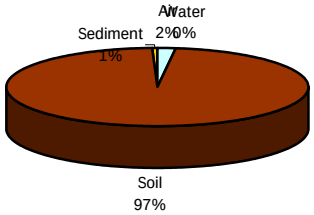
The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.
The equilibrium distribution reaction residence time calculated for this substance can be measured in years, and is comparable to that of pentachlorobenzene (2 years). Reactive residence time is more than 10 times shorter than advective residence time, indicating potential for transport to other regions is low.



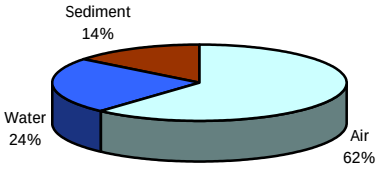
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	948	days	2.60	years
Reaction Residence Time:	1018	days	2.79	years
Advection Residence Time:	13900	days	38.08	years

Details of Level II calculation for: EPA p,p'-DDT

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	170	1.64E+08	4.03E+08	1.72E+01	4.21E+01	5.933
Water	5500	1.95E+07	1.55E+08	2.04E+00	1.62E+01	1.825
Soil	17000	8.67E+09	0	9.06E+02	0	90.631
Sediment	55000	5.96E+07	9.46E+07	6.23E+00	9.88E+00	1.611
Total		8.92E+09	6.53E+08	9.32E+02	6.82E+01	100.000
Reaction + Advection		9.57E+09		1000		

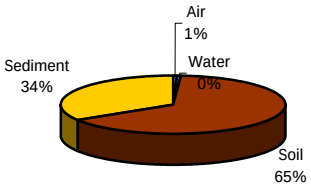
ChemSCORER Beta101 - Level III Model Results

EPA p,p'-DDT

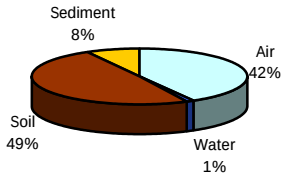
Emission to Air

Emissions to air partition predominantly to soil and sediment.

Steady State Distribution



Reactive Removal



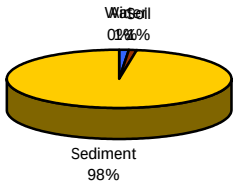
	Persistence
(hours)	18593.0
(days)	774.7
(years)	2.1

Persistence of air emissions is comparable to that of hexachlorobenzene (2200 days).

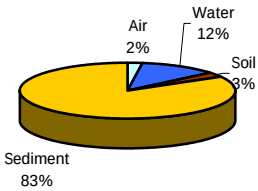
Emission to Water

Emissions to water partition significantly to sediment and may migrate to soil.

Steady State Distribution



Reactive Removal



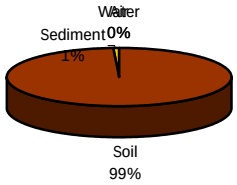
	Persistence
(hours)	67715.2
(days)	2821.5
(years)	7.7

Persistence of water emissions is comparable to that of hexachlorobenzene (2300 days).

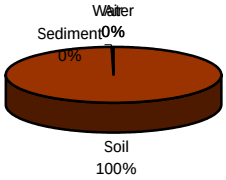
Emission to Soil

Emissions to soil remain predominantly in the soil compartment.

Steady State Distribution



Reactive Removal

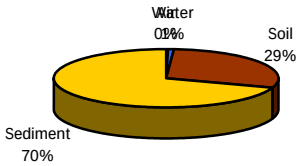


	Persistence
(hours)	24653.0
(days)	1027.2
(years)	2.8

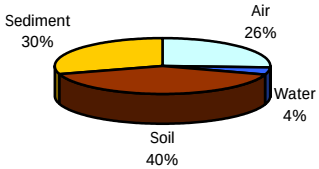
Persistence of soil emissions is comparable to that of hexachlorobenzene (3200 days).

Emission to All 3

Steady State Distribution



Reactive Removal



	Persistence
(hours)	33935.6
(days)	1414.0
(years)	3.9

Persistence under the standard emission scenario is comparable to that of hexachlorobenzene (2300 days).

Details of Level III calculation for: EPA p,p'-DDT

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	1.02E+05	8.82E+04	1.21E+07	6.32E+06	1.86E+07
Water	0	1000	0	5.71E+03	9.22E+05	6.75E+05	6.61E+07	6.77E+07
Soil	0	0	1000	3.29E+01	2.64E+03	2.45E+07	1.89E+05	2.47E+07
All 3	600	300	100	6.31E+04	3.30E+05	9.90E+06	2.36E+07	3.39E+07
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	417	11	492	80	1000
Water	0	1000	0	23	116	27	833	1000
Soil	0	0	1000	0	0	997	2	1000
All 3	600	300	100	257	42	403	298	1000

ChemSCORER Beta101 - Transport Model Results

EPA p,p'-DDT

TaPL II - Equilibrium distribution Characteristic Travel Distance

Under equilibrium partitioning conditions, this chemical is likely to be transported by both air and water.

TaPL III - Mode of entry assessments

Emission to air - Characteristic Travel Distance in Air

Characteristic Travel Distance in air is moderate, and is comparable to that of DDT (830 km). This chemical may be found in remote areas, but is not necessarily transported over very long distances.

Emission to water - Characteristic Travel Distance in Water

Characteristic Travel Distance in water is high, and is comparable to that of toxaphene (9700 km). This chemical may be subject to long range transport in surface and ocean waters.

Emission to soil - Effective Travel Distance

Emissions directly to soil are not expected to partition significantly to air or water, and are not likely to be subject to transport.

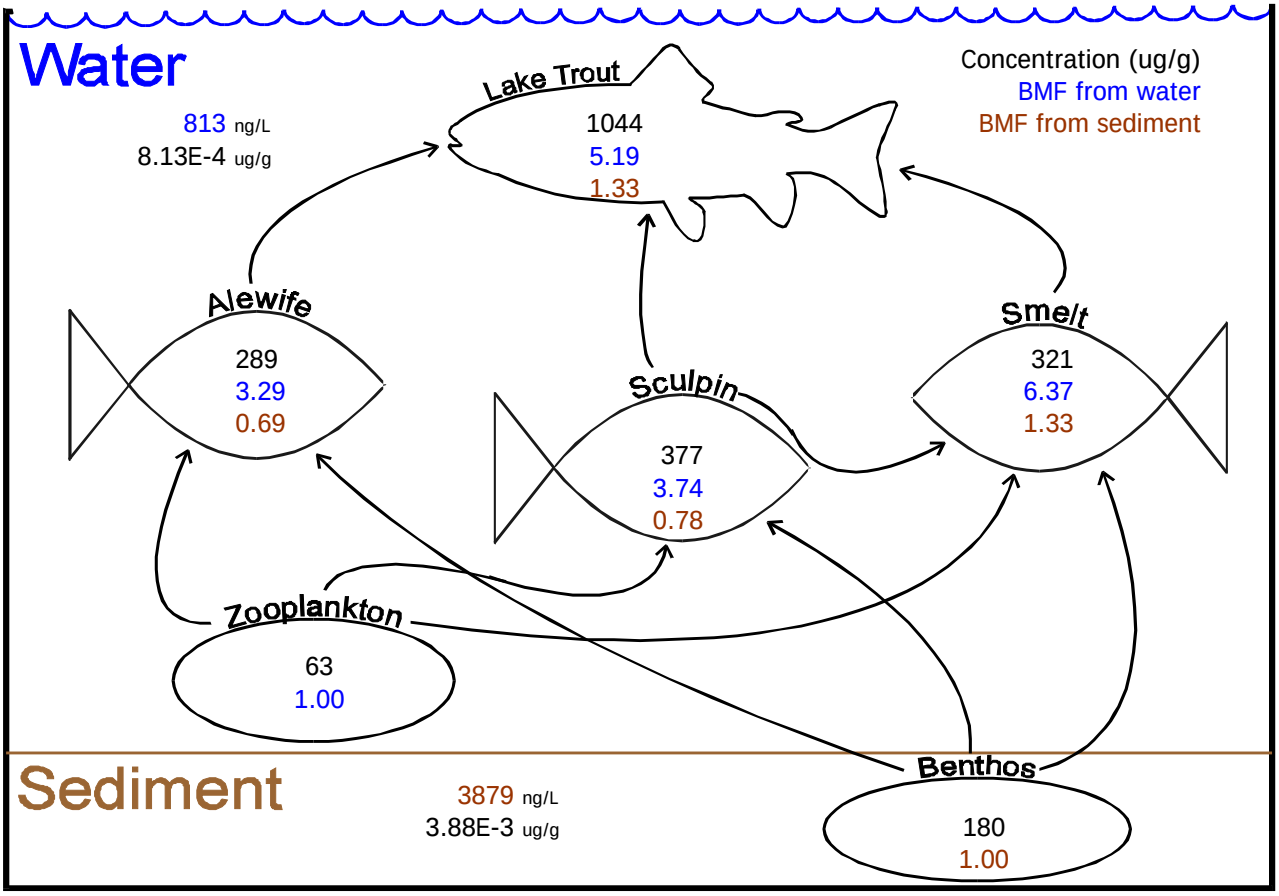
ChemSCORER Beta101 - Toxicity and Bioaccumulation
EPA p,p'-DDT

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



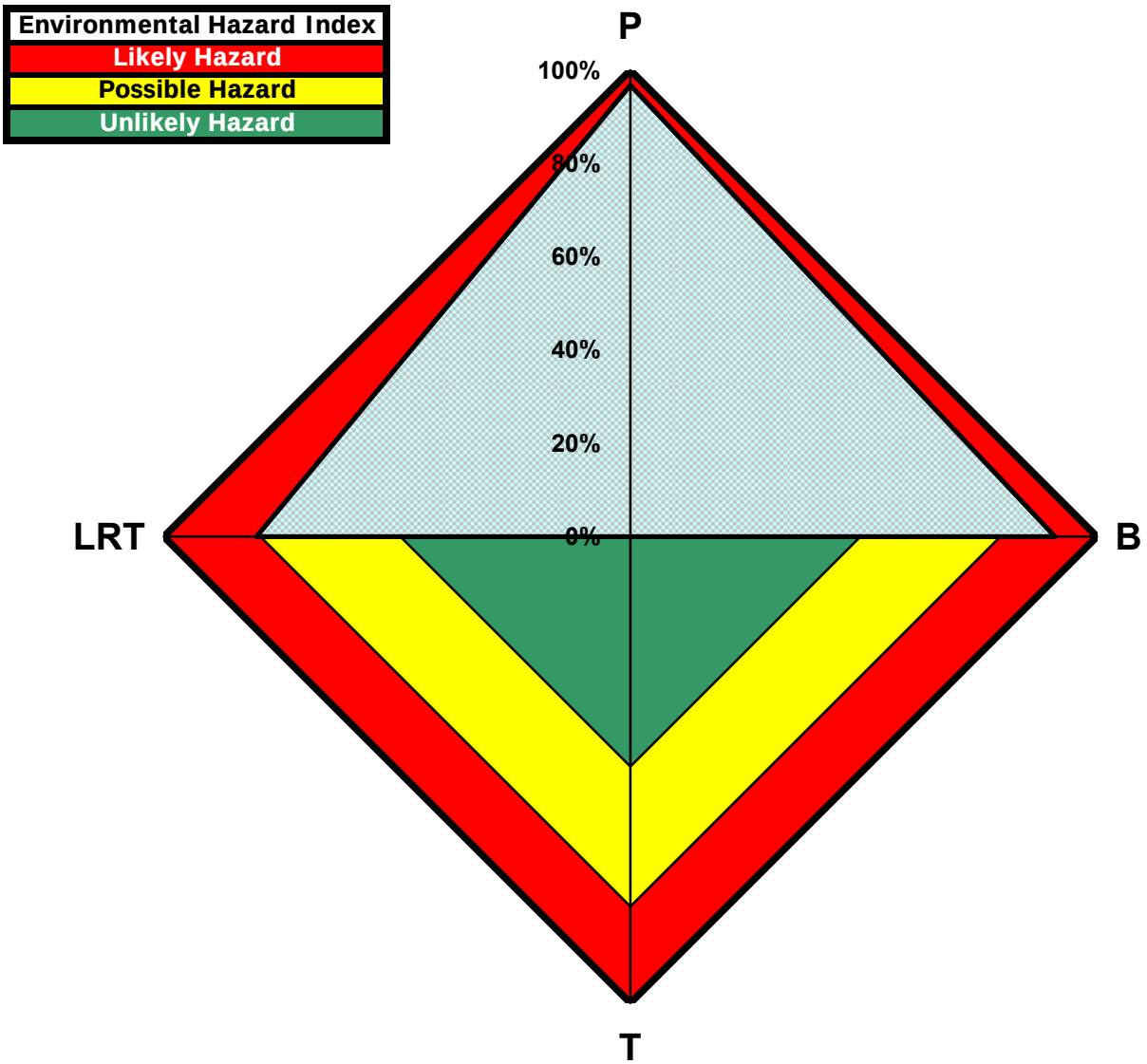
Overall Bioaccumulation Factor, Lake Trout / Water : 1285014

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.

ChemSCORER Beta101 Assessment - Summary Ranking

EPA Toxaphene



Summary Rankings for: EPA Toxaphene

This chemical ...

is more PERSISTENT (P) than **97 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **91 %** of chemicals in the reference set.

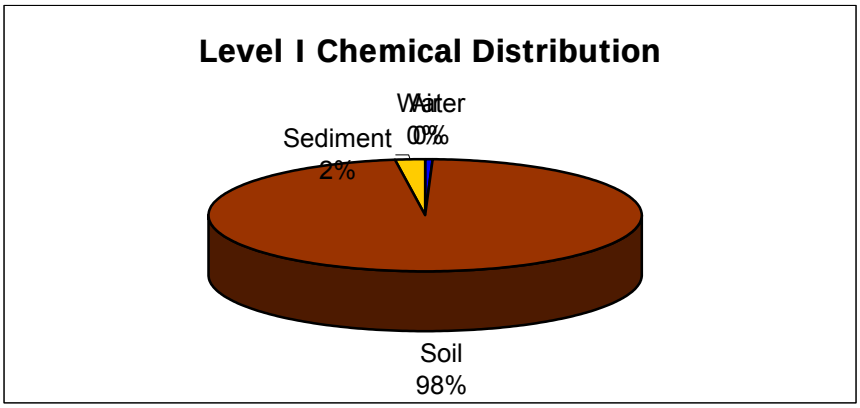
No data on mammalian toxicity was supplied.

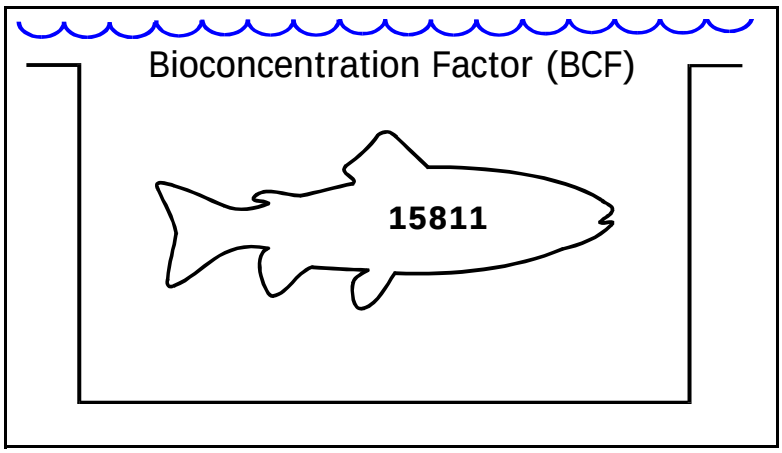
has greater LONG RANGE TRANSPORT (LRT) than **80 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA Toxaphene

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is greater than the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. In the absence of rapid metabolism by organisms, this substance is expected to bioaccumulate.

Details of Level I calculation for: EPA Toxaphene

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	7.47E-13	3.09E-10	2.61E-07	31	0.031
Water	2.27E+00	4.20E-09	1.74E-06	1.74E-06	348	0.348
Soil	1.41E+04	2.61E-05	1.08E-02	4.51E-03	97384	97.384
Sediment	2.82E+04	5.23E-05	2.16E-02	9.02E-03	2164	2.164
Suspended Sediment	8.82E+04	1.63E-04	6.76E-02	4.51E-02	68	0.068
Biota (Fish)	3.59E+04	6.64E-05	2.75E-02	2.75E-02	5	0.005
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

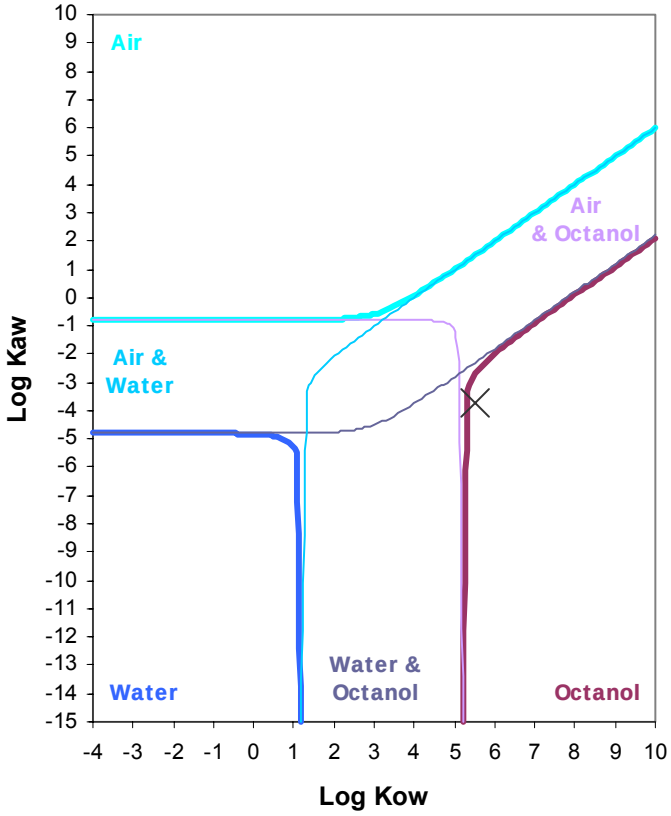
Input Parameters			Partition Coefficients		Three Solubilities	
					(g/m^3)	
Molar Mass	413.8	g/mol				
Vapor Pressure	1	Pa	Log Kow	5.50	Air	1.67E-01
Aqueous Solubility	938.7407107	g/m^3	Log Kaw	-3.75	Water	9.39E+02
Log Kow	5.5		Log Koa	9.25	Octanol	2.97E+08
Melting Point	-999	deg C				

ChemSCORER Beta101 - Level II Model Results

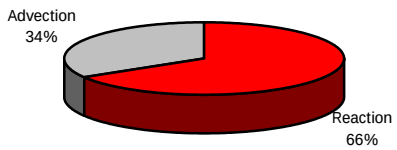
EPA Toxaphene

Equilibrium Partitioning Persistence Information

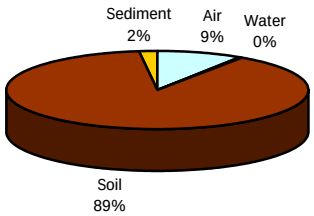
The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.
The equilibrium distribution reaction residence time calculated for this substance is greater than five years, and is comparable to that of hexachlorobenzene (7.6 years). Reactive and advective residence times are comparable, indicating the substance may be subject to long range transport.



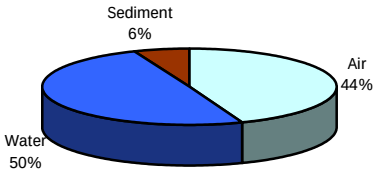
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	1998	days	5.48	years
Reaction Residence Time:	3009	days	8.24	years
Advection Residence Time:	5951	days	16.30	years

Details of Level II calculation for: EPA Toxaphene

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	170	1.64E+08	4.03E+08	6.05E+01	1.48E+02	20.875
Water	55000	5.72E+06	4.54E+08	2.10E+00	1.67E+02	16.889
Soil	55000	1.60E+09	0	5.89E+02	0	58.853
Sediment	55000	3.56E+07	5.65E+07	1.31E+01	2.08E+01	3.384
Total		1.81E+09	9.14E+08	6.64E+02	3.36E+02	100.000
Reaction + Advection		2.72E+09		1000		

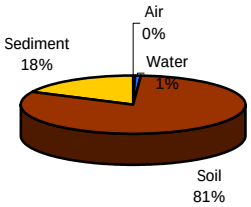
ChemSCORER Beta101 - Level III Model Results

EPA Toxaphene

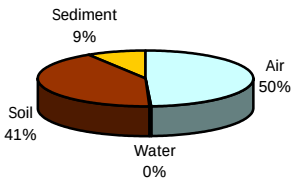
Emission to Air

Emissions to air partition predominantly to soil and sediment.

Steady State Distribution



Reactive Removal



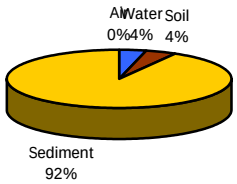
	Persistence
(hours)	40506.1
(days)	1687.8
(years)	4.6

Persistence of air emissions is comparable to that of hexachlorobenzene (2200 days).

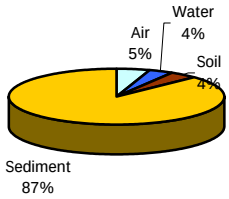
Emission to Water

Emissions to water partition significantly to sediment and may migrate to soil.

Steady State Distribution



Reactive Removal



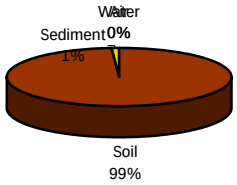
	Persistence
(hours)	75396.3
(days)	3141.5
(years)	8.6

Persistence of water emissions is comparable to that of hexachlorobenzene (2300 days).

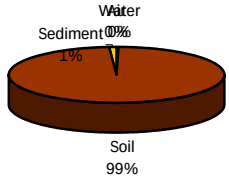
Emission to Soil

Emissions to soil remain predominantly in the soil compartment.

Steady State Distribution



Reactive Removal

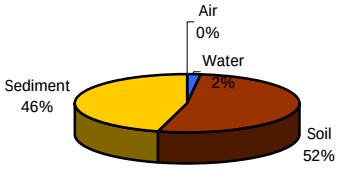


	Persistence
(hours)	79244.1
(days)	3301.8
(years)	9.0

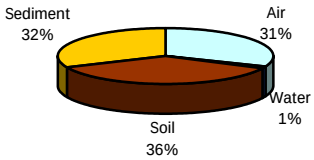
Persistence of soil emissions is comparable to that of hexachlorobenzene (3200 days).

Emission to All 3

Steady State Distribution



Reactive Removal



	Persistence
(hours)	54846.9
(days)	2285.3
(years)	6.3

Persistence under the standard emission scenario is comparable to that of hexachlorobenzene (2300 days).

Details of Level III calculation for: EPA Toxaphene

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	1.20E+05	2.96E+05	3.29E+07	7.16E+06	4.05E+07
Water	0	1000	0	1.23E+04	2.86E+06	3.36E+06	6.92E+07	7.54E+07
Soil	0	0	1000	3.75E+02	4.08E+04	7.82E+07	9.86E+05	7.92E+07
All 3	600	300	100	7.60E+04	1.04E+06	2.86E+07	2.51E+07	5.48E+07
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	491	4	415	90	1000
Water	0	1000	0	50	36	42	871	1000
Soil	0	0	1000	2	1	986	12	1000
All 3	600	300	100	310	13	360	317	1000

ChemSCORER Beta101 - Transport Model Results

EPA Toxaphene

TaPL II - Equilibrium distribution Characteristic Travel Distance

Under equilibrium partitioning conditions, this chemical is likely to be transported by both air and water.

TaPL III - Mode of entry assessments

Emission to air - Characteristic Travel Distance in Air

Characteristic Travel Distance in air is moderate, and is comparable to that of DDT (830 km). This chemical may be found in remote areas, but is not necessarily transported over very long distances.

Emission to water - Characteristic Travel Distance in Water

Characteristic Travel Distance in water is high, and is comparable to that of toxaphene (9700 km). This chemical may be subject to long range transport in surface and ocean waters.

Emission to soil - Effective Travel Distance

Emissions directly to soil are not expected to partition significantly to air or water, and are not likely to be subject to transport.

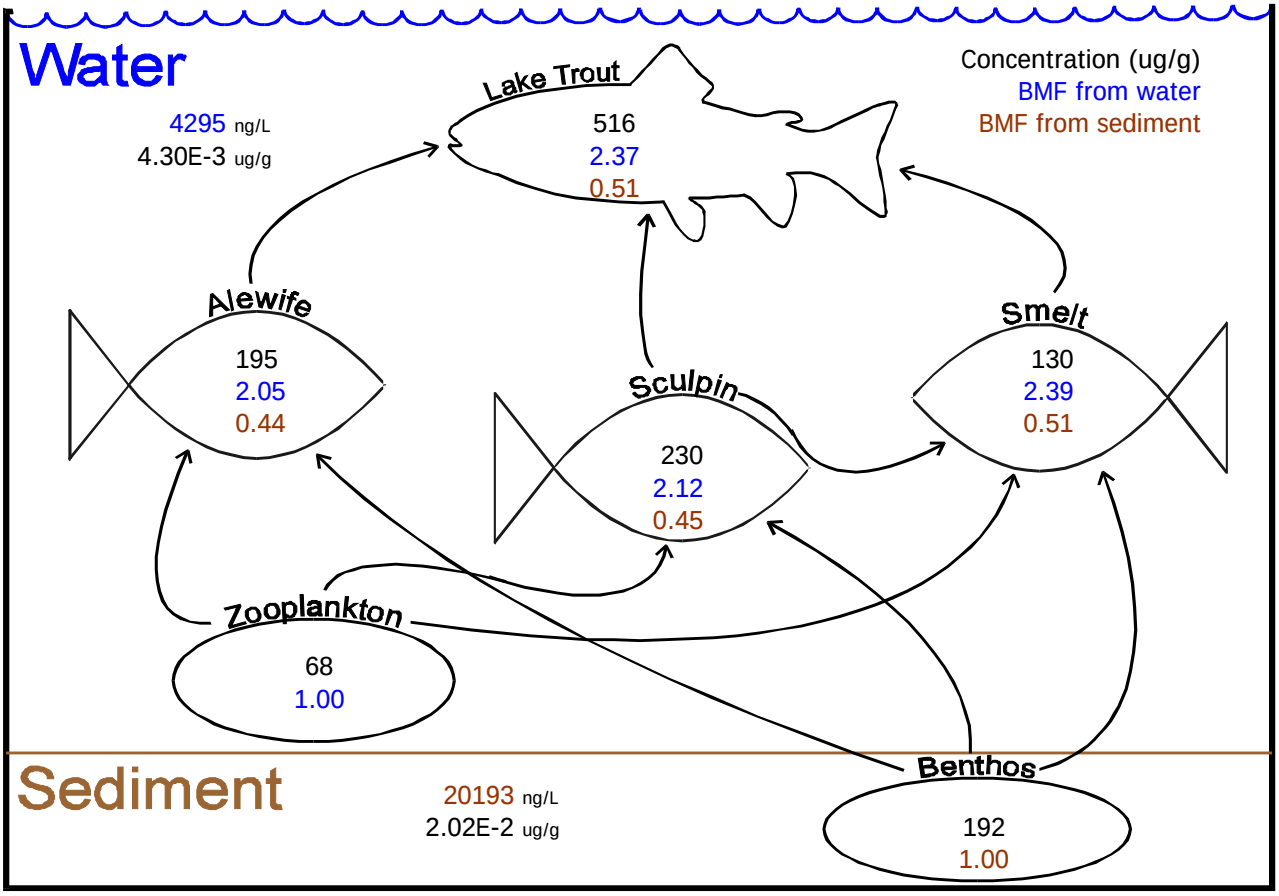
ChemSCORER Beta101 - Toxicity and Bioaccumulation
EPA Toxaphene

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



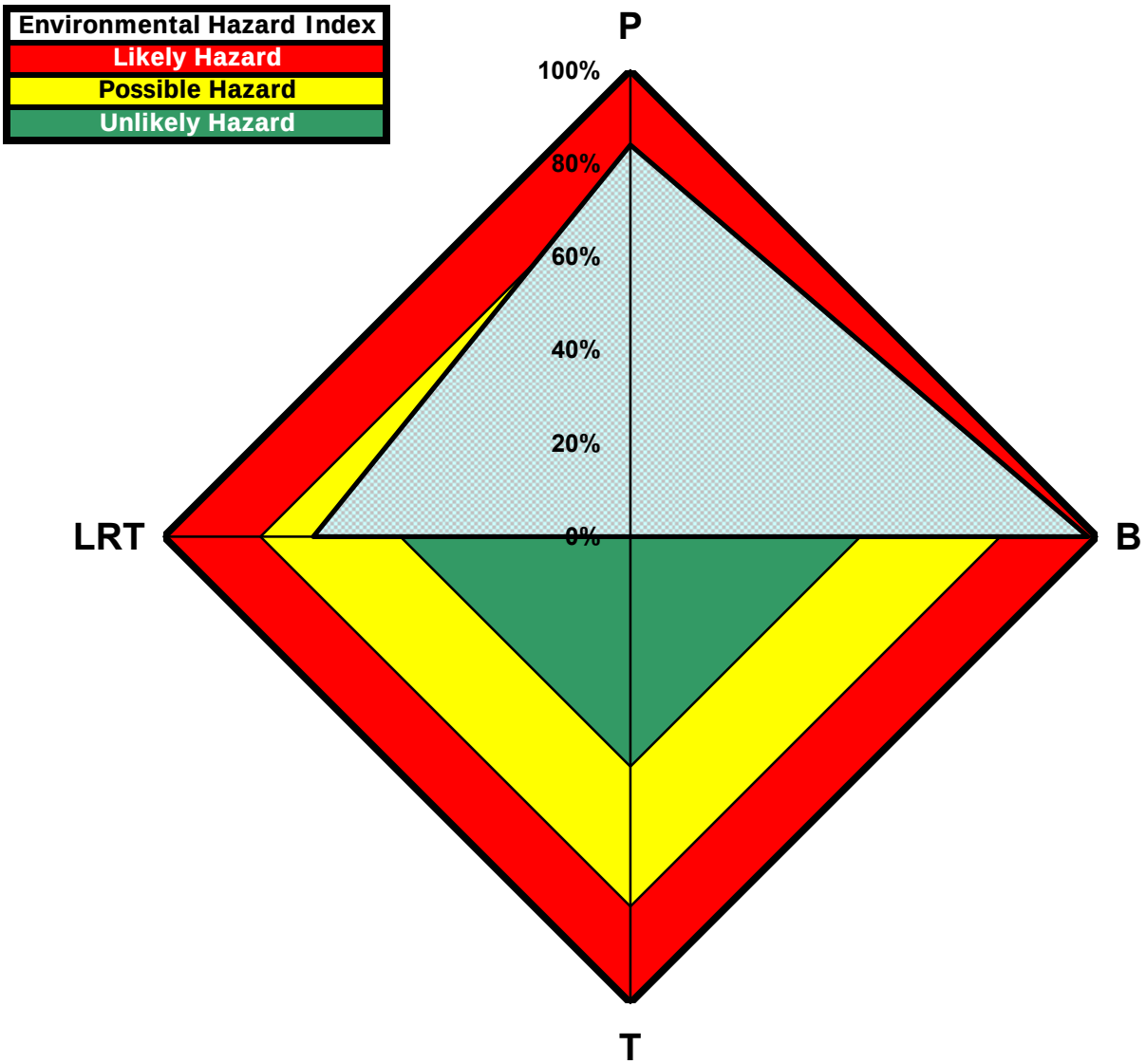
Overall Bioaccumulation Factor, Lake Trout / Water : 120143

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.

ChemSCORER Beta101 Assessment - Summary Ranking

EPA Octachlorostyrene



Summary Rankings for: EPA Octachlorostyrene

This chemical ...

is more PERSISTENT (P) than **84 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **98 %** of chemicals in the reference set.

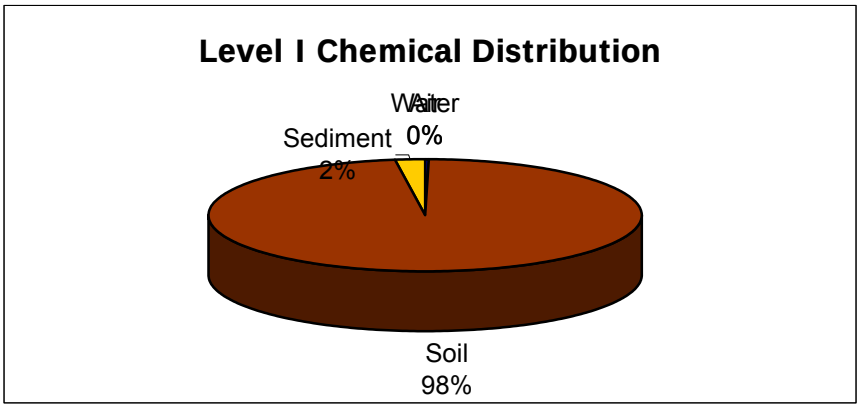
No data on mammalian toxicity was supplied.

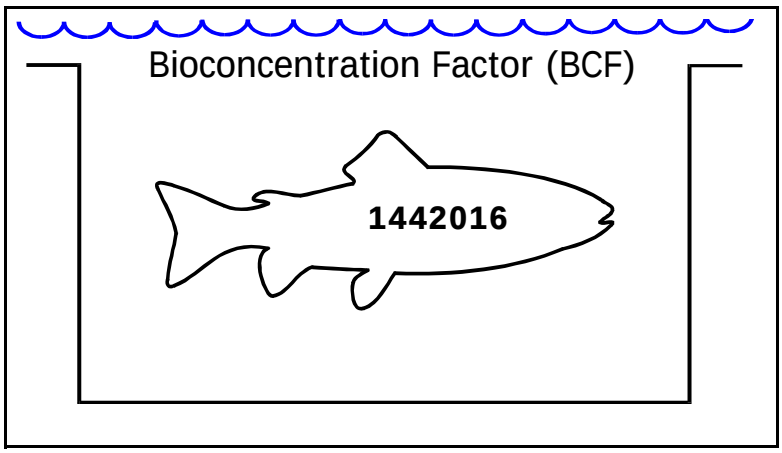
has greater LONG RANGE TRANSPORT (LRT) than **68 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA Octachlorostyrene

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is substantially greater than the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. In the absence of metabolism by organisms, this substance may bioaccumulate similar to DDT (BCF 63000) or PCBs (BCFs up to 300000).

Details of Level I calculation for: EPA Octachlorostyrene

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	2.96E-12	1.13E-09	9.50E-07	113	0.113
Water	6.85E-03	5.03E-11	1.91E-08	1.91E-08	4	0.004
Soil	3.89E+03	2.86E-05	1.08E-02	4.52E-03	97640	97.640
Sediment	7.78E+03	5.71E-05	2.17E-02	9.04E-03	2170	2.170
Suspended Sediment	2.43E+04	1.79E-04	6.78E-02	4.52E-02	68	0.068
Biota (Fish)	9.88E+03	7.26E-05	2.76E-02	2.76E-02	6	0.006
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

Input Parameters			Partition Coefficients		Three Solubilities	
Molar Mass	379.71	g/mol			(g/m^3)	
Vapor Pressure	0.00176	Pa	Log Kow	7.46	Air	2.70E-04
Aqueous Solubility	0.0045776	g/m^3	Log Kaw	-1.23	Water	4.58E-03
Log Kow	7.46		Log Koa	8.69	Octanol	1.32E+05
Melting Point	-999	deg C				

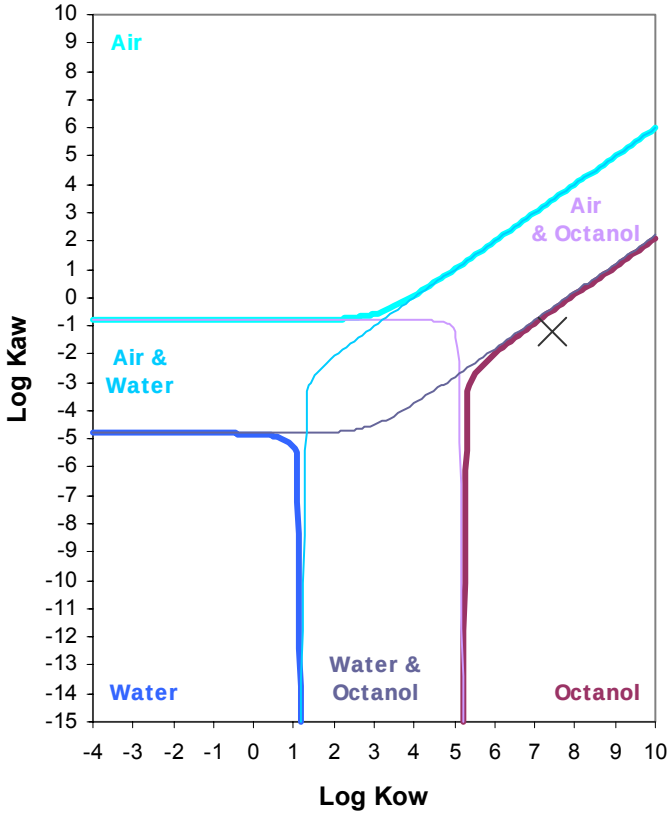
ChemSCORER Beta101 - Level II Model Results

EPA Octachlorostyrene

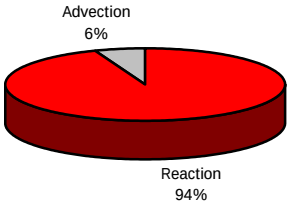
Equilibrium Partitioning Persistence Information

The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.

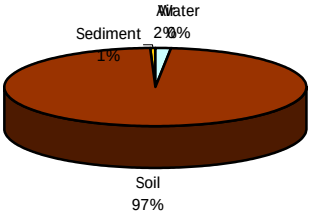
The equilibrium distribution reaction residence time calculated for this substance can be measured in years, and is comparable to that of pentachlorobenzene (2 years). Reactive residence time is more than 10 times shorter than advective residence time, indicating potential for transport to other regions is low.



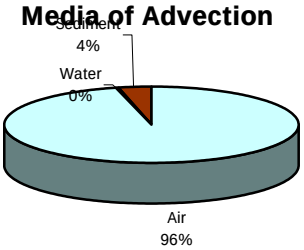
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	204	days	0.56	years
Reaction Residence Time:	217	days	0.59	years
Advection Residence Time:	3552	days	9.73	years

Details of Level II calculation for: EPA Octachlorostyrene

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	227	1.23E+08	4.03E+08	1.68E+01	5.51E+01	7.197
Water	3600	2.64E+05	1.37E+06	3.60E-02	1.87E-01	0.022
Soil	3600	6.74E+09	0	9.21E+02	0	92.057
Sediment	14400	3.74E+07	1.56E+07	5.11E+00	2.13E+00	0.724
Total		6.90E+09	4.20E+08	9.43E+02	5.74E+01	100.000
Reaction + Advection		7.32E+09		1000		

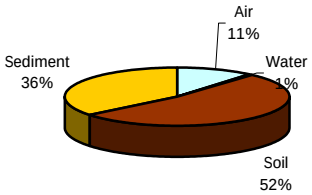
ChemSCORER Beta101 - Level III Model Results

EPA Octachlorostyrene

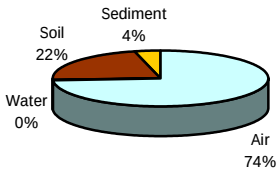
Emission to Air

Emissions to air partition significantly to soil and sediment.

Steady State Distribution



Reactive Removal



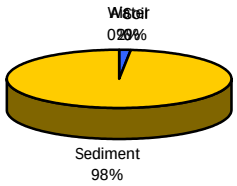
	Persistence
(hours)	2183.77
(days)	90.99
(years)	0.25

Persistence of air emissions is comparable to that of the tetrachlorobenzenes (110 days).

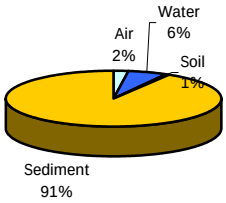
Emission to Water

Emissions to water partition significantly to sediment and may migrate to soil.

Steady State Distribution



Reactive Removal



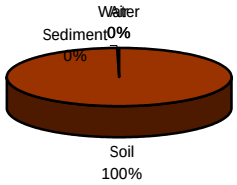
	Persistence
(hours)	19318.84
(days)	804.95
(years)	2.21

Persistence of water emissions is comparable to that of hexachlorobenzene (2300 days).

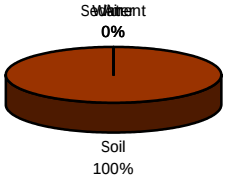
Emission to Soil

Emissions to soil remain predominantly in the soil compartment.

Steady State Distribution



Reactive Removal

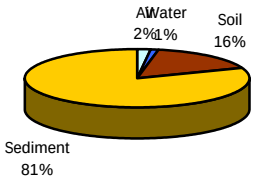


	Persistence
(hours)	5201.88
(days)	216.74
(years)	0.59

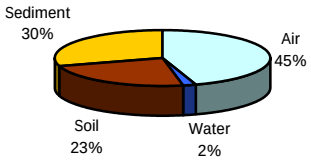
Persistence of soil emissions is comparable to that of the tetrachlorobenzenes (250 days).

Emission to All 3

Steady State Distribution



Reactive Removal



	Persistence
(hours)	7626.10
(days)	317.75
(years)	0.87

Persistence under the standard emission scenario is comparable to that of the tetrachlorobenzenes (130 days).

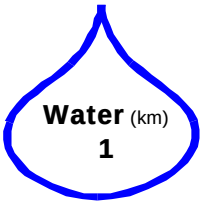
Details of Level III calculation for: EPA Octachlorostyrene

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	2.42E+05	1.21E+04	1.15E+06	7.81E+05	2.18E+06
Water	0	1000	0	7.53E+03	2.94E+05	3.57E+04	1.90E+07	1.93E+07
Soil	0	0	1000	3.01E+01	1.55E+02	5.19E+06	1.00E+04	5.20E+06
All 3	600	300	100	1.48E+05	9.56E+04	1.22E+06	6.16E+06	7.63E+06
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	739	2	221	38	1000
Water	0	1000	0	23	57	7	913	1000
Soil	0	0	1000	0	0	999	0	1000
All 3	600	300	100	450	18	235	297	1000

ChemSCORER Beta101 - Transport Model Results

EPA Octachlorostyrene

TaPL II - Equilibrium distribution Characteristic Travel Distance



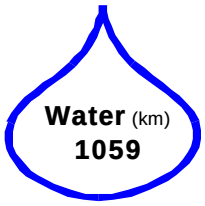
Under equilibrium partitioning conditions, this chemical is likely to be transported most effectively in air.

TaPL III - Mode of entry assessments

Emission to air - Characteristic Travel Distance in Air

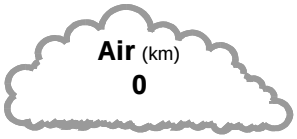
Characteristic Travel Distance in air is high, and is comparable to that of hexachlorinated PCBs (4200 km). This chemical may be subject to long range transport and deposition in the arctic.

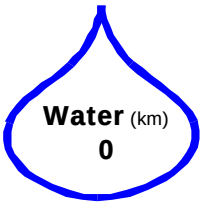
Emission to water - Characteristic Travel Distance in Water



Characteristic Travel Distance in water is moderate, and is comparable to that of chlorobenzene (1300 km). This chemical may be subject to transport in surface and near-shore marine waters.

Emission to soil - Effective Travel Distance





Emissions directly to soil are not expected to partition significantly to air or water, and are not likely to be subject to transport.

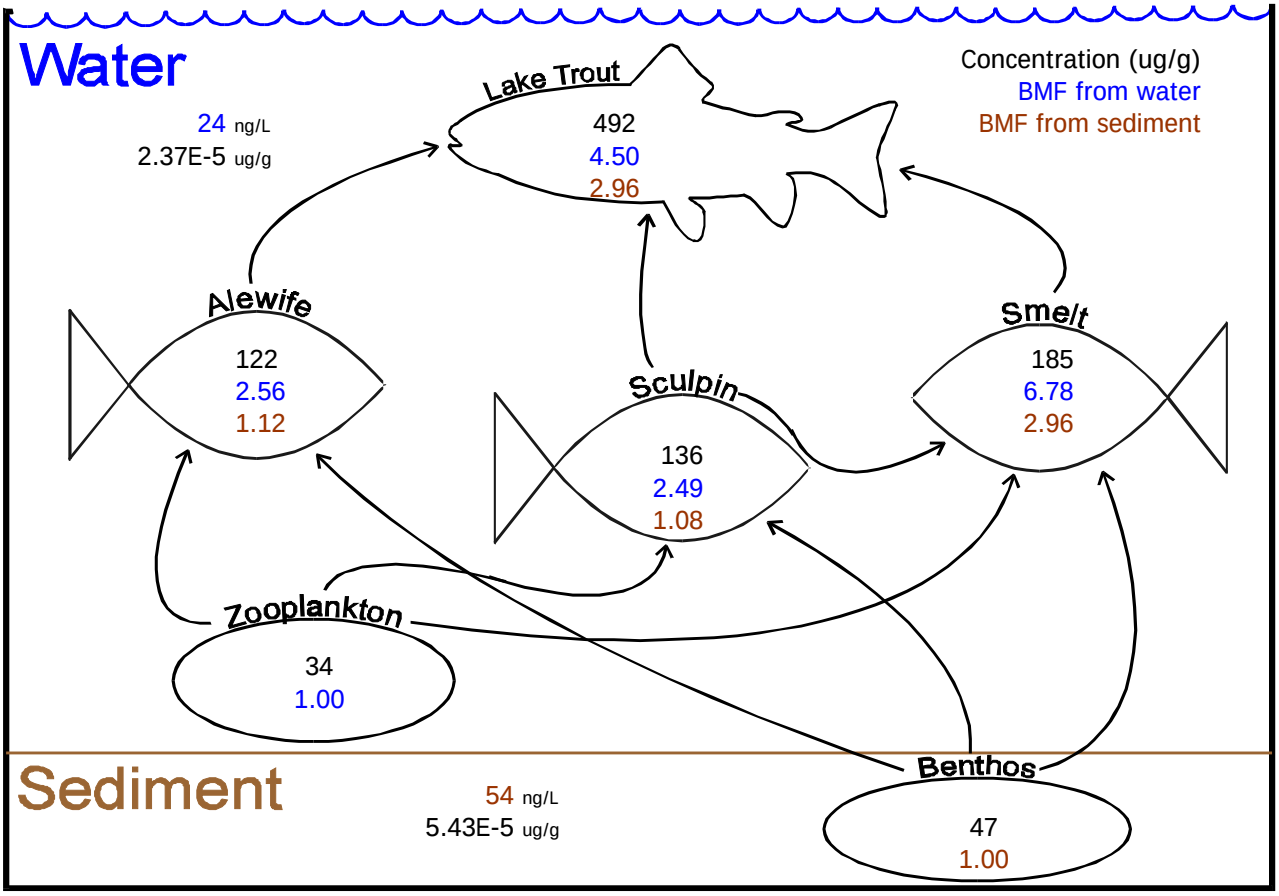
ChemSCORER Beta101 - Toxicity and Bioaccumulation
EPA Octachlorostyrene

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



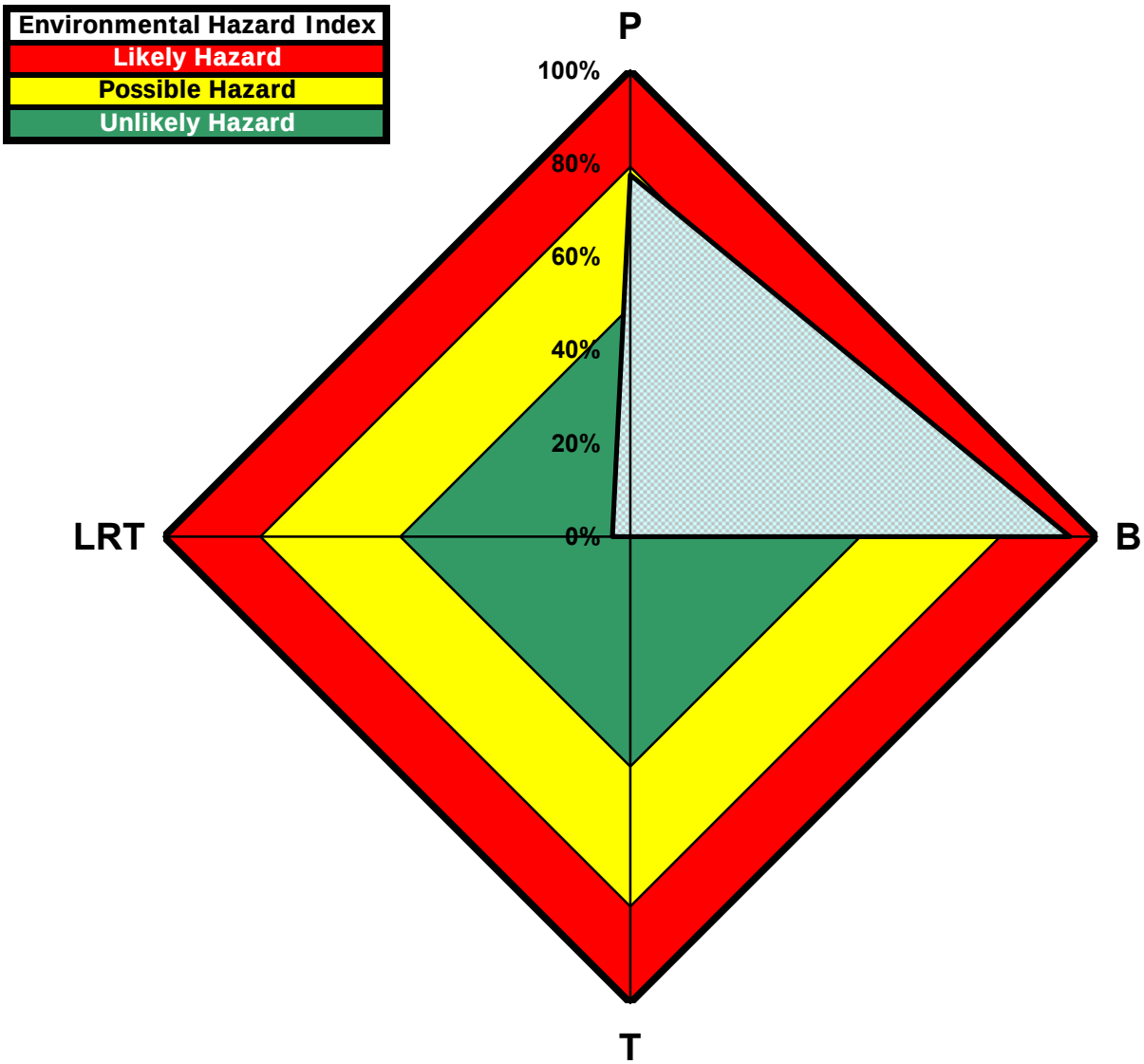
Overall Bioaccumulation Factor, Lake Trout / Water : 20770986

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.

ChemSCORER Beta101 Assessment - Summary Ranking

EPA B[a]p



Summary Rankings for: EPA B[a]p

This chemical ...

is more PERSISTENT (P) than **78 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **94 %** of chemicals in the reference set.

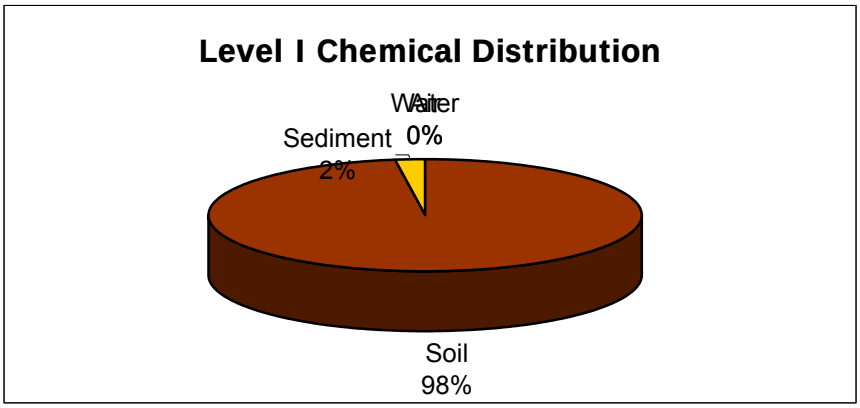
No data on mammalian toxicity was supplied.

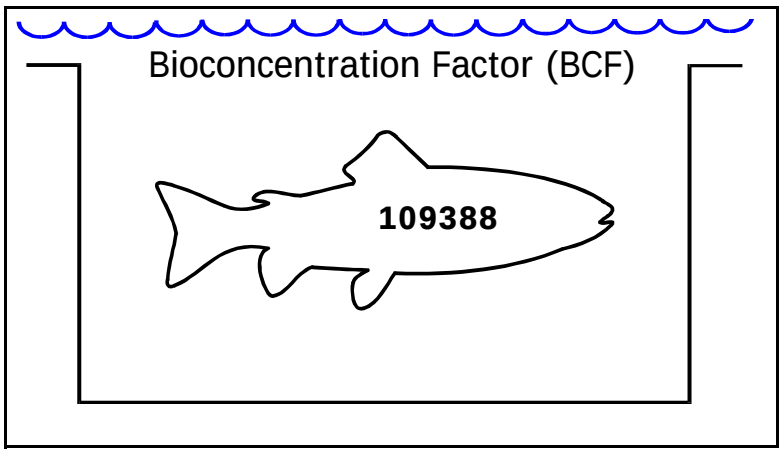
has greater LONG RANGE TRANSPORT (LRT) than **4 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA B[a]p

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is substantially greater than the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. In the absence of metabolism by organisms, this substance may bioaccumulate similar to DDT (BCF 63000) or PCBs (BCFs up to 300000).

Details of Level I calculation for: EPA B[a]p

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	3.46E-14	8.74E-12	7.37E-09	1	0.001
Water	1.16E+01	9.99E-10	2.52E-07	2.52E-07	50	0.050
Soil	5.01E+05	4.30E-05	1.09E-02	4.52E-03	97704	97.704
Sediment	1.00E+06	8.61E-05	2.17E-02	9.05E-03	2171	2.171
Suspended Sediment	3.13E+06	2.69E-04	6.79E-02	4.52E-02	68	0.068
Biota (Fish)	1.27E+06	1.09E-04	2.76E-02	2.76E-02	6	0.006
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

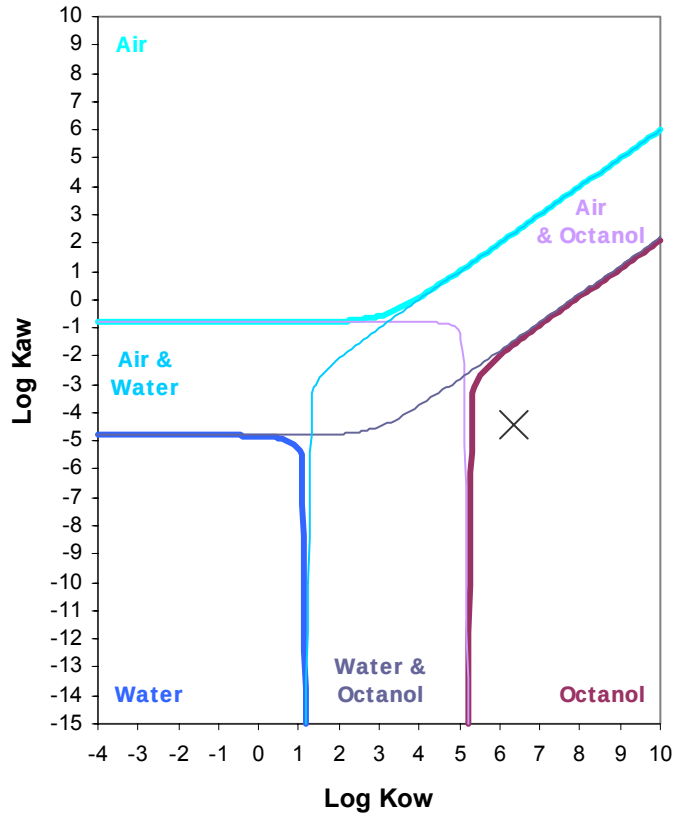
Input Parameters			Partition Coefficients		Three Solubilities	
					(g/m^3)	
Molar Mass	252.3	g/mol				
Vapor Pressure	1	Pa	Log Kow	6.34	Air	1.02E-01
Aqueous Solubility	2937	g/m^3	Log Kaw	-4.46	Water	2.94E+03
Log Kow	6.34		Log Koa	10.80	Octanol	6.43E+09
Melting Point	177.5	deg C				

ChemSCORER Beta101 - Level II Model Results

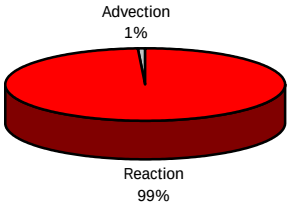
EPA B[a]p

Equilibrium Partitioning Persistence Information

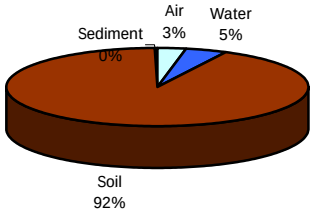
The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.
The equilibrium distribution reaction residence time calculated for this substance can be measured in years, and is comparable to that of pentachlorobenzene (2 years). Reactive residence time is more than 10 times shorter than advective residence time, indicating potential for transport to other regions is low.



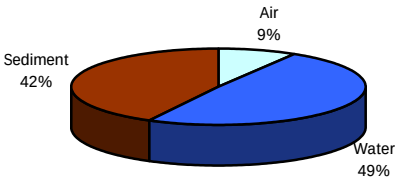
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	308	days	0.84	years
Reaction Residence Time:	311	days	0.85	years
Advection Residence Time:	40615	days	111.27	years
Details of Level II calculation for:	EPA B[a]p			

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	1.52	1.84E+10	4.03E+08	2.95E+01	6.46E-01	3.012
Water	56.08151099	2.88E+10	2.33E+09	4.61E+01	3.73E+00	4.983
Soil	5487.166023	5.70E+11	0	9.13E+02	0	91.288
Sediment	28140	2.47E+09	2.00E+09	3.96E+00	3.21E+00	0.717
Total		6.19E+11	4.74E+09	9.92E+02	7.59E+00	100.000
Reaction + Advection		6.24E+11		1000		

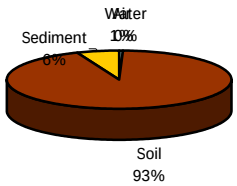
ChemSCORER Beta101 - Level III Model Results

EPA B[a]p

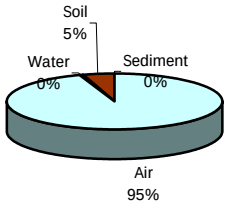
Emission to Air

Emissions to air partition predominantly to soil and sediment.

Steady State Distribution



Reactive Removal



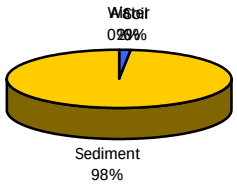
Persistence	
(hours)	397.21
(days)	16.55
(years)	0.05

Persistence of air emissions is comparable to that of chlorobenzene (250 hours).

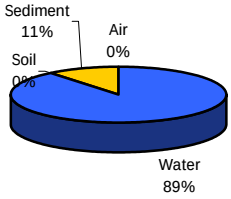
Emission to Water

Emissions to water partition significantly to sediment and may migrate to soil.

Steady State Distribution



Reactive Removal



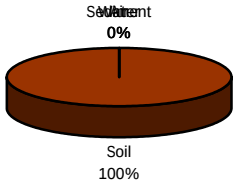
Persistence	
(hours)	4491.44
(days)	187.14
(years)	0.51

Persistence of water emissions is comparable to that of the tetrachlorobenzenes (140 days).

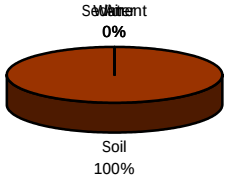
Emission to Soil

Emissions to soil remain predominantly in the soil compartment.

Steady State Distribution



Reactive Removal

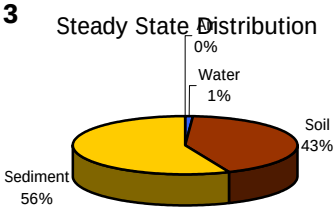


Persistence	
(hours)	7914.82
(days)	329.78
(years)	0.90

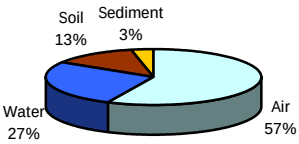
Persistence of soil emissions is comparable to that of the tetrachlorobenzenes (250 days).

Emission to All 3

Steady State Distribution



Reactive Removal



Persistence	
(hours)	2377.24
(days)	99.05
(years)	0.27

Persistence under the standard emission scenario is comparable to that of the tetrachlorobenzenes (130 days).

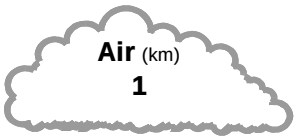
Details of Level III calculation for: EPA B[a]p

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	2.08E+03	3.91E+02	3.71E+05	2.40E+04	3.97E+05
Water	0	1000	0	5.27E-01	7.21E+04	9.40E+01	4.42E+06	4.49E+06
Soil	0	0	1000	3.89E-02	6.37E+01	7.91E+06	3.90E+03	7.91E+06
All 3	600	300	100	1.25E+03	2.19E+04	1.01E+06	1.34E+06	2.38E+06
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	948	5	47	1	1000
Water	0	1000	0	0	891	0	109	1000
Soil	0	0	1000	0	1	999	0	1000
All 3	600	300	100	569	270	128	33	1000

ChemSCORER Beta101 - Transport Model Results

EPA B[a]p

TaPL II - Equilibrium distribution Characteristic Travel Distance



Under equilibrium partitioning conditions, this chemical is likely to be transported most effectively in water.

TaPL III - Mode of entry assessments

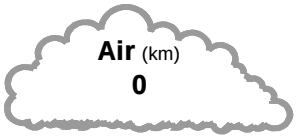
Emission to air - Characteristic Travel Distance in Air

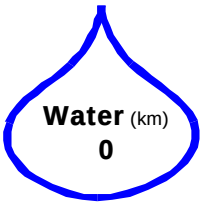
Characteristic Travel Distance in air is low. This chemical is not likely to be transported a significant distance in the atmosphere.

Emission to water - Characteristic Travel Distance in Water

Characteristic Travel Distance in water is low. This chemical is not likely to be transported a significant distance in water.

Emission to soil - Effective Travel Distance





Emissions directly to soil are not expected to partition significantly to air or water, and are not likely to be subject to transport.

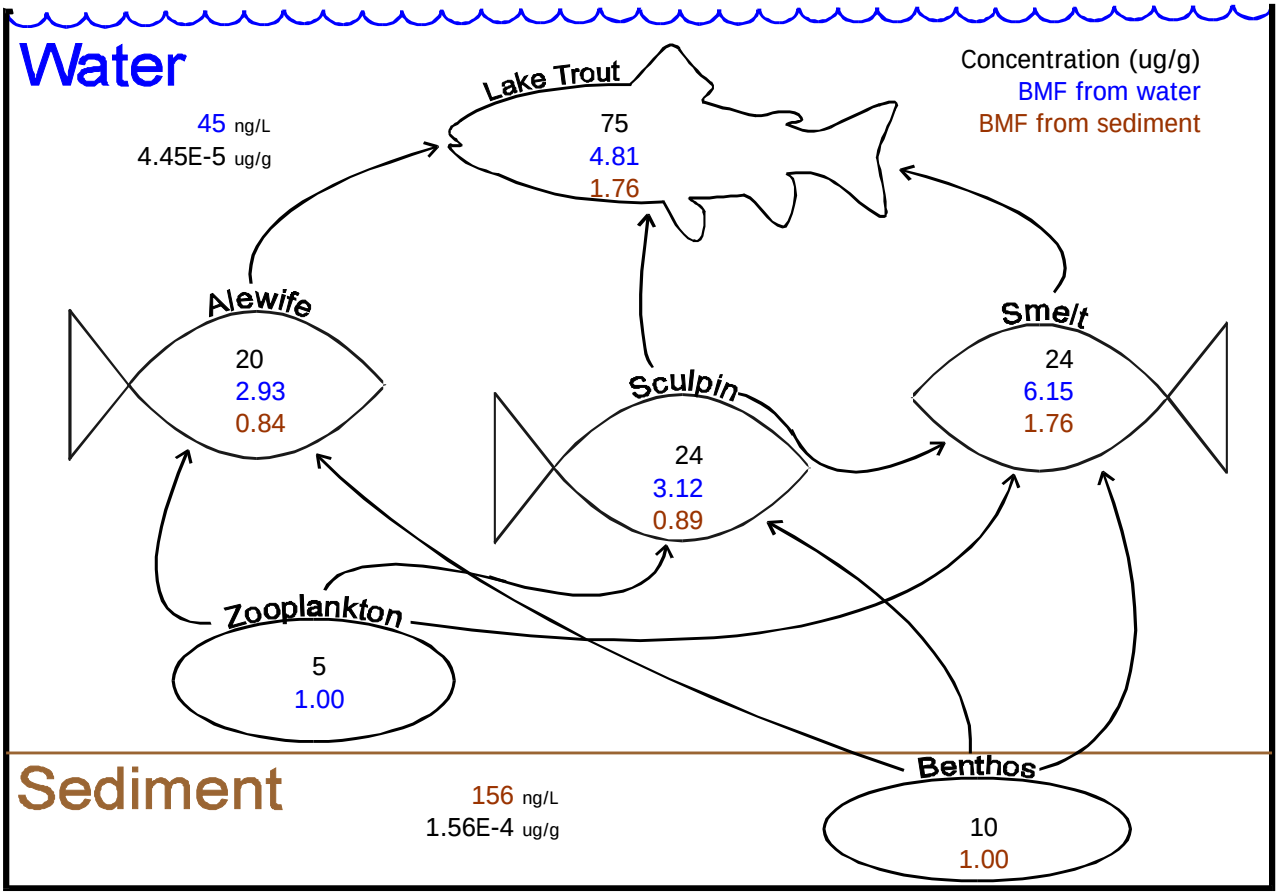
ChemSCORER Beta101 - Toxicity and Bioaccumulation
EPA B[a]p

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



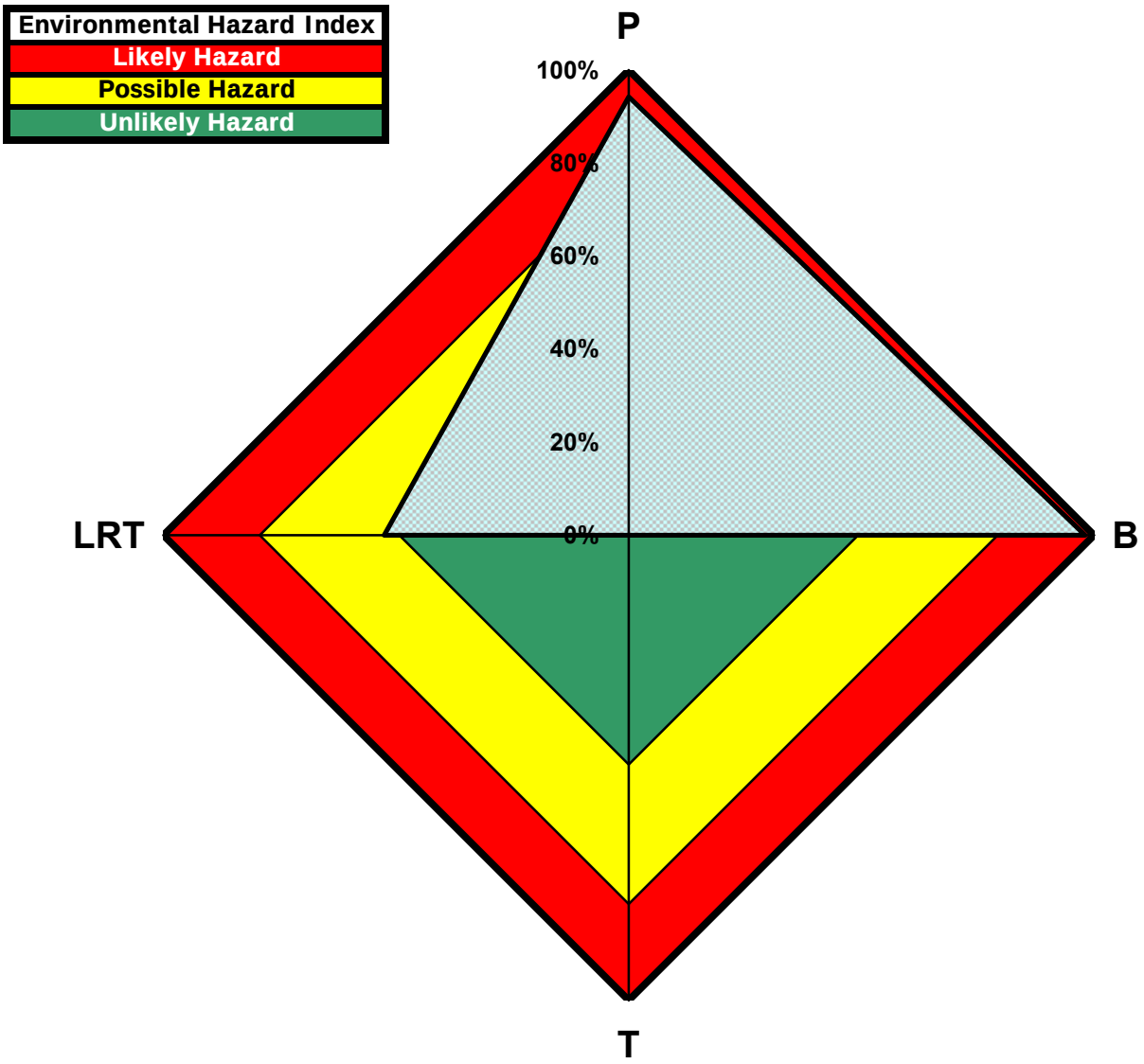
Overall Bioaccumulation Factor, Lake Trout / Water : 1683335

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.

ChemSCORER Beta101 Assessment - Summary Ranking

EPA Mirex



Summary Rankings for: EPA Mirex

This chemical ...

is more PERSISTENT (P) than **94 %** of chemicals in the reference set.

is more BIOACCUMMULATIVE (B) than **98 %** of chemicals in the reference set.

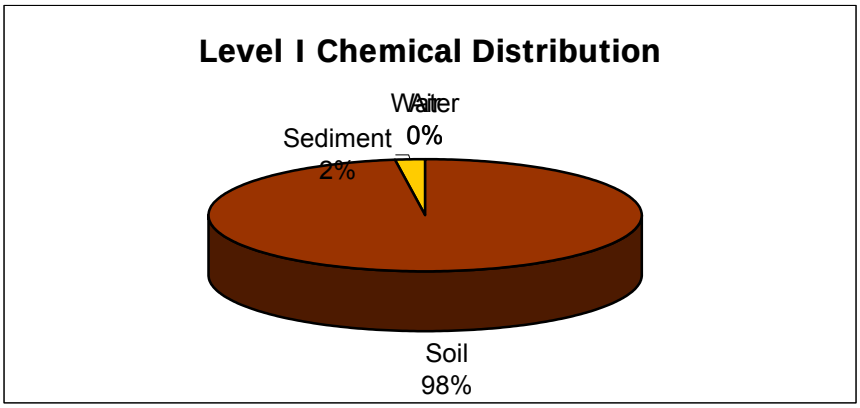
No data on mammalian toxicity was supplied.

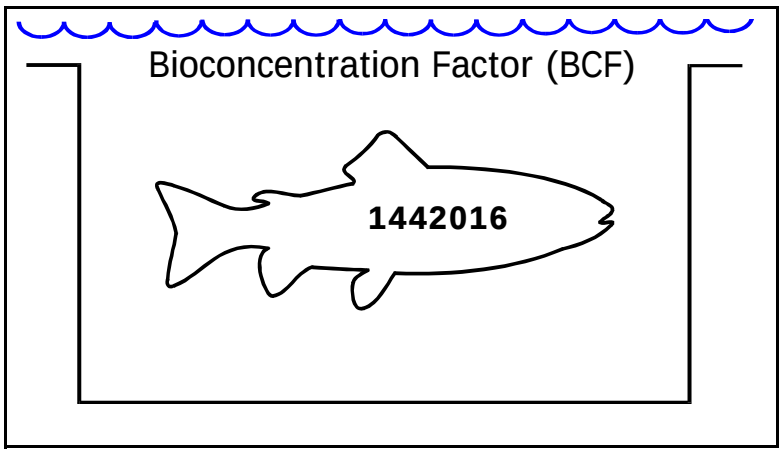
has greater LONG RANGE TRANSPORT (LRT) than **53 %** of chemicals in the reference set.

ChemSCORER Beta101 - Level I Model Results

EPA Mirex

The Level I chemical distibution represents long term equilibrium partitioning of the chemical. Many persistent chemicals partition predominantly to soils. Long range transport usually requires partitioning (at least 1%) to one of the mobile media (air or water).





The calculated BCF is substantially greater than the generally accepted cut-off between bioaccumulative and non-bioaccumulative substances of 5000. In the absence of metabolism by organisms, this substance may bioaccumulate similar to DDT (BCF 63000) or PCBs (BCFs up to 300000).

Details of Level I calculation for: EPA Mirex

Equilibrium Chemical Distribution

Compartment	Z	Concentration			Amount	
	(mol/m^3Pa)	(mol/m^3)	(mg/L)	(ug/g)	kg	%
Air	4.03E-04	5.69E-13	3.10E-10	2.62E-07	31	0.031
Water	2.49E-02	3.51E-11	1.91E-08	1.91E-08	4	0.004
Soil	1.41E+04	1.99E-05	1.09E-02	4.52E-03	97720	97.720
Sediment	2.82E+04	3.98E-05	2.17E-02	9.05E-03	2172	2.172
Suspended Sediment	8.82E+04	1.24E-04	6.79E-02	4.52E-02	68	0.068
Biota (Fish)	3.59E+04	5.06E-05	2.76E-02	2.76E-02	6	0.006
Total					100000	100.000

Physical Chemical Data and Partition Coefficients

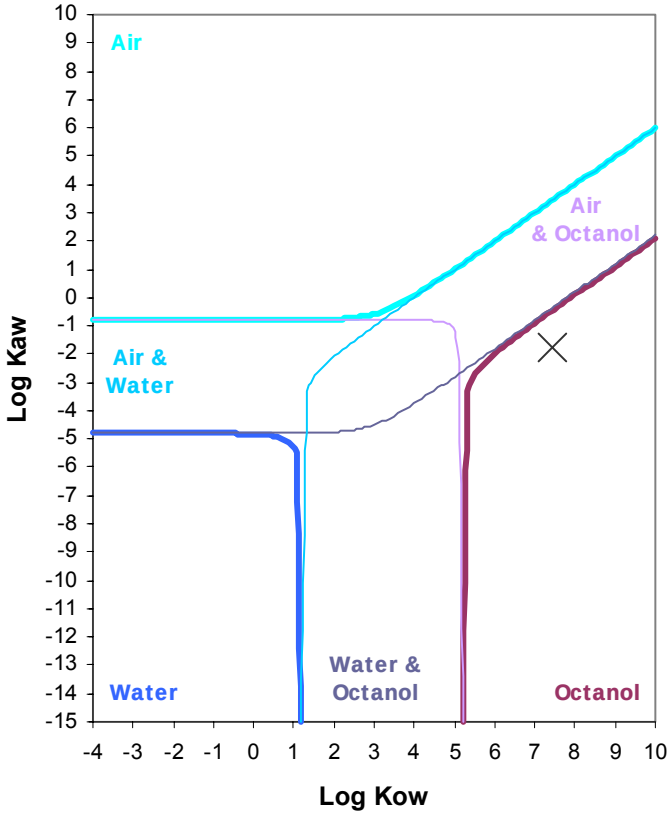
Input Parameters			Partition Coefficients		Three Solubilities	
					(g/m^3)	
Molar Mass	545.59	g/mol				
Vapor Pressure	1	Pa	Log Kow	7.46	Air	2.20E-01
Aqueous Solubility	13.57130365	g/m^3	Log Kaw	-1.79	Water	1.36E+01
Log Kow	7.46		Log Koa	9.25	Octanol	3.91E+08
Melting Point	-999	deg C				

ChemSCORER Beta101 - Level II Model Results

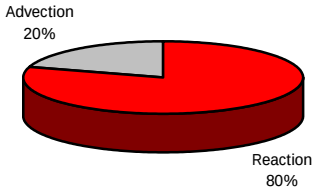
EPA Mirex

Equilibrium Partitioning Persistence Information

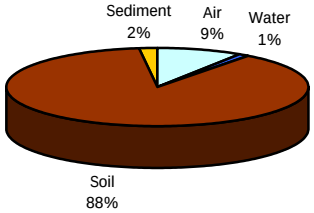
The figure at right identifies environmental media that have a controlling influence on the overall rate of reactive degradation of this substance. Substances that fall near the center of the diagram are expected to accumulate in all media, and overall persistence will be influenced by all degradation rates. The relative importance of advection and reaction to the regional-scale removal of this substance, and the media from which these processes take place are depicted in the pie charts below.
The equilibrium distribution reaction residence time calculated for this substance is greater than five years, and is comparable to that of hexachlorobenzene (7.6 years). Reactive and advective residence times are comparable, indicating the substance may be subject to long range transport.



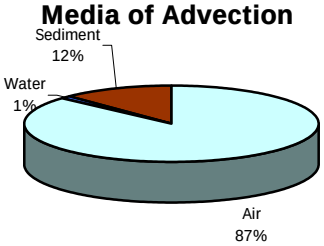
Removal Pathways



Media of Reaction



Media of Advection



Overall Residence Time:	2370	days	6.49	years
Reaction Residence Time:	2975	days	8.15	years
Advection Residence Time:	11655	days	31.93	years
Details of Level II calculation for:	EPA Mirex			

Removal Processes - Equilibrium Distribution

Compartment	Half-life (hours)	D Values Reaction (mol/Pa h)	D Values Advection (mol/Pa h)	Loss Rates Reaction (kg/h)	Loss Rates Advection (kg/h)	Removal %
Air	170	1.64E+08	4.03E+08	7.19E+01	1.76E+02	24.839
Water	170	2.03E+07	4.97E+06	8.87E+00	2.18E+00	1.105
Soil	55000	1.60E+09	0	7.00E+02	0	70.030
Sediment	55000	3.56E+07	5.65E+07	1.56E+01	2.47E+01	4.026
Total		1.82E+09	4.65E+08	7.97E+02	2.03E+02	100.000
Reaction + Advection		2.29E+09		1000		

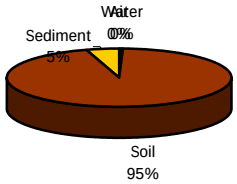
ChemSCORER Beta101 - Level III Model Results

EPA Mirex

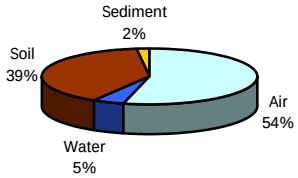
Emission to Air

Emissions to air partition predominantly to soil and sediment.

Steady State Distribution



Reactive Removal



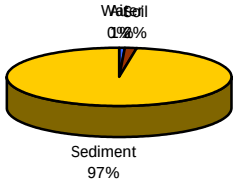
	Persistence
(hours)	32993.3
(days)	1374.7
(years)	3.8

Persistence of air emissions is comparable to that of hexachlorobenzene (2200 days).

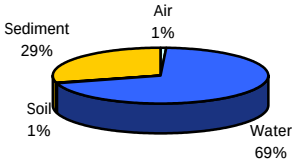
Emission to Water

Emissions to water partition significantly to sediment and may migrate to soil.

Steady State Distribution



Reactive Removal



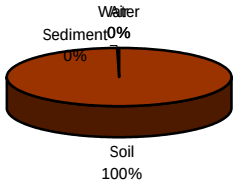
	Persistence
(hours)	23637.6
(days)	984.9
(years)	2.7

Persistence of water emissions is comparable to that of hexachlorobenzene (2300 days).

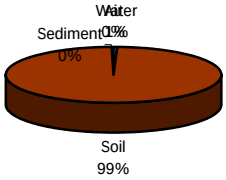
Emission to Soil

Emissions to soil remain predominantly in the soil compartment.

Steady State Distribution



Reactive Removal

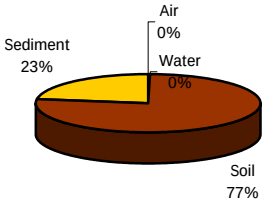


	Persistence
(hours)	78901.2
(days)	3287.6
(years)	9.0

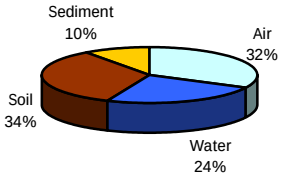
Persistence of soil emissions is comparable to that of hexachlorobenzene (3200 days).

Emission to All 3

Steady State Distribution



Reactive Removal



	Persistence
(hours)	34777.4
(days)	1449.1
(years)	4.0

Persistence under the standard emission scenario is comparable to that of hexachlorobenzene (2300 days).

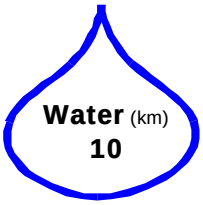
Details of Level III calculation for: EPA Mirex

	Emission Rate (kg/h)			Inventory at Steady State (kg)				
	Air	**Water**	**Soil**	**Air**	**Water**	**Soil**	**Sediment**	**Total**
Air	1000	0	0	1.32E+05	1.19E+04	3.13E+07	1.60E+06	3.30E+07
Water	0	1000	0	1.73E+03	1.71E+05	4.09E+05	2.31E+07	2.36E+07
Soil	0	0	1000	7.46E+01	1.36E+03	7.87E+07	1.84E+05	7.89E+07
All 3	600	300	100	7.97E+04	5.86E+04	2.67E+07	7.89E+06	3.48E+07
	Emission Rate (kg/h)			Reaction Loss Rate (kg/h)				
Air	1000	0	0	538	48	394	20	1000
Water	0	1000	0	7	697	5	290	1000
Soil	0	0	1000	0	6	992	2	1000
All 3	600	300	100	325	239	337	99	1000

ChemSCORER Beta101 - Transport Model Results

EPA Mirex

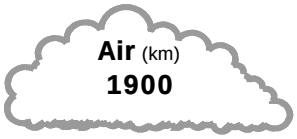
TaPL II - Equilibrium distribution Characteristic Travel Distance



Under equilibrium partitioning conditions, this chemical is likely to be transported most effectively in air.

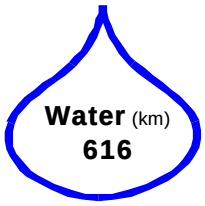
TaPL III - Mode of entry assessments

Emission to air - Characteristic Travel Distance in Air



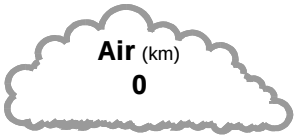
Characteristic Travel Distance in air is moderate, and is comparable to that of DDT (830 km). This chemical may be found in remote areas, but is not necessarily transported over very long distances.

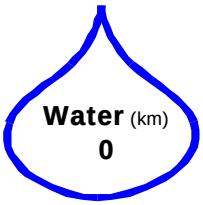
Emission to water - Characteristic Travel Distance in Water



Characteristic Travel Distance in water is low. This chemical is not likely to be transported a significant distance in water.

Emission to soil - Effective Travel Distance





Emissions directly to soil are not expected to partition significantly to air or water, and are not likely to be subject to transport.

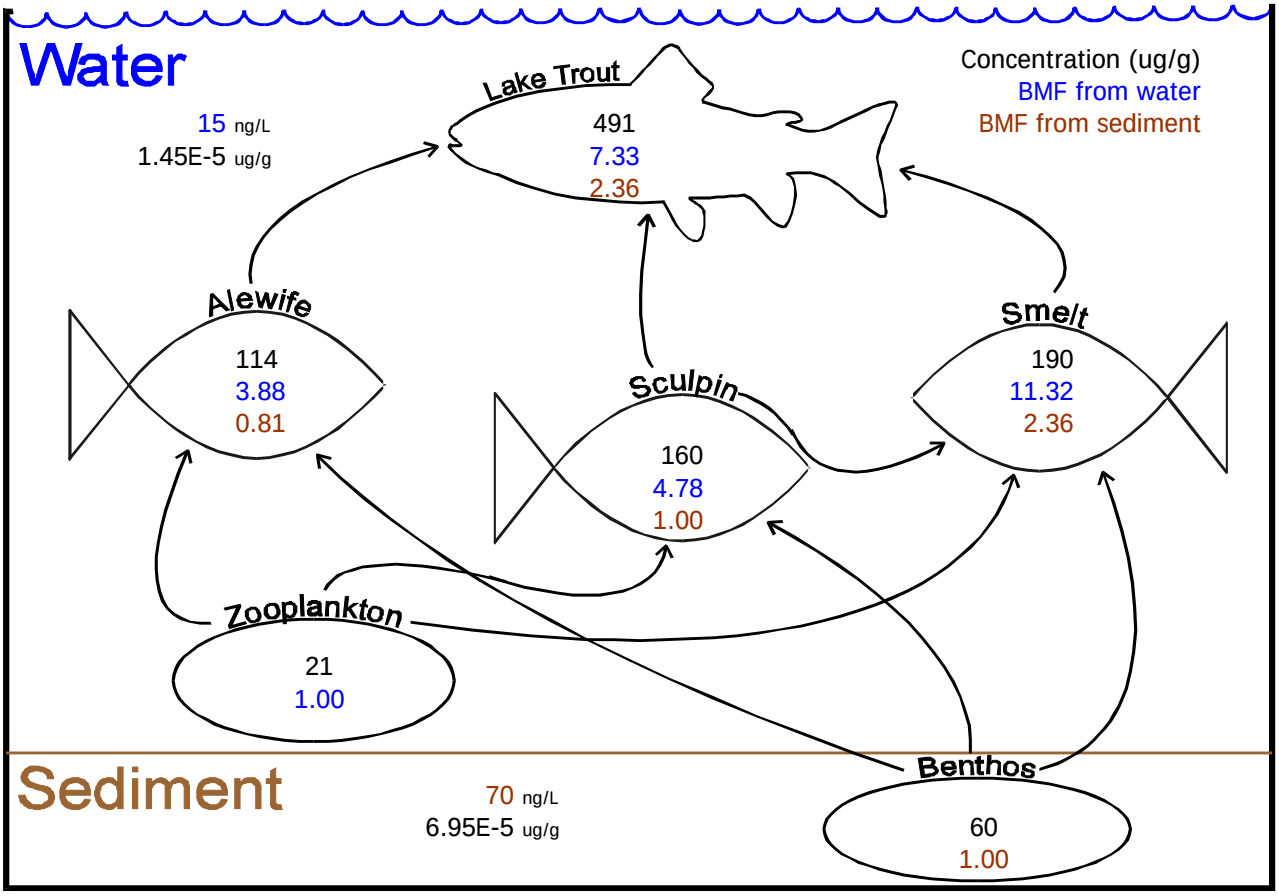
ChemSCORER Beta101 - Toxicity and Bioaccumulation
EPA Mirex

Toxicity Information

No mammalian toxicity data was supplied.

No aquatic toxicity data was supplied.

Evaluative Aquatic Foodweb



Overall Bioaccumulation Factor, Lake Trout / Water : 33808120

Notes on Terminology:

Bioconcentration (BCF) - Increase in contaminant concentration from water to fish.
Biomagnification (BMF) - Increase in contaminant concentration from food to fish.
Bioaccumulation (BAF) - Total contaminant concentration increase due to BCF and BMF.