Appendix D

SCREENING PROCESS FOR CHEMICALS

TABLE OF CONTENTS

D.1 Screening Procedure

For each chemical, the information listed in Table D.1 was assembled.

Environmental levels were taken from published and unpublished sources. These are identified in Tables D.2 and D.3.

Under the heading chemical properties, the octanol/water partition coefficient data (log K_{ow}) consist of both experimental and estimated values. The estimated data were calculated on the basis of chemical structure, via the fragment constant methods of Hansch and Leo[1]. The estimated log K_{ow} data were obtained from the University of Minnesota-Duluth's computer database, ISHOW (Information System for Hazardous Organics in Water) and from the EPA Duluth Research Laboratory (ERL-Duluth) computerized chemical property estimation system, UNICORN. In several instances when neither ISHOW nor UNICORN could produce an estimate of log K_{ow}, the partition coefficient was hand calculated using Hansch and Leo's method as presented by Lyman, et al.[2]. Experimentally derived log K_{ow} data were chosen in preference to estimated data. Such data were taken, when available, from the ISHOW database and from references identified in Tables D.2 and D.3.

The LC50 aquatic toxicity data are experimentally derived from the ISHOW database and from references identified in Tables D.2 and D.3. An attempt was made to fill the data gaps using the prototype UNICORN system to estimate LC50 values. However, after a review of the output, it was decided that the system had serious limitations in its ability to predict toxicity

---

1 Corwin Hansch and Albert Leo, Substituent Constants for Correlation Analysis in Chemistry and Biology, John Wiley and Sons, New York, 1979.

2 Warren J. Lyman, William F. Reehl, and David H. Rosenblatt, Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Co., New York, 1982. pp. 1-1 to 1-38.

TABLE D.1

INFORMATION BASE

Identification

Chemical name
CAS - Chemical Abstracts Service Registry Number (a widely recognized numerical identifier)

Environmental Levels

Biota - low and high ambient levels
Sediment - low and high ambient levels
Water - low and high ambient levels

Chemical and Toxicological Properties

LC50 - the lethal concentration of the particular chemical in water that will kill 50% of a test batch of fish within a certain period of exposure
LD50 - the lethal dose that will kill 50% of animals when administered orally
Log Kow - the logarithm of the partition coefficient. (The partition coefficient is the ratio of the concentration of the particular chemical in an organic solvent (octanol) to its concentration in water and represents the tendency for the chemical to concentrate and potentially bioaccumulate in an organism.)
BCF - bioconcentration factor: the ratio of the concentration of the particular chemical in fish to its concentration in water (represents the degree of accumulation of a chemical in fish)

Criteria

EPA (U.S. Environmental Protection Agency)
- Water Quality Documents, Federal Register, November 28, 1980
- National Interim Primary and Secondary Drinking Water Regulations, Federal Register, March 12, 1982 and November 29, 1979

DOE (Canada Department of Environment)
- Guidelines for Surface Water Quality, Vol. I, Inorganic Chemical Substances, 1979

MOE (Ontario Ministry of the Environment)
- Water Management Goals, Policies, Objectives and Implementation Procedures of the Ministry of the Environment, 1978

IJC (International Joint Commission)
- Great Lakes Water Quality Agreement, 1978

NHW (Canada Department of National Health and Welfare)
- Guidelines for Canadian Drinking Water, 1978

FDA (U.S. Food and Drug Administration)
- Action Levels for Poisonous or Deleterious Substances in Human and Animal Feed, 1981

NY (New York State)
- New York State Ambient Water Quality Regulatory and Guidance Criteria, August 3, 1983

TABLE D.2

REFERENCE CODES FOR CHEMICAL PROPERTIES, ENVIRONMENTAL LEVELS AND CRITERIA OF CHEMICALS

CHEMICAL	CHEMICAL PROPERTIES			ENVIRONMENTAL LEVELS						CRITERIA		LEGEND
	LogKow	LC50	BCF	AW-L	AW-H	AB-L	AB-H	AS-L	AS-H	AQC	BIC	
Acenaphthene	4*	1						33	33	1		LogKow: logarithm of partition coefficient (octanol/water)
Acenaphthylene	2							13	33			
Acetone	1	1			27							
Aldrin	4	1	4						28	7	5	LC50: lethal concentration that will kill 50% of a species within a specified period
1-Aminonaphthalene	3							22	22			
Aniline	2	1						22	22			
Anthracene	2	3							22			
Benzaldehyde	1	1		9	9		21		34			BCF: bioconcentration factor
Benz(a)anthracene	2	3	4		20				13	7		
Benzene	1	1	1	31	10			33	33	7		AW-L: ambient water level (min. value)
Benzene sulfonamide	1				34							
Benzo(b)fluoranthene	3				20			33	33	7		
Benzo(k)fluoranthene	3	3			20			7	7	7		AW-H: ambient water level (max. value)
Benzofluorene	3	3							20			
Benzoic acid	1	1										
Benzo(g.h.i.)perylene	3	3			20			7	33			AB-L: ambient biota level (min. value)
Benzo(a)pyrene	2	3	1		20			33	33	7		
Benzo(e)pyrene	3	3							7			
Benzo thiazole	1				34				34			AB-H: ambient biota level (max. value)
Benzyl alcohol	4	1							34			
Benzyl benzoate	3								34			
Benzylbutyl phthalate	2	1	1					33	33	1		AS-L: ambient sediment level (min. value)
N-Benzyl-N-ethylaniline	3							22	22			
Benzylidene-4,4'-bis(N,N-dimethylaniline)	3							22	22			
alpha-BHC	1	4		9	9	3	3			7	6	AS-H: ambient sediment level (max. value)
beta-BHC	1	4			27	9	9			7	6	
BHC	1	4							23	7	6	
Biphenyl	1	4	1						8		5	AQC: aquatic criteria
Bis(2-ethylhexyl) Phthalate	2	1	1		31			33	33	7		
Bromoform	4	1	4		16					7		BIC: biota criteria
Butanal	1	1			10							
Isobutanal	2	3										

NOTES: LD50 reference not shown; all LD50 data from the summary report by EPS. Sediment criteria references not shown; all are from Ontario MOE dredging guidelines.

* See Table D.3 for explanation of reference codes.

TABLE D.2 (Continued)

CHEMICAL	CHEMICAL PROPERTIES			ENVIRONMENTAL LEVELS						CRITERIA	
	LogKow	LC50	BCF	AW-L	AW-H	AB-L	AB-H	AS-L	AS-H	AQC	BIC
Butanol	1	1		9	9						
Isobutanol	4	1									
t-Butanol	2	1		9	9						
2-Butanone	1	1			27						
t-Butylphenol	3	3	3								
Carbon disulfide	1	1			25						
Carbon tetrachloride	4	1	1		27						
Chlordane	4	1	1		9		18	4	4	7	
Chloroanthracene	3	3	3								
Chlorobenzene	1	4	1		23			33	33	1	
Chlorodibromoethane	3	3	3		9						
Chlorodibromomethane	4	3			25			33	33	7	
Chloro(difluorochloromethyl)benzene	3	3	3								
Chloroform	1	1		31	17			33	33	7	
Chlorohydroxybenzophenone	3	3	3						8		
Chlorohydroxyphenothiazine	3		3								
Chloromethozybenzophenone	3	3	3								
Chloromethylbis(phenylmethyl)benzene	3	3	3						8		
Chloromethyldiphenylmethane	3	3	3						8		
Chloronaphthalene	4	3							8	1	
Chloronitrobenzene	3							30	30		
(Chlorophenyl)cyclohexene	3							30	30		
Chlorotoluene	1	1		2	2				23		
2-Chloro(trifluoromethyl)benzene	2	3					9				
3-Chloro(trifluoromethyl)benzene	2	3			27						
4-Chloro(trifluoromethyl)benzene	2	3					9				
Chrysene	3	3			20				22	7	
Corosene	3								7		
Cumene	1	1			9						
2,4-D	2	1	4		1					3	5
DCPA	2	1					21	33	33		
p,p-DDD	4	1	4	9	9		9	4	4	1	4
DDE	4	3	1	9	9		18	4	4	1	3
o,p-DDT	4	3						4	4	1	4
p,p-DDT	2	4	1					4	4	1	4
DDT	2	4	1	9	9	9	9			1	4
2,4-Decadienal	3						21				
Dibenz(a,h)anthracene	3				20			13	7		
Dibenzofuran	3	3							34		

TABLE D.2 (Continued)

CHEMICAL	CHEMICAL PROPERTIES			ENVIRONMENTAL LEVELS						CRITERIA	
	LogKow	LC50	BCF	AW-L	AW-H	AB-L	AB-H	AS-L	AS-H	AQC	BIC
Dibromomethane	2				27					1	
Di-n-butyl phthalate	4	1	1		34			33	13	1	
Di-t-butylquinone	5								34		
Dichloroanthracene	1	3									
1,2-Dichlorobenzene	1	1	4	1	1			33	33	1	
1,3-Dichlorobenzene	1	1	4		27			33	33	1	
1,4-Dichlorobenzene	1	1	4	1	1		26	33	33	1	
Dichlorobromoethane	3	3	3	9	9						
Dichlorobromomethane	2	3		31	17					7	
1,1-Dichloroethane	1	1						33	33	7	
1,2-Dichloroethane	1	1			15					7	
1,2-Dichloroethylene	2	1						33	33	1	
Dichloromethylbis(phenylmethyl)benzene	3		3						23		
Dichloromethyldiphenylmethane	3	3	3						23		
Dichloronapthalene	3	3	4						23	1	
Dichlorophenanthrene	3							30	30	1	
Dichlorophenol	1	1								1	
2,4-Dichloro-2-phenoxybutyric acid	2										
2,4-Dichloro-2-phenoxyethanol	3		3								
1,2-Dichloropropane	1	1						33	33	7	
Dichloropropane	2	1								7	
Dichloropropene	2	3								1	
Dichloroquinone	5							30	30		
2,6-Dichlorotoluene	2	/									
Dichlorotoluene	2	3		2	2				23		
Dichloro(trifluoromethyl)benzene	3	3	3								
2,3-Dichloro(trifluoromethyl)benzene	3	3	3				9				
2,4-Dichloro(trifluoromethyl)benzene	3						9				
3,4-Dichloro(trifluoromethyl)benzene	3	3					9				
Dichloro(trifluoromethyl)benzophenone	3	3			8						
Dicyclohexyl phthalate	2	3							34	3	
Dieldrin	2	1	3	9	9	9	9	4	4	3	5
Diethylbenzene	3	3	3		9						
Diethylcyclohexanone	3	3							34		
Diethyl disulfide	1	3									
Diethyl ether	1	1			27						
Diethyl phthalate	4	1						33	33	3	
Dimethyl adipate	1	3							34		
4-(Dimethylamino)benzophenone	3								29		
Dimethylaniline	2			9	9						

TABLE D.2 (Continued)

CHEMICAL	CHEMICAL PROPERTIES			ENVIRONMENTAL LEVELS						CRITERIA	
	LogKow	LC50	BCF	AW-L	AW-H	AB-L	AB-H	AS-L	AS-H	AQC	BIC
Dimethyl disulphide	1				27						
Dimethylheptadienone	3	3	3						34		
Dimethylphenanthrene	3	3	3						34		
Dimethyl phthalate	4	1							34	3	
N,N-Dimethyl-2-propenoamide	3				34						
Dinitroanisole	3								34		
Dioctyl phthalate	2	3	4		34				13		
Diphenylamine	2		1						34	3	
Diphenylcyclohexane	3	3	3						34		
Diphenyldifluoromethane	3	3									
1,2-Diphenylhydrazine	1	1						33	33	7	
Endosulfan	4	1	4	9	9	9	9	4	4	3	5
Endrin	4	1	1		9		9	4	4	3	5
Ethylbenzene	1	1			27			33	33	7	
3-Ethyl-4-menthylmaleic anhydride	5								34		
Ethyltoluene	3	3									
Fluoranthene	4	1			20			33	33	7	
Fluorene	1	3			27			33	33		
(2-Fluoroethyl)pentachlorobenzene	3							30	30		
Fluorotrichloromethane	1								12	7	
Furan	1	3									
Heptachlor	2	1	1				9		5	3	5
Heptachlor epoxide	2	3	1	9	9	9	9	4	4		3
Heptachlorodibenzofuran	3							30	30	3	
Heptachlorotoluene	3	3	3						23		
Hexachlorobenzene	2	1	3		9	9	9	4	33	7	
Hexachlorobutadiene	2	1	4	1	1		9		24	7	
Hexachlorodibenzofuran	3							30	30		
Hexachlorotoluene	3	3	3						23		
Hexanal	3	3			10						
Hexane	2	3			10						
Hexenone	3	3		9	9						
4-Hydroxybenzaldehyde	3						21				
Indeno(1,2,3-cd)pyrene	3								13		
Isophorone	2	1					21			1	
Lindane	1	1	1	2	2		9	4	4	3	6
Methoxychlor	1	1	1				21	33	33	7	
Methylanthracene	3	3						20			
2-Methylbutanoic acid	3						21				

TABLE D.2 (Continued)

CHEMICAL	CHEMICAL PROPERTIES			ENVIRONMENTAL LEVELS						CRITERIA	
	LogKow	LC50	BCF	AW-L	AW-H	AB-L	AB-H	AS-L	AS-H	AQC	BIC
Methylcoumarin	3	3						34			
Methyldibenzofuran	3	3						34			
Methylene-4,4'-bis(N,N-dimethylaniline)	3							22	22		
Methylene chloride	1	1			27			33	33	7	
Methylfluorene	3	3									
Methylfuran	3	3									
5-Methyl-3-hexen-2-one	3						21				
Methylnaphthalene	3			9	9		21		34		
o-Methyloxime-3-pentanone	3								34		
Methyl palmitate	2	3							34		
Methylpentene	3	4									
Methylphenanthrene	1	3							20		
Methyl pivalate	3	3	3						34		
Methylpyrene	3	3							34		
Mirex	2	1	1	9	9	9	9	4	4	3	3
Naphthalene	4	1	1		27			33	33	1	
N-Nitrosodiphenylamine	1	1						33	33	7	
3-Nonen-2-one	3						21				
Octachlorodibenzofuran	3							30	30		
Octachlorostyrene	3	3	1			9	9		24		
PCB-Aroclor 1242	4	4	4						19		
PCB-Aroclor 1254	4	4	4						28		
PCB-Aroclor 1260	4	4	4	31	31						
PCB	4	4	4			9	9				
Pentachloroanisole	2	3			9						
Pentachlorobenzene	1	1	1	9	9	9	9		23	1	
Pentachlorobiphenyl	2	1	1					33	8		
Pentachlorobiphenylene	3							30	30		
Pentachlorocarbazole	3							30	30		
Pentachlorodibenzofuran	3							30	30		
Pentachlorodifluoronaphthalene	3							30	30		
Pentachlorofluorene	3							30	30		
Pentachloromethylbis(phenylmethyl)benzene	3		3	9	9				23		
Pentachlorophenyl fluoromethyl ether	3							30	30		
Pentachlorophenol	1	1	1		9		9			7	
Pentachlorotoluene	3	3		9	9			8	8		
Pentane	4	4			27						
Perylene	2	3						7	7	1	
Phenanthrene	2	3	1		22				28		

TABLE D.2 (Continued)

CHEMICAL	CHEMICAL PROPERTIES			ENVIRONMENTAL LEVELS						CRITERIA	
	LogKow	LC50	BCF	AW-L	AW-H	AB-L	AB-H	AS-L	AS-H	AQC	BIC
Phenol	4	1			9				34	3	
Phenothiazine	3			9	9				8		
Phenylacetaldehyde	1						21				
Phenylacetic acid	1						21				
Phenylnapththalene	1	3							34		
Piperidinone	3						21				
Propanol	1	1			27						
Pyrene	4							33	33	1	
Silvex	2	1		1	1					1	
Styrene	1	1		9	9						
2,4,5-T	2	1		1	1						
TCDD	3	4	4		27	3	9				
1,2,3,4-Tetrachlorobenzene	4	4		1					4	1	
1,2,4,5-Tetrachlorobenzene	2	4		1					4	1	
Tetrachlorobenzene	4	4				9	9			1	
Tetrachlorobiphenyl	2	1	1					33	8	3	4
Tetrachlorocarbazole	3						30				
Tetrachlorodibenzofuran	3					30	30				
1,1,2,2-Tetrachloroethane	2	1			27			33	33	7	
Tetrachloroethene	4	1	1	1	1			33	33	1	
Tetrachloromethyl-bis-(phenylmethyl)benzene	3		3	9	9				23		
Tetrachlorophenanthrene	3							30	30		
2,3,4,6-Tetrachlorophenol	1	1					18				
Tetrachlorotoluene	1	3		9	9				23		
Tetrahydrofuran	1	1			27					7	
N,N,N',N'-Tetramethylbenzidine	3								29		
(Tetramethylbutyl)phenol	3	3		9	9						
Toluene	4	1	4	10	10			33	28	7	
Tribromomethane	1	1						33	33	1	
Trichloroanthracene	3	3	3	9	9						
1,2,4-Trichlorobenzene	2	4			1			33	33	1	
1.2.3-Trichlorobenzene	2	4			1			6	6	1	
1,3,5-Trichlorobenzene	2	4						6	6	1	
Trichlorobenzene	2	4					9			1	
Trichlorobiphenyl	2	4	4					33	8	3	
Trichlorodiphenylmethane	3	3		9	9						
1,1,1-Trichloroethane	4	1		31	9			33	33	7	
Trichloroethene	1	1		31	15					7	
Trichloromethyl-bis-(phenylmethyl)benzene	3		3	9	9				23		

TABLE D.2 (Continued)

CHEMICAL	CHEMICAL PROPERTIES			ENVIRONMENTAL LEVELS						CRITERIA	
	LogKow	LC50	BCF	AW-L	AW-H	AB-L	AB-H	AS-L	AS-H	AQC	BIC
Trichloronaphthalene	2	3	4						8	1	
Trichlorophenanthrene	3							30	30		
Trichlorophenol	2	1	1	9	9						
2,4,5-Trichlorophenol	2	1	1				9				
2,4,6-Trichlorophenol	1	1					9	5	5	1	
2.4.5-Trichlorotoluene	3	3		9	9						
Trichlorotoluene	3	3							23		
Trichlorotrifluoroethane	2	3									
(Trifluoromethyl)benzene	1	3		9	9						
Trimethylbenzene	3	3								7	
Trimethylbiphenyl	3						21				
Trimethylphenanthrene	3	3							34		
3A,6,6-Trimethyl-3A,4,5,6-tetrahydro-2-coumaranone	3	3							34		
o-Xylene	3	4		9	31					7	
m-Xylene	1	1						33	33	7	
2,4-Xylenol	2	1						33	33	1	
Zytron	1						21	33	33		
Aluminum		4		9	9			4	4	7	
Antimony		6		17	17				28	7	
Arsenic	4	4		9	9		9		9	7	5
Barium		6		17	17				12	1	
Beryllium		6		17	31				28	7	
Cadmium	4	4	4	9	9		26		28	1	
Chromium		4	4	9	9	9	9		13	1	
Copper		4		17	31		26	4	4	2	5
Cyanide		4			9			4	4	1	
Lead		4	4	17	31		26	4	4	1	5
Manganese		4	4					4	4	1	
Mercury		4	4		17				13	1	3
Nickel		4	4	9	31		26	4	4	7	
Selenium		4	4		17				28	7	
Silver		6		27	31				28	7	
Thallium		6							13	7	
Zinc		4	4	31	31		26	4	4	3	

TABLE D.3

KEY TO REFERENCE CODES

REFERENCE #	SOURCE
Chemical Properties	
1	ISHOW computer database, an experimental value
2	ISHOW computer database, an estimated value
3	UNICORN computer modelling system, an estimated value
4	Summary report data
5	Hand-calculated estimate via methods in Handbook of Chemical Property Estimation Methods
6	EPA Water Quality Criteria Documents
Environmental Levels	
1	"Comparison of Niagara River Water Quality with Health Department Drinking Water Standards"; Niagara River Drinking Water Work Group
2	"Niagara River - Raw Water Quality Data - Organics"; Niagara River Drinking Water Work Group
3	"Niagara River Edible Portion Fish Analyses"; Ontario MOE
4	"NYDEC Statistical Analysis System - EPA GLNPO Sediment Data"
5	"NYDEC Statistical Analysis System - Environment Canada Sediment Data"
6	"NYDEC Statistical Analysis System - Ontario MOE Sediment Data"
7	"PNA Sediment Concentrations From Four Niagara River Sites"; NYDEC

TABLE D.3 (Continued)

REFERENCE #	SOURCE
8	"Organic Compounds Found Near Dump Sites in Niagara Falls, New York"; EST 15(10), 1981, Hites, Roland et al.
9	Summary Report data
10	"Niagara River Water Quality Update"; Ontario MOE, 6/23/82
11	"Priority Pollutant Loadings to the Niagara River from Lake Erie and the Buffalo River"; NYDEC Bureau of Water Research, 5/82-4/83
12	"Niagara Frontier Sampling Results"; attached to memo - Randy Braun to Roland Hemmett, 3/29/83
13	"Lake Erie Survey"; Randy Braun, 6/29-30/82
14	"Analysis of Water for Total TCDD"; Environment Canada, transmittal - Dave Pascoe to Peter Crabtree, 6/13/83
15	"Data Collected on Sub-project II-9, Water Quality Surveillance Network Sampling"; attached to memo of Dr. Collin to NRTC, 12/2/82
16	"Analysis of Water Samples Submitted to EMSL by the Office of Health Research for Purgeable Organic Compounds"; attached to memo - Thomas Bellar (Physical and Chemical Methods Branch) to Dwight Ballinger (Environmental Monitoring and Support Laboratory - Cincinnati), 1/17/80
17	"Environmental Monitoring at Love Canal"; EPA 600/4-82-030a, May 1982
18	"Organochlorine Contaminant Monitoring of Fish in Lake Erie and the Niagara River Basin"; Edward Kuzia, NYDEC, June 1982
19	"Contaminants in the Bottom Sediments of the Niagara River - May 1981"; K.W. Kuntz, Water Quality Branch, Ontario Region
20	"Investigation of Polycyclic Aromatic Hydrocarbon Dischargers to Water in the Vicinity of Buffalo, NY"; Edward Kuzia, 4/83

TABLE D.3 (Continued)

REFERENCE #	SOURCE
21	"1981 Buffalo Area Fish Contaminant Study - Composite Sample of Two Whole Fish"; attached memo - Dave DeVault to Tony Kizlauskas, Great Lakes National Program Office 6/30/83
22	"Niagara River Toxics Committee/Times Beach Disposal Area"; attached to letter, Robert Hardimen, Army Corps of Engineers, to Dr. Collin, NYDEC
23	"Quarterly Report - Niagara River Sediment Data - 7/82 to 9/82"; attached to communication - Roland Hites to Ann Alford - Stevens, Indiana University
24	"History of Lake Ontario Contamination from the Niagara River by Sediment Radioidating and Chlorinated Hydrocarbon Analysis"; Jrl. of Great Lakes Research, 9(2), 1983, Durham, R.W., and Oliver, G.G.
25	"Volatile Hydrocarbon Contaminants in the Niagara River and Lake Ontario"; Jrl. of Great Lakes Research 9(2), 1983, Kaiser, K.L. et al.
26	"DOE Data Summary-Spottail Shiners"; K.W. Kuntz, Environment Canada, 1982
27	"Niagara River Toxics Committee Report, Chapter II, Ambient Measurements"; P.B. Kauss, 8/8/83
28	"Analytical Data From Scajaquada Creek and Two Mile Creek"; RECRA Environmental Laboratories, 1982-1983
29	"Aromatic Amines in and Near the Buffalo River"; Ronald Hites and Charles R. Nelson, EST 14(9), 1980, P. 1147
30	"Buffalo River Fish and Sediment Analysis"; memo, Douglas Kuehl to Vacys Saulys, 12/8/82
31	"Report on 1982 Data from Sub-Project II-9 Water Quality Surveillance Network Sampling"; transmitted by Robert Collin, 9/14/83
32*	"New Niagara River Chemicals"; memo of 10/12/82, R. Collin to V. Saulys

TABLE D.3 (Continued)

REFERENCE #	SOURCE
33	"1981 EPA Buffalo Area Sediment Survey"; (GLNPO)
34	Kauss, P., Compounds Identified in Niagara River Water and Sediment Samples by GC/MS, (8/25-9/5)
35*	Collin, R., Toxic Chemical Found in the Niagara River
Criteria Values	
1	Environmental Protection Agency, Water Quality Documents, Federal Register, November 28, 1980 Environmental Protection Agency, National Interim Primary and Secondary Drinking Water Regulations, Federal Register, March 12, 1982 and November 29, 1979
2	Environment Canada, Guidelines For Surface Water Quality Vol. 1 Inorganic Chemical Substances, Inland Waters Directorate, Water Quality Branch, Ottawa, 1979
3	Ontario Ministry of the Environment, Water Management Goals, Policies, Objectives and Implementation Procedures of the Ministry of the Environment, 1978
4	International Joint Commission, Great Lakes Water Quality Agreement of 1978, Canada and United States, 1978
5	Canadian Department of National Health and Welfare, Guidelines for Canadian Drinking Water Quality, 1978
6	Food and Drug Administration, Action Levels for Poisonous or Deletrious Substances in Human and Animal Feed, 1981
7	New York State Department of Environmental Conservation, New York State Ambient Water Quality Regulatory and Guidance Criteria, August 3, 1983

*References to qualitatively identified compounds.

for a number of chemical structures. Furthermore, estimates were not applicable to compounds having high log K_{ow} values (>5.3). Therefore, LC50 estimates obtained in this manner were deleted from the data base.

The LD50 toxicity data (oral-rat) were obtained from references included in the Tables D.2 and D.3. Experimentally derived bioconcentration factor data (BCF) were taken from the ISHOW computerized database and from references included in the Tables D.2 and D.3. BCF data were also estimated via the UNICORN system, when no experimental data were available.

The aquatic criteria (Table D.4) consist of concentrations of pollutants which, when exceeded, are considered to pose a threat to aquatic life and drinking water. Similarly, criteria for biota (Table D.5) are based on protection of human health from pollutants ingested through fish consumption. Sediment criteria (Table D.6) were based on Ontario MOE dredging guidelines, since these proved to be the most sensitive of those available for this medium. For each environmental medium (water, sediment, biota), the most stringent criterion for each chemical was selected as the trigger point for the sorting exercise.

The information summarized in Table 6.1 was entered into a computerized data base from which it is possible to extract specific information on environmental levels and characteristics for each chemical.

A screening process was developed to sort the 261 chemicals into three major groups and is depicted in Figure D.1. These groups were given the following definitions:

Group I - chemicals requiring immediate attention (They are found at levels greater than or equal to environmental or human health criteria or are considered to pose a human health or environmental risk based on the screening mechanism.).

TABLE D.4

AQUATIC CRITERIA (mg/L)

COMPOUND	EPA-DW	EPA-AQ	DOE	MOE	IJC	NY	KEY TO CRITERIA
Acenaphthene		1.70E+00					
Aldrin		3.00E-03		1.00E-06*	1.00E-03	1.00E-06	AQ: Aquatic criteria
Benz(A)anthracene						2.00E-04	DW: Drinking water standard
Benzene		5.30E+00				1.50E-03	EPA: Environmental Protection Agency
Benzo(B)fluoranthene						2.00E-04	ambient water quality criteria
Benzo(k)fluoranthene						2.00E-04	
Benzo(A)pyrene						2.00E-04	
Benzylbutyl phthalate		3.00E-03				5.00E-02	DOE: Environment Canada criteria
BHC-(α)		1.00E-01				1.00E-05	
BHC-(β)		1.00E-01				1.00E-05	MOE: Ministry of the Environment criteria
BHC		1.00E-01				1.00E-05	
Bis(2-ethylhexyl) phthalate		3.00E-03				6.00E-04	IJC: International Joint Commission
Bromoform	1.00E-01	1.10E+01				5.00E-02	NY: New York State Dept. of Environmental Conservation criteria
Carbon tetrachloride		3.52E+01				3.00E-04	
Chlordane		4.30E-06		6.00E-05	6.00E-05	4.00E-06	
Chlorobenzene		5.00E-02				5.00E-02	NOTE: The most stringent criteria for each reference source are listed. The most stringent criterion out of all reference sources is underlined for each chemical. Multiple underlinings indicate a tie for the most stringent criterion.
Chlorodibromomethane	1.00E-01	1.10E+01				2.00E-04	
Chloroform	1.00E-01	1.24E+00					
Chloronaphthalene		1.60E+00				2.00E-04	
Chrysene						1.00E-01	
2,4-D	1.00E-01			4.00E-03			
DDD-(p,p')**		1.00E-06		3.00E-06	3.00E-06	1.00E-06	
DDE**		1.00E-06		3.00E-06	3.00E-06	1.00E-06	
DDT-(o,p)**		1.00E-06		3.00E-06		1.00E-06	
DDT-(p,p')**		1.00E-06		3.00E-06	3.00E-06	1.00E-06	
DDT**		1.00E-06		3.00E-06	3.00E-06	1.00E-06	
Dibromomethane		1.10E+01					
Di-n-butyl phthalate		3.00E-03		4.00E	4.00E-03	4.00E-03	Numerical values for the criteria are expressed using "E" notation. This notation is equivalent to using power of 10; e.g., 3.00 E-03 = 3 x 10^{-3}, and 3.52 E+01 = 3.52 x 10 = 35.2).
1,2-Dichlorobenzene		7.63E-01					
1,3-Dichlorobenzene		7.63E-01					
1,4-Dichlorobenzene		7.63E-01					
Dichlorobromomethane	1.00E-01	1.10E+01				5.00E-02	
1,1-Dichloroethane						5.00E-02	
1,2-Dichloroethane		2.00E+01				1.00E-03	

* MOE and IJC criterion for Aldrin includes Dieldrin.

** Actual criterion is for sum total of DDT and its metabolites.

TABLE D.4 (Continued)

COMPOUND	EPA-DW	EPA-AQ	DOE	MOE	IJC	NY
1,2-Dichloroethylene		1.16E+01				
Dichloronaphthalene		1.60E+00				
Dichlorophenol		7.00E-02				
1,2-Dichloropropane		5.70E+00				5.00E-02
Dichloropropane		5.70E-00				5.00E-02
Dichloropropene		2.44E-01				
Dicyclohexyl phthalate		3.00E-03		0.20E-03		
Dieldrin		1.90E-06		1.00E-06*	1.00E-06	
Diethyl phthalate		3.00E-03		0.20E-03	0.20E-03	5.00E-02
Dimethyl phthalate		3.00E-03		0.20E-03	0.20E-03	5.00E-02
Dioctyl phthalate		3.00E-03		0.20E-03		5.00E-02
1,2-Diphenylhydrazine		2.70E-01				1.00E-05
Endosulfan		5.60E-05		3.00E-06		3.00E-06
Endrin	2.00E-03	2.30E-06		2.00E-06	2.00E-06	2.00E-06
Ethylbenzene		3.20E+01				5.00E-02
Fluoranthene		3.98E+00				2.00E-04
Fluorotrichloromethane		1.10E+01				5.00E-02
Heptachlor		3.80E-06		1.00E-06**	1.00E-06	1.00E-06
Heptachlor epoxide		3.80E-06		1.00E-06**	1.00E-06	1.00E-06
Hexachlorobenzene		5.00E-02				4.00E-05
Hexachlorobutadiene		9.30E-03				4.00E-04
Isophorone		1.17E+02				
Lindane	4.00E-03	8.00E-05		1.00E-05	1.00E-05	1.00E-05
Methoxychlor	1.00E-01					3.00E-05
Methylene chloride	1.00E-01	1.00E+01				1.00E-02
Mirex				1.00E-06	1.00E-06	
Naphthalene		6.20E-01				
N-Nitrosodiphenylamine		5.85E+00				1.40E-02
PCB-Aroclor 1242***		1.40E-05		1.00E-06		1.00E-06
PCB-Aroclor 1254***		1.40E-05		1.00E-06		1.00E-06
PCB-Aroclor 1260***		1.40E-05		1.00E-06		1.00E-06
PCB***		1.40E-05		1.00E-06		1.00E-06
Pentachlorobenzene		5.00E-02				
Pentachlorobiphynyl***		1.40E-05		1.00E-06		
Pentachlorophenol		3.20E-03		1.00E-03		4.00E-04
Phenol		1.56E+00		1.00E-03		5.00E-03
Pyrene						2.00E-04
Silvex	1.00E-02					1.00E-02
2,3,7,8,-TCDD						1.00E-09

* MOE and IJC criterion for Aldrin includes Dieldrin.
** Actual MOE and IJC criterion is for sum of Heptachlor and Heptachlor epoxide.
*** Actual criterion is for total Polychlorinated Biphenyl.

TABLE D.4 (Continued)

COMPOUND	EPA-DW	EPA-AQ	DOE	MOE	IJC	NY
1,2,3,4-Tetrachloro-benzene		5.00E-02				
1,2,4,5-Tetrachloro-benzene		5.00E-02				
Tetrachlorobiphenyl**		1.40E-05		1.00E-06		
1,1,2,2-Tetrachlorethane		2.40E+00				3.00E-04
Tetrachloroethene		8.40E-01				2.00E-03
Tetrahydrofuran						5.00E-02
Toluene		1.75E+01				1.00E-02
Tribromomethane	1.00E-01	1.10E+01				
1,2,4-Trichlorobenzene		5.00E-02				
1,2,3-Trichlorobenzene		5.00E-02				
1,3,5-Trichlorobenzene		5.00E-02				
Trichlorobenzene		5.00E-02				
Trichlorobiphenyl*		1.40E-05		1.00E-06		
1,1,1-Trichloroethane		1.80E+01				5.00E-02
Trichloroethene		2.19E+01				5.00E-03
Trichloronaphthalene		1.60E+00				
2,4,6-Trichlorophenol		9.70E-01				
Trichlorophenol		9.70E-01				
Trimethylbenzene						5.00E-02
Xylene-(m)						5.00E-02
Xylene-(o)						5.00E-02
2,4-Xylenol		2.12E+00				
Antimony		1.60E+00				5.00E-02
Arsenic	5.00E-02	4.00E-02	5.00E-02	5.00E-02		1.00E-02
Barium	1.10E+00					1.00E+00
Beryllium		5.30E-03		1.10E-02		1.10E-03
Cadmium	1.00E-02	1.20E-05	2.00E-04	2.00E-04	2.00E-04	3.00E-01
Chromium	5.00E-02	2.90E-04	4.00E-02	1.00E-01	1.00E-01	5.00E-02
Copper	1.00E+00	5.60E-03	2.00E-03	5.00E-03		2.00E-01
Cyanide		3.50E-03		5.00E-02		1.00E-01
Lead	5.00E-02	7.50E-04	5.00E-03			9.90E-03
Manganese	5.00E-02					3.00E-01
Mercury	2.00E-03	2.00E-04	2.00E-04	5.00E-04		2.00E-04
Nickel		5.60E-02		2.50E-02	2.50E-02	1.50E-02
Selenium	1.00E-02	3.50E-02	1.00E-02	1.00E-02		1.00E-03
Silver	5.00E-02	1.20E-04				1.00E-04
Thallium		2.00E-02				2.00E-02
Zinc	5.00E+00	4.70E-02	5.00E-02	3.00E-02	3.00E-02	3.00E-01

* Actual criterion is for sum total of DDT and its metabolites.
** Actual criterion is for total Polychlorinated Biphenyl.

TABLE D.5

BIOTA CRITERIA (mg/kg)

COMPOUND	MOE	IJC	CDNHW	FDA	KEY TO CRITERIA
Aldrin	0.30E+00	0.30E+00	1.00E-01	0.30E+00	CDNHW: Canadian Dept. of National Health & Welfare criteria
Biphenyl			1.10E+02		
Chlordane				0.30E+00	FDA: FDA criteria
DDD-(p,p')*	1.00E+00	1.00E+00	5.00E+00	5.00E+00	IJC: International Joint Commission
DDE*	1.00E+00	1.00E+00	5.00E+00	5.00E+00	MOE: Ministry of the Environment criteria
DDT-(o,p)*	1.00E+00	1.00E+00	5.00E+00	5.00E+00	
DDT-(p,p')*	1.00E+00	1.00E+00	5.00E+00	5.00E+00	
2,4-D			2.05E+02		
Dieldrin	0.30E+00	0.30E+00	0.10E+00	0.30E+00	NOTE: The most stringent criteria for each reference source are listed. The most stringent criterion out of all reference sources is underlined for each chemical. Multiple underlinings indicate a tie for the most stringent criterion.
Diphenylamine			1.00E+01		
Endosulfan			1.00E-01		
Endrin	0.30E+00	0.30E+00	2.00E-02	0.30E+00	
Heptachlor	0.30E+00	0.30E+00	1.00E-01	0.30E+00	
Heptachlor epoxide	3.00E-01	3.00E-01		3.00E-01	
Lindane	0.30E+00	0.30E+00	0.20E+00		
Mirex	1.00E-01		1.00E-01	1.00E-01	
PCB-Aroclor 1242**	2.00E+00	1.00E-01		5.00E+00	
PCB-Aroclor 1254**	2.00E+00	1.00E-01		5.00E+00	Numerical values for the criteria are expressed using "E" notation. This notation is equivalent to using power of 10; e.g., 3.00 E-03 = 3 x 10^{-3}, and 3.52 E+01 = 3.52 x 10 = 35.2).
PCB-Aroclor 1260**	2.00E+00	1.00E-01		5.00E+00	
Pentachlorobiphenyl**	2.00E+00	1.00E-01		5.00E+00	
Tetrachlorobiphenyl**	2.00E+00	1.00E-01		5.00E+00	
2,3,7,8,-TCDD	2.00E-05		2.00E-05		
Arsenic			1.00E-01		
Copper			5.00E+01		
Lead			5.00E-01		
Mercury	5.00E-01	5.00E-01	5.00E-01	1.00E+00	

* Actual criterion is for sum total of DDT and its metabolites.
** Actual criterion is for total Polychlorinated Biphenyl.

TABLE D.6

SEDIMENT CRITERIA
(mg/kg)

COMPOUND	MOE
PCB-Aroclor 1242*	5.00E-02
PCB-Aroclor 1254*	5.00E-02
PCB-Aroclor 1260*	5.00E-02
Pentachlorobiphenyl*	5.00E-02
Tetrachlorobiphenyl*	5.00E-02
Trichlorobiphenyl*	5.00E-02
Arsenic	8.00E+00
Cadmium	1.00E+00
Chromium	2.50E+01
Copper	2.50E+01
Cyanide	1.00E-01
Lead	5.00E+01
Mercury	3.00E-01
Nickel	2.50E+01
Silver	5.00E-01
Zinc	1.00E+02

* Actual criterion is for total Polychlorinated Biphenyls.

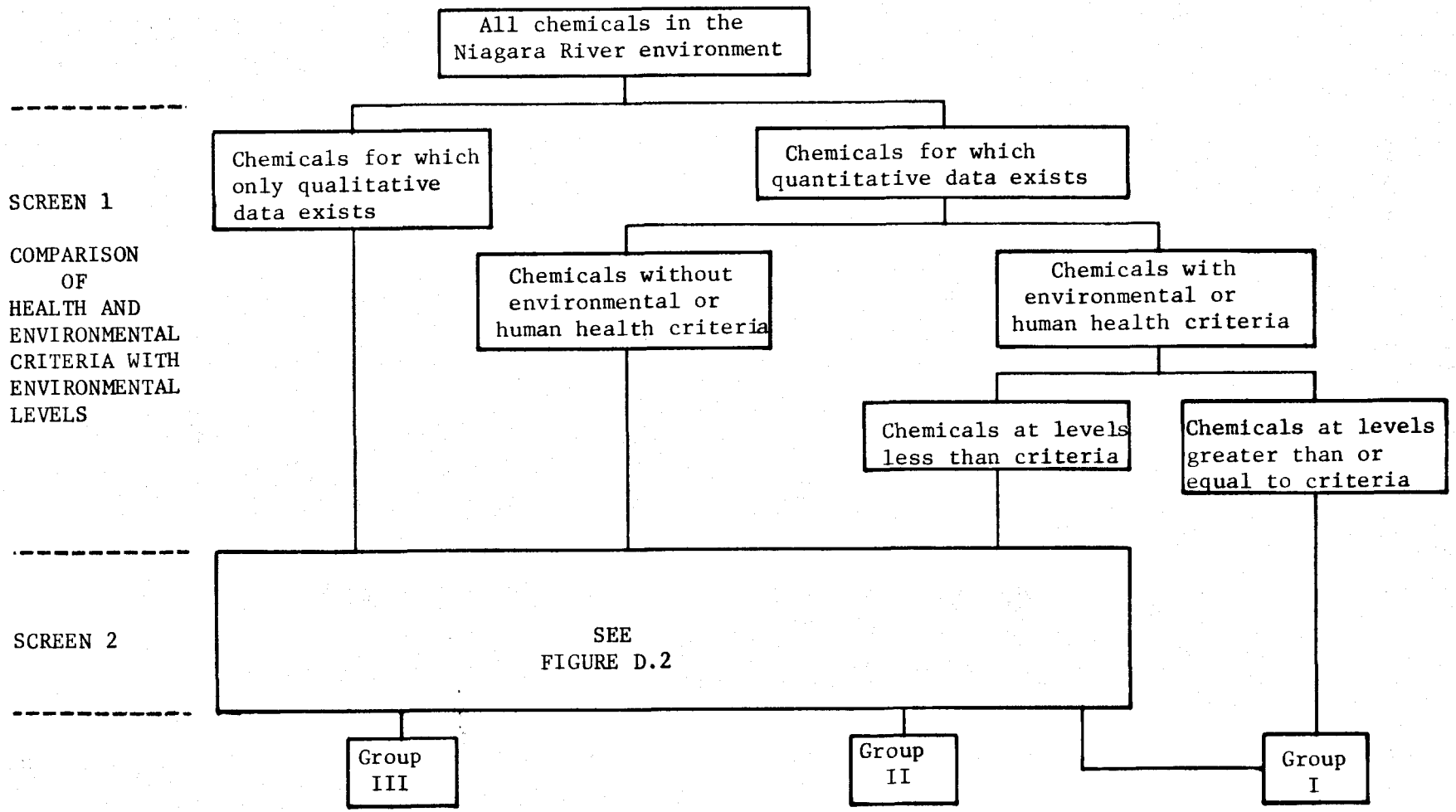


FIGURE D.1 SCREENING PROCESS FOR EVALUATING CHEMICALS (GENERAL)

Group II - chemicals requiring continuing and in some cases new efforts in the area of environmental measurement, characteristics and inventory (They do not demand immediate regulatory action but do require additional attention to clarify their environmental significance.).

Group III - chemicals which should require minimal attention (They are considered to pose neither health nor environmental risks based on the screening mechanism.).

Figure D.1 can be split into two distinct screens. The first screen involves separating the chemicals into two groups: chemicals for which quantitative data exist for one or more of the environmental media (biota, sediment, water), and chemicals for which only qualitative information is available, indicating that the chemical is present in the environment at a low, undefined level in a particular medium. Chemicals measured only qualitatively were routed to the second screen. Chemicals measured quantitatively had their environmental levels compared to agency criteria.

Chemicals that were found in the environment at levels less than criteria, and chemicals for which criteria do not exist, were routed to the second screen. Chemicals with environmental levels greater than or equal to criteria were immediately assigned to Group I (chemicals requiring immediate attention).

The second screen in the process (Figure D.2) involved the use of the 1982 Annual Report of the Committee on the Assessment of Human Health Effects of Great Lakes Water Quality (Health Effects Committee or HEC). That report used as its base the chemicals found in the Great Lakes ecosystem. Each chemical was reviewed based on toxicity and exposure and categorized in Tables 7.1-7.5 of the 1982 report. Table D.7 presents the classifications for each of the HEC tables. Also involved in the screen is a modified version of the Michigan Critical Materials Register scoring methodology. That system uses a hazard assessment methodology which considers acute

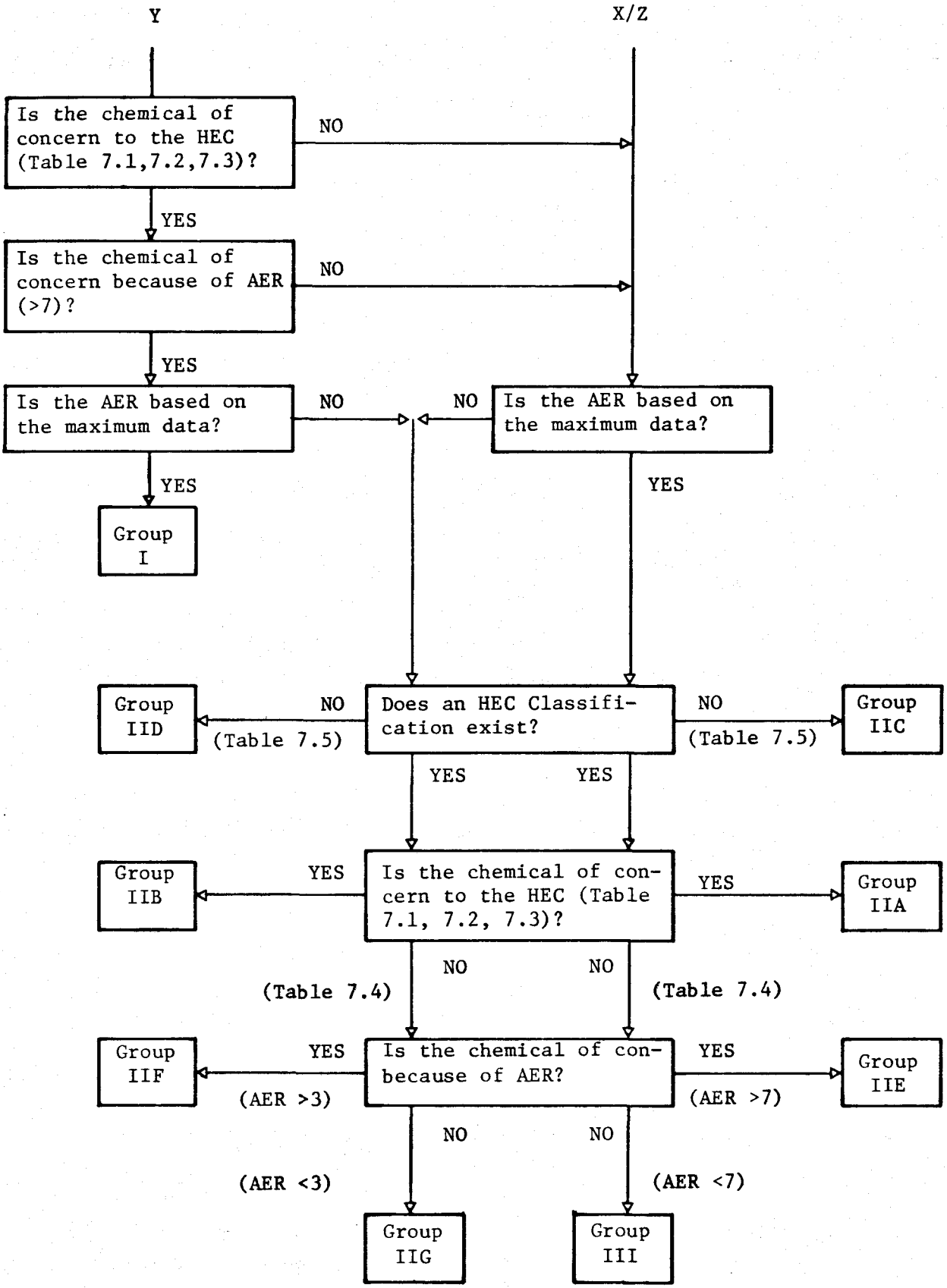


FIGURE D.2 SCREENING PROCESS FOR EVALUATING CHEMICALS (SCREEN 2)

TABLE D.7

IJC HEC CLASSIFICATIONS OF GREAT LAKES CONTAMINANTS

HEC TABLE NUMBERS	TABLE TITLES
7.1	Chemicals Found in the Great Lakes Which May Impact on Human Health in the Event of High Local Contamination
7.2	Chemicals Found in the Great Lakes With Known Effects in Mammals That Are Currently Subjected to Regulatory Monitoring
7.3	Chemicals Found in the Great Lakes With the Potential to Impact on Health That Are Not Currently Subject to Regulatory Monitoring But for Which Surveillance Should be Considered.
7.4	Chemicals Found in the Great Lakes of Minimal Current Concern From a Human Health Perspective
7.5	Chemicals Found in the Great Lakes for Which There Are Insufficient Data Available to Conduct a Health Hazard Assessment

toxicity, carcinogenicity, mutagenicity, terato-genicity, persistence, bioaccumulation and other adverse effects (including subacute and chronic toxicity, feto or embryotoxicity, phytotoxicity, and aesthetics). Chemicals are numerically scored as to their hazard and can then be ranked in order of concern. The modification was necessitated because of the lack of data for the majority of chemicals in the NRTC inventory. The classification criteria used were limited to bioaccumulation and acute aquatic and mammalian toxicity. The numerical score was calculated using two data elements: bioaccumulation and acute toxicity, derived from the Michigan Critical Materials Register. If the bioaccumulation score was unavailable, the Log K_{ow} score as found in ISHOW was substituted. Acute toxicity scores were derived by using the LD50 or LC50 values. Where both LD50 and LC50 values were available, the more limiting value was used to calculate the score. The final score, which can range from 0 to 14 (increasing with increasing environmental significance), was derived by adding the individual bioaccumulation (or Log K_{ow}) and acute toxicity (LC50 or LD50) scores. The

score derived has been referred to as an "acute effects ranking" (AER). The scoring does not take account of chronic toxicity, carcinogenicity, teratogencity, persistence, or mutagenicity and thus is highly limited in this respect.

In some cases insufficient information was available; and, therefore, the AER score was based solely on bioaccumulation or acute toxicity (ie., one of these pieces of information could not be obtained). AER scores as given in the tables of this report are followed by a number (either 1 or 2) in parentheses to indicate whether only one or both data elements are used. For example, a score of 7(2) indicates that the AER is 7 and that both data elements (bioaccumulation and acute toxicity) are available. A score of 7(1) indicates that one of the data elements is not available and the score is that much less reliable.

The HEC categorization and the AER score were used jointly to make a final assignment of each chemical entering the second screen in Figure D.1 into Group I, II or III.

Figure D.2 should be referred to for ease in clarifying the actual screen 2 process. Screen 2 is entered through one of three points (X, Y, or Z) in Figure D.1. These corresponding points are marked at the top of Figure 2. Chemicals entering screen 2 at point Y (chemicals found quantitatively but without environmental and human health criteria) were checked first against the HEC classification. Those of concern to the HEC with an AER greater than or equal to 7, based on both data elements, were considered to be of sufficient concern to warrant inclusion in Group I. Chemicals not of concern to the HEC, or with an AER score of less than 7 or with only one AER data element were directed to Groups II or III. Chemicals entering Screen 2 from points X or Z also were directed to Groups II or III.

The majority of chemicals in the NRTC inventory, because of the lack of characteristics data, fall into Group II. For that reason it was thought necessary to subdivide Group II into more manageable groups based on HEC

classifications and AER scores. Figure D.2 shows the subdivision into Groups IIA-G. Chemicals were assigned to each of these groups based on the following:

Group IIA - Chemicals in this group have been reviewed by the HEC and have been found to be of concern (ie., Table 7.1, 7.2 or 7.3). Their AER scores were calculated using both data elements.

Group IIB - This group is similar to Group IIA except that the AER score was calculated based on only one data element.

Group IIC - This group includes chemicals for which an AER score has been calculated based on both data elements but for which no HEC classification exists, either because data were lacking (ie., Table 7.5) or because the chemical was not considered by the HEC.

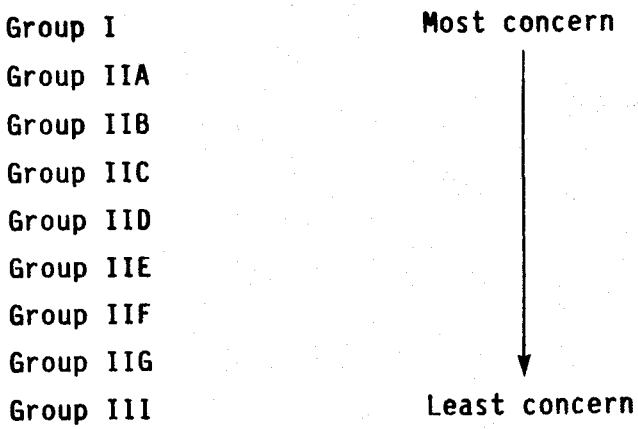
Group IID - This group is similar to Group IIC except that the AER score was calculated based on only one data element.

Group IIE - This group contains chemicals reviewed by the HEC and found to be of no concern (ie., Table 7.4). The AER score, which is greater than or equal to 7, indicates a potential problem based on both data elements.

Group IIF - Group IIF chemicals were also considered to be of no concern to the HEC (Table 7.4). Their AER scores were based on only one data element and for that reason a score greater than or equal to 3 was designated to be sufficient for inclusion in this group.

Group IIG - Based on the HEC classification of no concern and an AER score of less than 3 these chemicals are not considered to warrant much attention. Their AER scores were based on only one data element.

To show the relative significance among the groups they are ranked below in order of decreasing concern:



It can be seen that each chemical was assigned to one of the nine groups based on several factors: its environmental level, its environmental or human health criteria, and consideration of its HEC classification and AER score.