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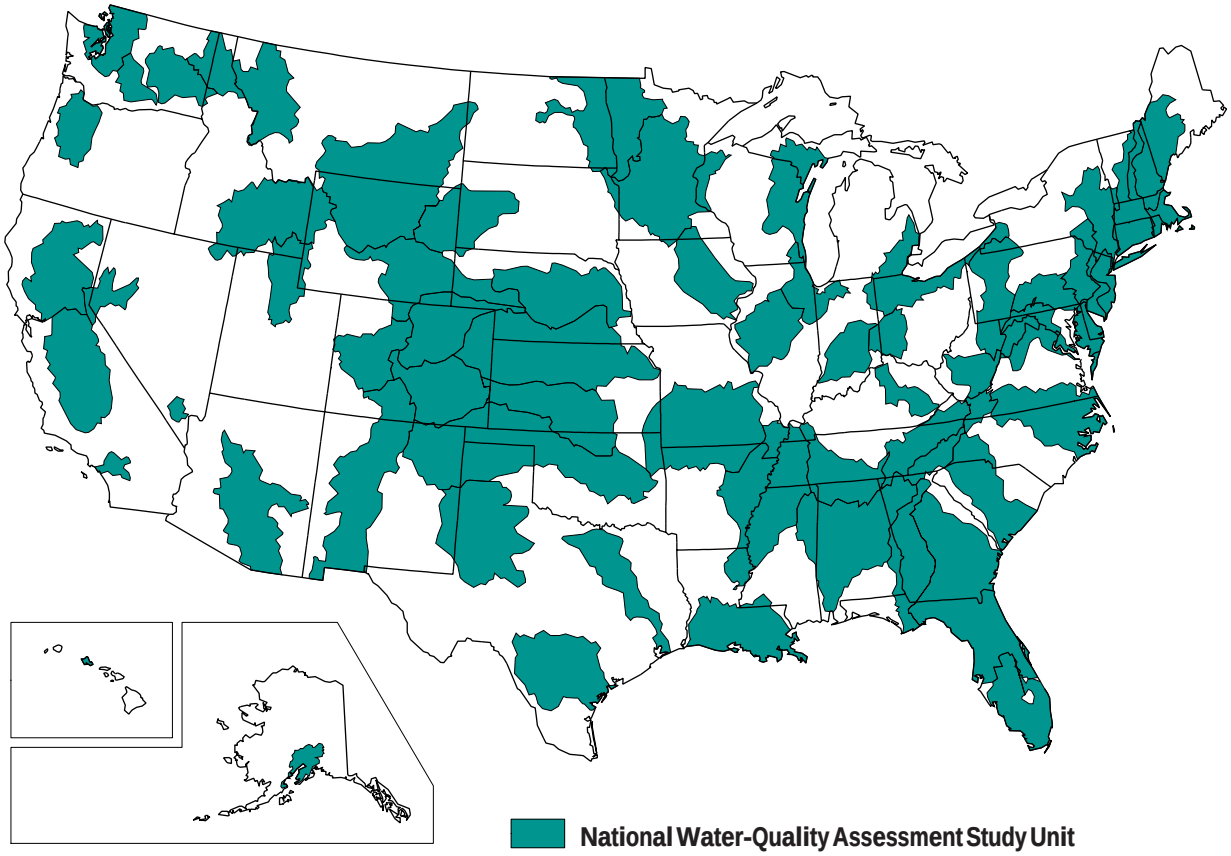
NATIONAL WATER-QUALITY ASSESSMENT PROGRAM

Selection Procedure and Salient Information for Volatile Organic Compounds Emphasized in the National Water-Quality Assessment Program

Open-File Report 99-182



U.S. Department of the Interior
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By David A. Bender, John S. Zogorski, Michael J. Halde, and Barbara L. Rowe

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U.S. Department of the Interior

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Rapid City, South Dakota: 1999

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FOREWORD

The mission of the U.S. Geological Survey (USGS) is to assess the quantity and quality of the earth resources of the Nation and to provide information that will assist resource managers and policymakers at Federal, State, and local levels in making sound decisions. Assessment of water-quality conditions and trends is an important part of this overall mission.

One of the greatest challenges faced by water-resources scientists is acquiring reliable information that will guide the use and protection of the Nation's water resources. That challenge is being addressed by Federal, State, interstate, and local water-resource agencies and by many academic institutions. These organizations are collecting water-quality data for a host of purposes that include: compliance with permits and water-supply standards; development of remediation plans for a specific contamination problem; operational decisions on industrial, wastewater, or water-supply facilities; and research on factors that affect water quality. An additional need for water-quality information is to provide a basis on which regional and national-level policy decisions can be based. Wise decisions must be based on sound information. As a society we need to know whether certain types of water-quality problems are isolated or ubiquitous, whether there are significant differences in conditions among regions, whether the conditions are changing over time, and why these conditions change from place to place and over time. The information can be used to help determine the efficacy of existing water-quality policies and to help analysts determine the need for and likely consequences of new policies.

To address these needs, the Congress appropriated funds in 1986 for the USGS to begin a pilot program in seven project areas to develop and refine the National Water-Quality Assessment (NAWQA) Program. In 1991, the USGS began full implementation of the program. The NAWQA Program builds upon an existing base of water-quality studies of the USGS, as well as those of other Federal, State, and local agencies. The objectives of the NAWQA Program are to:

• Describe current water-quality conditions for a large part of the Nation's freshwater streams, rivers, and aquifers.

• Describe how water quality is changing over time.

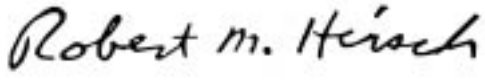
• Improve understanding of the primary natural and human factors that affect water-quality conditions.

This information will help support the development and evaluation of management, regulatory, and monitoring decisions by other Federal, State, and local agencies to protect, use, and enhance water resources.

The goals of the NAWQA Program are being achieved through ongoing and proposed investigations of 59 of the Nation's most important river basins and aquifer systems, which are referred to as Study Units. These Study Units are distributed throughout the Nation and cover a diversity of hydrogeologic settings. More than two-thirds of the Nation's freshwater use occurs within the 59 Study Units and more than two-thirds of the people served by public water-supply systems live within their boundaries.

National synthesis of data analysis, based on aggregation of comparable information obtained from the Study Units, is a major component of the program. This effort focuses on selected water-quality topics using nationally consistent information. Comparative studies will explain differences and similarities in observed water-quality conditions among study areas and will identify changes and trends and their causes. The first topics addressed by the national synthesis are pesticides, nutrients, volatile organic compounds, and aquatic biology. Discussions on these and other water-quality topics will be published in periodic summaries of the quality of the Nation's ground and surface water as the information becomes available.

This report is an element of the comprehensive body of information developed as part of the NAWQA Program. The program depends heavily on the advice, cooperation, and information from many Federal, State, interstate, Tribal, and local agencies and the public. The assistance and suggestions of all are greatly appreciated.



Robert M. Hirsch
Chief Hydrologist

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ABBREVIATIONS AND ACRONYMS

Listed below are abbreviations and acronyms that are used frequently in this report:

AQUIRE	AQUatic toxicity Information REtrieval—The U.S. Environmental Protection Agency's data base for aquatic toxicity; effect concentrations that follow designate the least-to-most sensitive toxic effects on aquatic organisms observed during testing:
	LC_{50} Median lethal concentration (50 percent mortality)
	EC_{50} Median effective concentration (affects 50 percent of species with an endpoint other than mortality)
	LOEC Lowest observed effective concentration (lowest concentration producing an effect)
	LOEL Lowest observed effective level
	MATC Maximum acceptable toxicant concentration (hypothetical mean between NOEC and LOEC)
	NOEC No-observed effective concentration (highest concentration at which observed effects are not significant)
CAS	Chemical Abstract Service
CWQC	Chronic water-quality criteria established by the USEPA
DWEL	Drinking-water equivalent level (USEPA Drinking Water Health Advisories)
IRIS	Integrated Risk Information System, USEPA's data base for risk assessment and risk management information
IUPAC	International Union of Pure and Applied Chemistry
MCL	Maximum contaminant level
MCLG	Maximum contaminant level goal
NAWQA	U.S. Geological Survey National Water-Quality Assessment Program
NWQL	U.S. Geological Survey National Water-Quality Laboratory
P&T GC/MS	Purge-and-trap gas chromatography/mass spectrometry
µg/L	Microgram per liter
USEPA	U.S. Environmental Protection Agency
USGS	U.S. Geological Survey
VOC	Volatile organic compound

Selection Procedure and Salient Information for Volatile Organic Compounds Emphasized in the National Water-Quality Assessment Program

By David A. Bender, John S. Zogorski, Michael J. Halde, *and* Barbara L. Rowe

ABSTRACT

Volatile organic compounds (VOCs) are organic compounds with chemical and physical properties that allow the compounds to move freely between water and air. Many products contain VOCs including fuels, solvents, paints, glues, adhesives, deodorizers, refrigerants, and fumigants. Because of human-health concerns, many VOCs have been the focus of national regulations, monitoring, and research during the past 10 to 20 years.

The selection procedure for VOC target analytes for emphasis in the U.S. Geological Survey's National Water-Quality Assessment (NAWQA) Program, completed in 1994-96, involved three sequential phases: (1) initial selection and preliminary screening of 130 candidate compounds on the basis of available information; (2) laboratory studies to ascertain the feasibility of analysis by purge-and-trap gas chromatography/mass spectrometry; and (3) analysis of groundwater, surface-water, and quality-control samples to ascertain the performance of laboratory methods on environmental samples. Preliminary screening considered several factors including: (1) physical properties; (2) human cancer rating; (3) noncancer human-health risk; (4) toxicity to freshwater aquatic organisms; (5) occurrence data for VOCs in ground water, surface water, and drinking water; (6) potential for atmospheric ozone depletion; (7) bioconcentration in aquatic organisms; and (8) use or potential use as a fuel oxygenate in gasoline. As a result of the selection procedure, 55 VOC target analytes were identified for additional study including 21 halogenated alkanes, 10 halogenated alkenes, 3 aromatic hydrocarbons, 9 alkyl benzenes, 6 halogenated aromatics, 4 ethers, 1 aldehyde, and 1 nitrile.

Of the 55 VOC target analytes, 29 have a national enforceable drinking-water regulation; 28 are classified as known, probable, or possible human carcinogens; 35 have noncancer human-health effects; and 33 are known to impart taste and odor to water. For the protection of freshwater biota, 33 of the 55 VOC target analytes have water-quality guidelines established by the U.S. Environmental Protection Agency, and 17 have water-quality guidelines established by Environment Canada.

Important physical, chemical, and biological properties governing aquatic behavior and fate of the VOC target analytes include: aqueous solubility, vapor pressure, Henry's law constant, octanol-water partitioning coefficient, sorption coefficient, half-life, and bioconcentration factor.

This report (1) describes the step-by-step procedure used to select NAWQA's VOC target analytes, (2) lists the VOC target analytes, and (3) provides human-health criteria, drinking-water regulations, aquatic toxicity criteria, and other information on each target analyte.

INTRODUCTION

Background

Volatile organic compounds (VOCs) are organic compounds with chemical and physical properties that allow the compounds to move freely between water and air. In general, these compounds have low molecular weights, high vapor pressures, and low-to-medium water solubilities (Rathbun, 1998). VOCs have been used extensively in industry, commerce, and households in the United States since the 1940's. Many products contain these compounds including, for example, fuels, solvents, paints, glues, adhesives, deodorizers, refrigerants, and fumigants.

Large quantities of VOCs are released to the environment as indicated by reports completed by commercial and industrial entities as part of the 1996 Toxics Release Inventory (U.S. Environmental Protection Agency, 1998). Data in this inventory show that 10 of the top 20 chemical compounds with the largest releases to the environment were VOCs, with combined VOC releases of almost 1 trillion pounds in 1996.

Many VOCs are toxic, and these compounds became a focus of a number of Federal regulations related to water quality starting in the 1970's (Leahy and Thompson, 1994; Pankow and Cherry, 1996). As many as 400 VOCs appear on regulatory lists associated with Federal acts (for example, Safe Drinking Water Act, Clean Water Act, Resource Conservation and Recovery Act, Clean Air Act, and Food Quality Protection Act).

VOCs and various pesticides are compounds of primary concern in surface and ground waters, and as such, both VOCs and pesticides were included in pilot studies of the U.S. Geological Survey's (USGS) National Water-Quality Assessment (NAWQA) Program (Hirsch and others, 1988) and in the full-scale NAWQA Program (Leahy and Thompson, 1994). A total of 60 VOCs (prior to NAWQA VOC target analyte selection) were analyzed in NAWQA's groundwater studies between 1993 and 1995, and a total of 88 VOCs (55 NAWQA VOC target analytes plus 33 additional VOCs) were analyzed in NAWQA's groundwater and surface-water studies completed in 1996-98.

The objectives of the NAWQA Program are to: (1) describe current water-quality conditions for a large part of the water resources of the United States; (2) define long-term trends or the absence of trends in water quality; and (3) identify and describe the primary factors affecting the observed water-quality conditions and trends (Hirsch and others, 1988). The NAWQA Program consists of two parts that include: (1) investigations of the water quality of river basins and aquifer systems; and (2) national synthesis assessments (Leahy and Thompson, 1994). The synthesis assessments focus on high-priority water-quality issues.

Initial national synthesis assessments described the occurrence of nutrients and pesticides in surface water and ground water. In 1994, a national study on VOCs was initiated because of the widespread occurrence of these compounds in water and the lack of information on factors related to their occurrence and behavior. The objectives of the VOC national synthesis are to: (1) determine the occurrence of VOCs in ground water and surface water, (2) identify probable sources of VOCs, and (3) describe the primary processes affecting the concentrations of VOCs in water resources of the United States. Within the national context, the VOC synthesis seeks to greatly expand knowledge concerning the significance of VOCs in ambient ground water and in surface water in relation to public health and aquatic toxicity. Determining the occurrence of VOCs in shallow ground water for selected subcategories of land use and defining natural and human factors that relate to VOC occurrence are planned, as well.

Selection of Volatile Organic Compounds for Emphasis

As part of planning NAWQA's national VOC synthesis, a subset of VOCs were selected for emphasis. Denoted as NAWQA VOC target analytes, these compounds are referred to herein as "VOC target analytes." The VOC target analytes are included on analytical schedules used in the NAWQA Program. Selection of VOC target analytes was done in 1994-96 utilizing three sequential phases: (1) initial selection of candidate analytes and preliminary screening on the basis of published and additional information; (2) laboratory studies to ascertain the feasibility of analysis by purge-and-trap gas chromatography/mass spectrometry (P&T GC/MS); and (3) analysis of ground water, surface water, and quality-control samples to ascertain the performance of field and laboratory methods on environmental samples.

Initial selection of candidate VOC target analytes was done in 1994 with emphasis on regulated

VOCs and on VOCs with potential regulation under the Safe Drinking Water Act and Clean Water Act. This was done because of the water-quality focus of regulations developed under these two acts and because of the direct linkage of water-quality data collected in the NAWQA Program to these two acts. Consequently, VOCs with known or suspected concern to human health and (or) aquatic toxicity were emphasized. Additional VOCs were considered initially because of concern with depletion of the atmosphere's ozone level, potential bioconcentration in aquatic organisms, or use as oxygenates in gasoline as part of Federally mandated programs.

The decision to continue the use of P&T GC/MS for analysis of VOCs in water samples collected by the NAWQA Program also was made in 1994. The decision to retain P&T GC/MS for the analysis of VOCs further reduced the number of candidate VOC target analytes. P&T GC/MS has been used extensively in the United States for the analysis of VOCs in samples of ambient ground water and drinking water since the mid-1980's. This methodology has been used since 1988 at the USGS National Water Quality Laboratory (NWQL), which analyzes NAWQA's water samples (Rose and Schroeder, 1995). Both unequivocal identification and sub-microgram-per-liter detection levels are achieved by the P&T GC/MS method (Connor and others, 1998).

Approximately 40 to 60 target analytes were sought for emphasis in NAWQA's national assessment of VOCs. This number appears reasonable for the assessment considering the large number of tasks required to assure the completion of the study's overall objectives. These tasks include for example: (1) implementation of analytical enhancements at the NWQL; (2) development and onsite testing of sampling equipment, spiking procedures, and a sample preservation method; (3) acquisition and spatial display of information on releases of VOC target analytes to the environment; (4) compilation, for each VOC target analyte, of physical and chemical properties, human-health effects, aquatic toxicity, uses, and behavior and fate attributes; and (5) summary of information from previous VOC occurrence and distribution studies, and compilation in some cases of the actual VOC analytical results.

The list of VOCs given emphasis in the NAWQA Program will need periodic updating. This will be attempted on about a 10-year cycle and be based on information similar to that used to select VOC target analytes for emphasis in the first cycle of NAWQA studies.

Purpose and Scope

The purposes of this report are to: (1) describe the procedure used to select VOC target analytes for emphasis in the NAWQA Program; (2) list the VOC target analytes; and (3) provide salient information on each VOC target analyte. As noted previously, the selection of VOC target analytes included initial screening on the basis of existing information, as well as laboratory and field studies for compounds previously not evaluated. Existing information reviewed for each candidate analyte included: (1) physical properties; (2) cancer rating; (3) noncancer human-health risk; (4) toxicity to aquatic organisms; (5) occurrence data for ground water, surface water, and drinking water; (6) potential for atmospheric ozone depletion; (7) bioconcentration by aquatic organisms; and (8) use or potential use as an oxygenate in gasoline. The laboratory study consisted of measuring several solutions of each candidate analyte to assess the accuracy and precision of analysis by P&T GC/MS. The extent of carryover from water samples containing each candidate analyte to laboratory blanks was also assessed in the laboratory. Water-sample validation included routine processing of ground-water and surface-water samples and concurrent analysis of equipment blanks, trip blanks, and spiked water samples at the NWQL.

The three-phase selection process resulted in the identification of 55 VOC target analytes. Information provided for each VOC target analyte includes: (1) drinking-water regulations, health advisories, cancer rating, risk of noncancer effects, and related information; and (2) water-quality guidelines and lowest observed toxicity level for aquatic organisms. Information sources for physical, chemical, and biological properties that are useful in predicting partitioning among water, air, and soil also are provided.

Acknowledgments

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SELECTION PROCEDURE FOR VOLATILE ORGANIC COMPOUND TARGET ANALYTES

The selection procedure for VOC target analytes and the final list of VOC target analytes are described in this section. The selection procedure involved three sequential phases (fig. 1): (1) development of an initial candidate analyte list and screening of each analyte on the basis of existing information; (2) assessment via laboratory studies of the feasibility of analysis by P&T GC/MS of the VOCs identified in Phase 1; and (3) water-sample validation of selected analytes by analysis of ground-water, surface-water, and quality-control samples using the USGS's analytical method for VOCs (Connor and others, 1998).

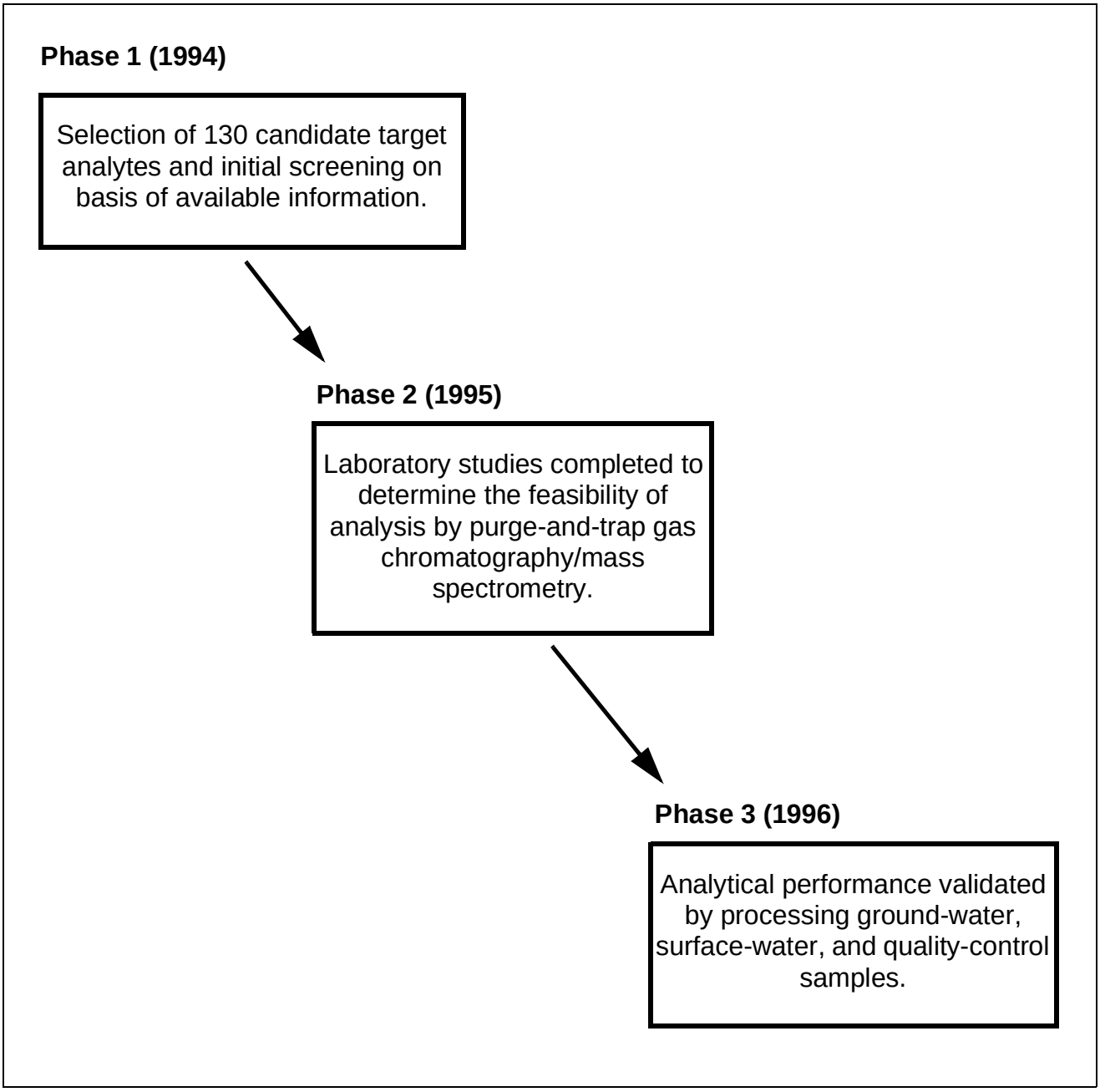

Figure 1. Schematic of the three-phase process used to select volatile organic compounds for emphasis in the National Water-Quality Assessment Program.

Identification and Initial Screening of Candidate Target Analytes

A total of 130 compounds were selected for initial screening (fig. 1, appendix 1). One-hundred twenty-four (124) compounds were from one or more regulatory lists associated with the Safe Drinking Water Act and Clean Water Act. Six additional compounds were included on the basis of: (1) listing as a carcinogen in the Toxics Release Inventory (chloromethyl methyl ether and *bis*-(2-chloroethyl) sulfide); (2) potential for ozone depletion (1,1,2-trichloro-1,2,2-trifluoroethane); or (3) use or potential use as a gasoline oxygenate (*tert*-amyl methyl ether, diisopropyl ether, and ethyl *tert*-butyl ether).

The 130 candidate analytes (appendix 1) then were screened by a six-step process (fig. 2). The first step was to determine if the candidate compounds had physical properties generally considered typical for VOCs. Vapor pressure, aqueous solubility, octanol-water partition coefficient, Henry's law constant, molecular weight, and melting point were the physical properties used in this initial screening (table 1). Eighty-nine candidate analytes (appendix 1) had properties typical of VOCs and were screened further. Forty-one compounds failing the physical-properties screen were not classified as volatile and received no further consideration.

The 89 remaining candidate analytes were evaluated further to determine if they were: (1) a serious human-health concern (fig. 2, steps 2 and 3); (2) toxic to aquatic organisms at low concentrations (fig. 2, step 4); (3) known to occur frequently in ground water, surface water, or drinking water (fig. 2, step 5); or (4) known to be important for other reasons, including the potential for atmospheric ozone depletion, bioaccumulation in aquatic organisms, or use as a gasoline oxygenate (fig. 2, step 6). Both carcinogenic and noncarcinogenic risks were considered to assess human-health concern. Freshwater, water-quality guidelines, and published aquatic toxicity data were used to assess aquatic-organism concerns. This additional screening was done sequentially (fig. 2, steps 2-6). Compounds were retained as VOC target analytes if they met any one of the four above-mentioned concerns.

Human carcinogenic potential was assessed (fig. 2, step 2) on the basis of the strength of evidence score (U.S. Environmental Protection Agency, 1996a). Cancer categories and associated criteria are:

- A - Human carcinogen—sufficient evidence in epidemiologic studies to support causal association between exposure and cancer;
- B_1 - Probable human carcinogen—limited evidence in epidemiological studies;
- B_2 - Probable human carcinogen—sufficient evidence from animal studies;
- C - Possible human carcinogen—limited or equivocal evidence from animal studies and inadequate or no data from human studies;
- D - Not classified—inadequate or no human and animal evidence of carcinogenicity; and
- E - No evidence of carcinogenicity for humans—no evidence of carcinogenicity in at least two adequate animal tests in different species or in adequate epidemiologic and animal studies.

Compounds indicated as either human carcinogens (category A) or probable human carcinogens (categories B_1 and B_2) were considered a serious human-health concern and were retained as VOC target analytes. Twenty-five compounds passing the physical properties screen in appendix 1 are classified by the U.S. Environmental Protection Agency (USEPA) as either known human carcinogens or probable human carcinogens; the remaining 64 compounds that are classified are identified as either C or D carcinogens. The 25 VOCs with an A, B_1, or B_2 classification were acrylamide, benzene, bromodichloromethane, bromoethene, chloroethane, chloroethene, *bis*-(2-chloroethyl) ether, *bis*-(2-chloroethyl) sulfide, *bis*-(chloromethyl) ether, chloromethyl methyl ether, 1,2-dibromo-3-chloropropane, 1,2-dibromoethane, 1,2-dichloroethane, dichloromethane, 1,2-dichloropropane, *cis*-1,3-dichloropropene, *trans*-1,3-dichloropropene, 1,4-dioxane, formaldehyde, 2-propenenitrile, tetrachloromethane, tribromomethane, trichloroethene, trichloromethane, and 1,2,3-trichloropropane.

Noncarcinogenic human-health effects (fig. 2, step 3) were assessed on the basis of the drinking-water equivalent level (DWEL). DWEL is the highest lifetime (70 years) exposure concentration in drinking water at which adverse noncarcinogenic health effects would not be expected to occur for a person with a body weight of 70 kilograms consuming 2 liters of water a day (Nowell and Resek, 1994). In the calculation of DWEL, 100-percent exposure to the compound is assumed to occur from drinking water. The DWEL value for each compound was obtained from the USEPA (1996a).

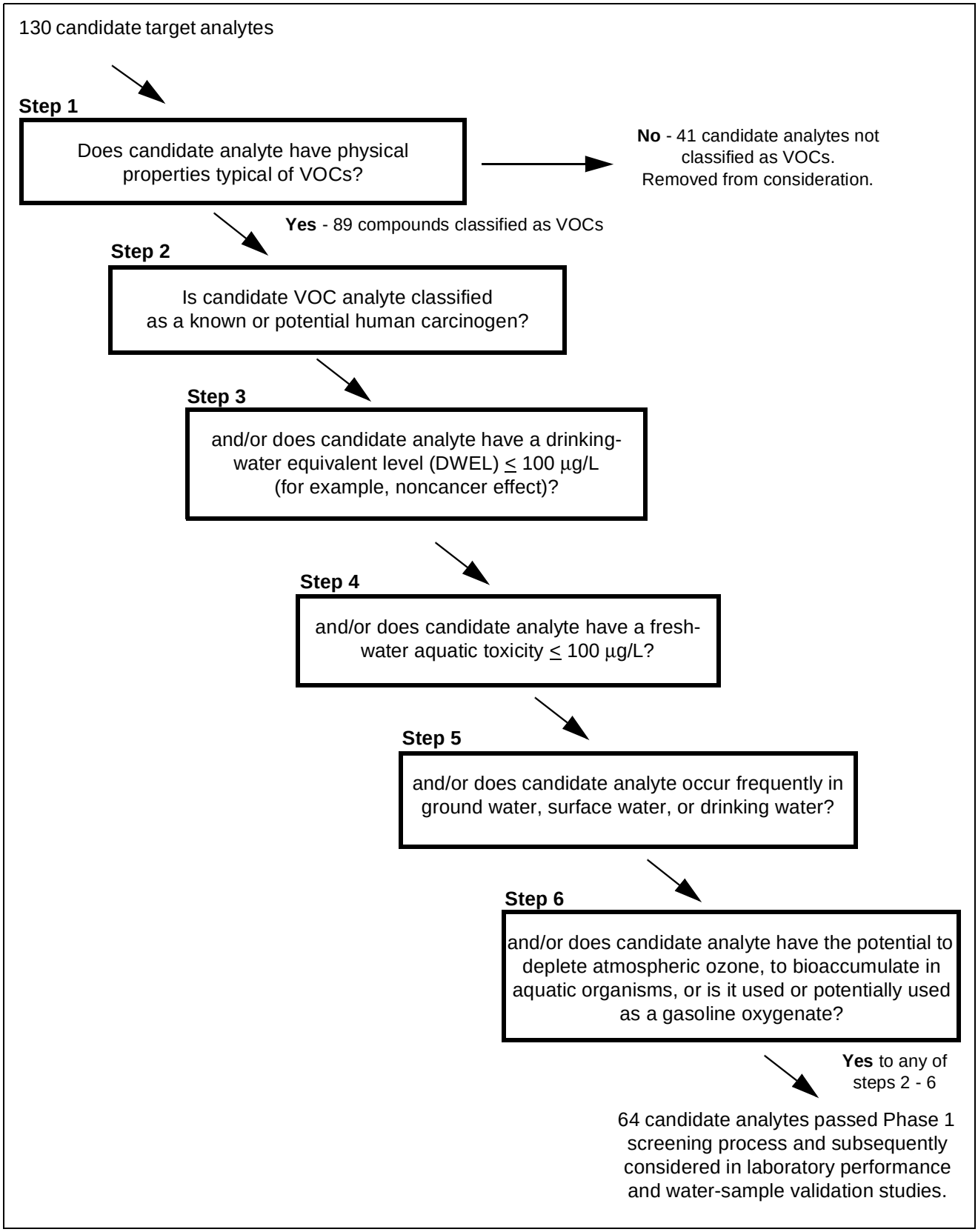

Figure 2. Schematic of six-step process used in Phase 1 to screen 130 candidate target analytes on the basis of available information. [≤, less than or equal to; µg/L, microgram per liter]

Table 1. Physical properties of volatile organic compounds (Mackay and Shiu,1990)

[--, dimensionless; >, greater than; <, less than]

Property	Unit of measurement	Boundary or range[1]
Vapor pressure	pascals	> 500
Aqueous solubility	grams per liter	< 10
Octanol-water partition coefficient	--	10 - 1,000
Henry's law constant	--	> 0.1
Molecular weight	grams per mole	< 160
Melting point	degrees Celsius	25

[1] Boundaries of properties apply for most compounds but are not totally exclusive.

Experience in the USGS, USEPA, and elsewhere indicates that in most natural water (that is, water resources not affected by point-source contamination) concentrations of VOCs in excess of 100 µg/L (micrograms per liter) are rare, and therefore, this concentration represents a conservative exposure threshold. Thirteen compounds passing the physical properties screen had DWELs of 100 µg/L or less (appendix 1), five of which were previously selected because of carcinogenic risks. This screening step identified eight additional VOC target analytes specifically because of the potential for noncarcinogenic health risk in concentration less than or equal to 100 µg/L. These eight VOCs were bromomethane, chloromethane, hexachlorobutadiene, hexachloroethane, naphthalene, pentachlorobenzene, 1,2,4-trichlorobenzene, and 1,1,2-trichloroethane.

Adverse aquatic-organism effects were assessed on the basis of the freshwater, chronic water-quality guidelines and aquatic toxicity study results from USEPA's AQUIRE data base (fig. 2, step 4). Water-quality guidelines for protection of freshwater biota have been published by the USEPA for 36 VOCs. These guidelines are based on the lowest observed effect level (LOEL). Again, a 100-µg/L concentration was selected as an appropriate upper threshold for selection of the target analyte on the basis of aquatic toxicity. Nine compounds that passed the physical screen had water-quality guidelines or evidence of aquatic toxicity at concentrations of 100 µg/L or less, three of which were previously selected because of noncarcinogenic risks. This screening step identified six additional VOC target analytes because of their toxicity to aquatic organisms. These six VOCs were *n*-butylbenzene, chlorobenzene, hexachlorocyclopentadiene, 2-propenal, *iso*-propylbenzene, and *n*-propylbenzene.

To assess which VOCs are most frequently occurring in ground water, surface water, and drinking water, the results of 45 studies were reviewed. Twenty-four of these studies were of regional or national scale. Requiring considerable effort, this step was deemed especially important to assure that frequently occurring compounds were selected as VOC target analytes. Results from previous studies by the USEPA Office of Ground Water and Drinking Water, the USGS NAWQA Program, the USGS Toxics Hydrology Program, USGS State programs, and several State agency ambient monitoring programs were compiled.

Three criteria for occurrence were used, any one providing the basis for selecting a compound for the VOC target analyte list:

1. Compounds were retained if they were detected in at least one sample in more than 30 percent of the 45 studies reviewed. This criterion was the broadest assessment of occurrence in that national, regional, State, and local studies were included.
2. Compounds were retained if they were detected at least once in more than 30 percent of 24 regional and national studies. Additionally, these compounds must have been target analytes for those studies. Finally, it was required that these compounds occurred frequently in the experience of the VOC analysis staff at the USGS's NWQL, which analyzes approximately 2,500 to 3,000 water samples for VOCs each year (D.L. Rose, USGS, oral commun., 1998).
3. Compounds were retained as noted in 2 (above) except that when staff at the NWQL did not indicate frequent occurrence, an alternate approach was used to confirm the potential for frequent occurrence. Individual studies were examined, occurrence data were compiled, and if frequent occurrence was indicated in two or more studies, the compound was selected as a target analyte.

A total of 20 additional compounds were selected as target analytes on the basis of frequency of occurrence in past monitoring studies. These compounds were chlorodibromomethane, 1,2-dichlorobenzene, 1,3-dichlorobenzene, 1,4-dichlorobenzene, 1,1-dichloroethane, 1,1-dichloroethene, *cis*-1,2-dichloroethene, *trans*-1,2-dichloroethene, dichlorodifluoromethane, 1,2-dimethylbenzene, 1,3-dimethylbenzene, 1,4-dimethylbenzene, ethylbenzene,

methylbenzene, methyl *tert*-butyl ether, styrene, tetrachloroethene, 1,1,1-trichloroethane, trichlorofluoromethane, and 1,2,4-trimethylbenzene.

The final step (fig. 2, step 6) in screening candidate analytes was to review the remaining 30 compounds to assure that target analytes were included for three topics of national interest (atmospheric ozone depletion, bioaccumulation in aquatic organisms, and gasoline oxygenates). Five additional VOCs were selected for the target analyte list for these reasons (appendix 1). 1,1,2-trichloro-1,2,2-trifluoroethane was selected because of its potential for atmospheric-ozone depletion, and 1,2,3-trichlorobenzene was selected because of its potential for bioaccumulation in aquatic organisms. *Tert*-amyl methyl ether, diisopropyl ether, and ethyl *tert*-butyl ether were selected because of their known or potential use as gasoline oxygenates.

Laboratory Performance Studies

Phase 1 of the selection process, just described (fig. 2), resulted in selection of 64 candidate VOC target analytes. Forty-eight of these 64 compounds were evaluated previously for analytical feasibility by P&T GC/MS, and these 48 compounds were included on NWQL's VOC analysis schedule 2090 used in the NAWQA Program from 1993 to 1995. Analysis by P&T GC/MS of these 48 compounds in ground-water and quality-control samples did not indicate any concern about sample stability or adverse matrix effects. Therefore, no additional evaluation of these 48 compounds was needed. The remaining 16 candidate VOC target analytes (table 2) required further laboratory evaluation.

Table 2. Evaluation of analysis of 16 volatile organic compound candidate target analytes by purge-and-trap gas chromatography/mass spectrometry on the basis of laboratory performance studies

[IUPAC, International Union of Pure and Applied Chemistry; P&T GC/MS, purge-and-trap gas chromatography/mass spectrometry; µg/L, micrograms per liter]

IUPAC name	Feasible to analyze by P&T GC/MS	Remarks
bromoethene	Yes	Performs well.
2-propenenitrile	Yes	Performs well.
hexachloroethane	Yes	Performs well.
2-propenal	Yes	Marginal performance, low precision, and not stable in acidified samples held 14 days and longer.
tert-amyl methyl ether	Yes	Performs well.
diisopropyl ether	Yes	Performs well.
ethyl *tert*-butyl ether	Yes	Performs well.
acrylamide	No	Not detectable by P&T GC/MS at levels up to 500 µg/L.
bis-(2-chloroethyl) ether	No	Poor purging efficiency and low response factor by P&T GC/MS; carryover contamination of high-level standards; co-elutes and has a similar ion with another compound.
bis-(2-chloroethyl) sulfide	No	Not stable for more than 40 minutes in water.
bis-(chloromethyl) ether	No	Not detectable by P&T GC/MS at levels up to 500 µg/L.
chloromethyl methyl ether	No	Not detectable by P&T GC/MS at levels up to 500 µg/L.
1,4-dioxane	No	Poor purging efficiency and low response factor by P&T GC/MS; carryover contamination of high-level standards.
formaldehyde	No	Not detectable by P&T GC/MS at levels up to 500 µg/L.
pentachlorobenzene	No	Unacceptable purging efficiency, elution time, and carryover; better analyzed by an extraction method.
hexachlorocyclopentadiene	No	Unacceptable purging efficiency, elution time, and carryover; better analyzed by an extraction method.

In 1995, the NWQL completed several laboratory studies to determine the feasibility of measuring 16 candidate VOC target analytes in water samples by P&T GC/MS. These studies assessed purging efficiency, instrument response, precision, carryover, analyte stability, and elution time. On the basis of results of these studies, 7 of the 16 compounds were analyzed adequately using P&T GC/MS. These seven compounds were bromoethene, 2-propenenitrile, hexachloroethane, 2-propenal, *tert*-amyl methyl ether, diisopropyl ether, and ethyl *tert*-butyl ether (table 2). Although 2-propenal was amenable to analysis by P&T GC/MS and retained as a target analyte, analysis of this compound was marginal because of lower precision, higher detection level, and instability in acidified samples held for 14 days or longer, as compared to the six previously noted compounds. Nine of the 16 compounds were not amenable to analysis by P&T GC/MS and were not selected as VOC target analytes. The "remarks" column of table 2 describes briefly the reason why analysis by P&T GC/MS was not feasible. The reader is referred to Connor and others (1998) for discussion of additional factors that led to deletion of these compounds from NWQL's VOC analysis schedules. As a result of Phase 2, 55 compounds were retained as target analytes.

Water-Sample Validation

To further assess the feasibility of P&T GC/MS analysis of the remaining seven candidate VOC target analytes (table 2), these compounds were included in 1996 as analytes on NWQL's VOC custom method 9090 (along with the other 48 VOC target analytes and 33 other VOCs). During 1996, the NAWQA Program used this method for the analysis of about 1,200 water samples including 900 samples of ground water and surface water, 200 sample blanks, and 100 matrix-spiked samples. This sample validation (Phase 3) confirmed the excellent performance of the P&T GC/MS analysis of six analytes previously analyzed in laboratory performance studies (table 2). Water-sample data also confirmed the marginal performance of the P&T GC/MS in analyzing for 2-propenal, which led to a NWQL decision to report all detections of this compound as estimated concentrations. For similar reasons, only estimated concentrations are reported for three other VOC target analytes—bromomethane, chloromethane, and dichlorodifluoromethane.

In summary, Phase 3 confirmed the analysis feasibility of seven candidate VOC target analytes including bromoethene, 2-propenenitrile, hexachloroethane, 2-propenal, *tert*-amyl methyl ether, diisopropyl ether, and ethyl *tert*-butyl ether.

List of Target Analytes

The selection process described heretofore resulted in a list of 55 VOCs for emphasis in the NAWQA Program. The 55 compounds are listed in table 3 by chemical subgroup. The Chemical Abstract Services (CAS) numbers and the USGS parameter codes are included to assist in compound identification; however, the International Union of Pure and Applied Chemistry (IUPAC) name is preferred and is used in this report. Many of the VOC target analytes have numerous alternative names and abbreviations. Select alternative names and abbreviations are given in table 3.

Halogenated alkanes frequently are named in the literature as "ethyls" rather than by the IUPAC name. For example, ethyl chloride is synonymous with chloroethane. Also, the chlorinated alkenes often appear in the literature as "ethylenes" rather than as the current IUPAC usage of "ethenes." For example, tetrachloroethylene is the same compound as tetrachloroethene. 1,3-dimethylbenzene and 1,4-dimethylbenzene (*m*- and *p*-xylene) have the same USGS parameter code because these isomers cannot be separated by the P&T GC/MS method. As such, concentrations reported under this parameter code are the sum for these two compound concentrations.

2-propenal is included as a VOC target analyte in table 3; however, it was deleted from VOC schedules at the NWQL in May 1998 because of erratic and poor instrument response after a new concentrator was installed. Poor performance is presumed to be associated with a moisture-control system in the new concentrator (D.L. Rose, USGS, oral commun., 1998). 2-propenal is included in subsequent sections of this report and retained as a NAWQA VOC target analyte because 2.5 years of acceptable data were collected by the NAWQA Program in 1996-98.

Table 3. Volatile organic compound target analytes (adapted from Rathbun, 1998)

[CAS, Chemical Abstract Services; USGS, U.S. Geological Survey; IUPAC, International Union of Pure and Applied Chemistry]

IUPAC name	CAS number	USGS parameter code	Select alternative name or abbreviation	Predominant use	Chemical formula	Molecular weight (gram/mole)
			Halogenated alkanes			
bromodichloromethane	75-27-4	32101	--	organic synthesis	$CHBrCl_2$	163.83
bromomethane[1]	74-83-9	34413	methyl bromide	fumigant	CH_3Br	94.94
chlorodibromomethane	124-48-1	32105	--	organic synthesis	$CHBr_2Cl$	208.29
chloroethane	75-00-3	34311	ethyl chloride	solvent	C_2H_5Cl	64.52
chloromethane[1]	74-87-3	34418	methyl chloride	refrigerant	CH_3Cl	50.49
1,2-dibromo-3-chloropropane	96-12-8	82625	DBCP	fumigant	$C_3H_5Br_2Cl$	236.33
1,2-dibromoethane	106-93-4	77651	EDB	fumigant	$C_2H_4Br_2$	187.87
dichlorodifluoromethane[1]	75-71-8	34668	Freon 12, CFC 12	refrigerant	CCl_2F_2	120.91
1,1-dichloroethane	75-34-3	34496	ethylidenedichloride	solvent	$C_2H_4Cl_2$	98.96
1,2-dichloroethane	107-06-2	32103	ethylenedichloride	solvent	$C_2H_4Cl_2$	98.96
dichloromethane	75-09-2	34423	methylene chloride	solvent	CH_2Cl_2	84.93
1,2-dichloropropane	78-87-5	34541	--	solvent	$C_3H_6Cl_2$	112.99
hexachloroethane	67-72-1	34396	--	metallurgy refining	C_2Cl_6	236.74
tetrachloromethane	56-23-5	32102	carbon tetrachloride	solvent	CCl_4	153.82
tribromomethane	75-25-2	32104	bromoform	solvent	$CHBr_3$	252.75
trichloromethane	67-66-3	32106	chloroform	solvent	$CHCl_3$	119.38
1,1,1-trichloroethane	71-55-6	34506	methyl chloroform	solvent	$C_2H_3Cl_3$	133.41
1,1,2-trichloroethane	79-00-5	34511	--	solvent	$C_2H_3Cl_3$	133.41
trichlorofluoromethane	75-69-4	34488	Freon 11, CFC 11	refrigerant	CCl_3F	137.37
1,2,3-trichloropropane	96-18-4	77443	--	solvent	$C_3H_5Cl_3$	147.43
1,1,2-trichloro-1,2,2-trifluoroethane	76-13-1	77652	Freon 113, CFC 113	refrigerant	$C_2Cl_3F_3$	187.38
			Halogenated alkenes			
bromoethene	593-60-2	50002	vinyl bromide	fire retardant	C_2H_3Br	106.96
chloroethene	75-01-4	39175	vinyl chloride	organic synthesis	C_2H_3Cl	62.50
1,1-dichloroethene	75-35-4	34501	--	organic synthesis	$C_2H_2Cl_2$	96.94
cis-1,2-dichloroethene	156-59-2	77093	--	solvent	$C_2H_2Cl_2$	96.94
trans-1,2-dichloroethene	156-60-5	34546	--	solvent	$C_2H_2Cl_2$	96.94
cis-1,3-dichloropropene	10061-01-5	34704	--	fumigant	$C_3H_4Cl_2$	110.97
trans-1,3-dichloropropene	10061-02-6	34699	--	fumigant	$C_3H_4Cl_2$	110.97
hexachlorobutadiene	87-68-3	39702	--	organic synthesis	C_4Cl_6	260.76
tetrachloroethene	127-18-4	34475	tetrachloroethylene, perchloroethylene, PCE	solvent	C_2Cl_4	165.83
trichloroethene	79-01-6	39180	trichloroethylene, TCE	solvent	C_2HCl_3	131.39

Table 3. Volatile organic compound target analytes (adapted from Rathbun, 1998)—Continued

[CAS, Chemical Abstract Services; USGS, U.S. Geological Survey; IUPAC, International Union of Pure and Applied Chemistry]

IUPAC name	CAS number	USGS parameter code	Select alternative name or abbreviation	Predominant use	Chemical formula	Molecular weight (gram/mole)
			Aromatic hydrocarbons			
benzene	71-43-2	34030	--	gasoline aromatic hydrocarbon	C_6H_6	78.12
naphthalene	91-20-3	34696	--	gasoline aromatic hydrocarbon	$C_{10}H_8$	128.19
styrene	100-42-5	77128	vinyl benzene	organic synthesis	C_8H_8	104.16
			Alkyl benzenes			
n-butylbenzene	104-51-8	77342	--	gasoline aromatic hydrocarbon	$C_{10}H_{14}$	134.22
1,2-dimethylbenzene	95-47-6	77135	o-xylene	gasoline aromatic hydrocarbon	C_8H_{10}	106.17
1,3-dimethylbenzene	108-38-3	85795	m-xylene	gasoline aromatic hydrocarbon	C_8H_{10}	106.17
1,4-dimethylbenzene	106-42-3	85795	p-xylene	gasoline aromatic hydrocarbon	C_8H_{10}	106.17
ethylbenzene	100-41-4	34371	--	gasoline aromatic hydrocarbon	C_8H_{10}	106.17
methylbenzene	108-88-3	34010	toluene	gasoline aromatic hydrocarbon	C_7H_8	92.15
iso-propylbenzene	98-82-8	77223	cumene	organic synthesis	C_9H_{12}	120.20
n-propylbenzene	103-65-1	77224	--	solvent	C_9H_{12}	120.20
1,2,4-trimethylbenzene	95-63-6	77222	--	organic synthesis	C_9H_{12}	120.20
			Halogenated aromatics			
chlorobenzene	108-90-7	34301	--	solvent	C_6H_5Cl	112.56
1,2-dichlorobenzene	95-50-1	34536	o-dichlorobenzene	solvent	$C_6H_4Cl_2$	147.01
1,3-dichlorobenzene	541-73-1	34566	m-dichlorobenzene	solvent	$C_6H_4Cl_2$	147.01
1,4-dichlorobenzene	106-46-7	34571	p-dichlorobenzene	fumigant	$C_6H_4Cl_2$	147.01
1,2,3-trichlorobenzene	87-61-6	77613	--	organic synthesis	$C_6H_3Cl_3$	181.45
1,2,4-trichlorobenzene	120-82-1	34551	--	solvent	$C_6H_3Cl_3$	181.45
			Ethers			
tert-amyl methyl ether	994-05-8	50005	TAME	oxygenate	$C_6H_{14}O$	102.18
diisopropyl ether	108-20-3	81577	DIPE	oxygenate	$C_6H_{14}O$	102.18
ethyl *tert*-butyl ether	637-92-3	50004	ETBE	oxygenate	$C_6H_{14}O$	102.18
methyl *tert*-butyl ether	1634-04-4	78032	MTBE	oxygenate	$C_5H_{12}O$	88.15
			Others (aldehydes and nitriles)			
2-propenal[1,2]	107-02-8	34210	acrolein	organic synthesis	C_3H_4O	56.06
2-propenenitrile	107-13-1	34215	acrylonitrile	organic synthesis	C_3H_3N	53.06

[1]All detections of these compounds are reported by the National Water Quality Laboratory as estimated concentrations.

[2]Deleted from list of volatile organic compounds analyzed by the National Water Quality Laboratory in May 1998, because of poor performance after installation of new equipment.

The VOC target analyte list includes 21 halogenated alkanes, 10 halogenated alkenes, 3 aromatic hydrocarbons, 9 alkyl benzenes, 6 halogenated aromatics, 4 ethers, 1 aldehyde, and 1 nitrile. Many of the VOC target analytes have been the focus of national regulations, monitoring, and research during the past 10 to 20 years. These include, for example, bromodichloromethane, chlorodibromomethane, tribromomethane, and trichloromethane, all of which are associated with the chlorination of drinking water; the fumigants 1,2-dibromo-3-chloropropane (DBCP) and 1,2-dibromoethane (EDB); the solvents tetrachloroethene (PCE) and trichloroethene (TCE); and the gasoline aromatic hydrocarbons benzene, methylbenzene (toluene), ethylbenzene, and dimethylbenzenes (xylenes), commonly referred to as BTEX compounds.

Most of the VOC target analytes have numerous uses in industry, commerce, and households (table 3). For example, the aromatic hydrocarbon, naphthalene, is used in the manufacturing of various organic chemicals, externally on livestock and poultry to control lice, as an ingredient of some moth repellents and toilet bowl deodorants, and formerly for intestinal vermifuge and wood preservative (Prager, 1995). Information about the amount of a compound's use for varied purposes is not systematically available for the United States. For the purpose of reporting frequency of occurrence information for VOCs in ground water and surface water, four predominant use categories are used in the NAWQA Program: (1) solvents, organic synthesis, and refrigerants; (2) fumigants; (3) gasoline aromatic hydrocarbons; and (4) gasoline oxygenates.

The predominant use for each VOC target analyte (table 3) is based on a review of available use information. These designations are applicable at the national level; the predominant use of a particular VOC may vary regionally and from location to location within a region. Therefore, it is appropriate that verification of actual use patterns be done in local, State, and regional studies.

SALIENT INFORMATION FOR TARGET ANALYTES

Additional information for each VOC target analyte is given in this section, including: (1) human-health and aesthetic concerns, cancer and noncancer risks, and drinking-water regulations, goals, and advisories; and (2) aquatic toxicity and water-quality guidelines. Also included is a listing and definition of salient physical, chemical, and biological properties and information sources for these properties.

Human-Health and Aesthetic Concerns and Drinking-Water Regulations

Human-health and aesthetic concerns, cancer and noncancer risks, and drinking-water regulations, goals, and advisories for the VOC target analytes are given in table 4. Unless noted otherwise, the information in table 4 was synthesized from two USEPA documents (U.S. Environmental Protection Agency, 1994, 1996a). Human-health concerns of VOC target analytes include: (1) cancer; (2) liver, kidney, lung, circulation, nervous- and respiratory-system effects; (3) eye, skin, and throat irritation; (4) mental confusion; and (5) damage to blood cells. All but eight of the VOC target analytes have known or suspected human-health concerns. Furthermore, 28 of the VOC target analytes are classified as known, probable, or possible carcinogens. Benzene and chloroethene are known human carcinogens. It is noteworthy that 27 of the 55 VOC target analytes have not been classified for carcinogenicity by the USEPA because of inadequate or no animal- and human-health evidence to assess carcinogenicity. At least 35 of the VOC target analytes have a noncancer human-health effect as evidenced by the existence of a DWEL concentration.

Thirty-three of the 55 VOC target analytes are known to impart taste or odor to water on the basis of published taste or odor threshold values. Table 4 lists threshold values and associated references for these 33 compounds. Entries in this table list the lowest reported taste and odor threshold value.

Drinking-water regulations, goals, and health advisories are listed in the last three columns of table 4. National drinking-water regulations have been established by the USEPA for 29 VOC target analytes. Twenty-five of these VOC target analytes are regulated individually, and each has a Maximum Contaminant Level (MCL). Four VOC target analytes—the trihalomethanes (bromodichloromethane, chlorodibromomethane, tribromomethane, and trichloromethane)—are regulated on the basis of the sum of the concentrations of these four compounds. A drinking-water regulation is a legally enforceable requirement that includes a MCL for the protection of human health that public water supplies can not exceed.

Table 4. Human-health and aesthetic concerns, and drinking-water regulations, goals, and advisories (U.S. Environmental Protection Agency, 1994, 1996a) for NAWQA volatile organic compound target analytes

[NAWQA, National Water-Quality Assessment; IUPAC, International Union of Pure and Applied Chemistry; Cancer risk E-5 level, concentration causing one additional death per 100,000 individuals; DWEL, drinking-water equivalent level; MCL, Maximum Contaminant Level; MCLG, Maximum Contaminant Level Goal; µg/L, micrograms per liter; THM, trihalomethane; --, no data]

IUPAC name	Human-health concern	Cancer rating[1]	Cancer risk E-5 level (µg/L)	DWEL (µg/L)	Taste or odor threshold (µg/L)	MCL (µg/L)	MCLG (µg/L)	Lifetime health advisory (µg/L)
		Halogenated alkanes						
bromodichloromethane (THM)	Cancer[2]	B_2	6	700	--	[3]100	0	--
bromomethane	Nervous system effects[4]	D	.82	50	--	--	--	10
chlorodibromomethane (THM)	Cancer[2]	C	--	700	--	[3]100	60	60
chloroethane	Eye, skin, and throat irritant[5]	B	--	--	[6]19	--	--	--
chloromethane	Mental confusion[4]	C	--	100	--	--	--	3
1,2-dibromo-3-chloropropane	Cancer[2]	B_2	.3	--	--	.2	0	--
1,2-dibromoethane	Cancer[2]	B_2	.004	--	--	0.05	0	--
dichlorodifluoromethane	Inhalation irritant[5]	D	1,000	5,000	--	--	--	1,000
1,1-dichloroethane	Circulatory system effects[4]	C	--	--	--	--	--	--
1,2-dichloroethane	Cancer[2]	B_2	4	--	[6]7,000	5	0	--
dichloromethane	Cancer[2]	B_2	50	2,000	[6]910	5	0	--
1,2-dichloropropane	Cancer, liver, and kidney effects[2]	B_2	6	--	[6]10	5	0	--
hexachloroethane	Cancer[5]	C	1	40	[7]10	--	--	1
tetrachloromethane	Cancer[2]	B_2	3	30	[6]520	5	0	--
tribromomethane (THM)	Cancer[2]	B_2	40	700	[6]300	[3]100	0	--
trichloromethane (THM)	Cancer[2]	B_2	60	400	[6]2,400	[3]100	0	--
1,1,1-trichloroethane	Liver, nervous system effects[2]	D	--	1,000	[6]970	200	200	200
1,1,2-trichloroethane	Liver, kidney, nervous system effects[2]	C	--	100	[6]50,000	5	3	3
trichlorofluoromethane	Mild irritant[4]	D	175	10,000	--	--	--	2,000
1,2,3-trichloropropane	Cancer[5]	B_2	50	200	--	--	--	40
1,1,2-trichloro-1,2,2-trifluoroethane	Nervous system effects[5]	--	210,000	--	--	--	--	--
		Halogenated alkenes						
bromoethene	Cancer[5]	--	--	--	--	--	--	--
chloroethene	Cancer[2]	A	.15	--	[6]3,400	2	0	--

Table 4. Human-health and aesthetic concerns, and drinking-water regulations, goals, and advisories (U.S. Environmental Protection Agency, 1994, 1996a) for NAWQA volatile organic compound target analytes—Continued

IUPAC name	Human-health concern	Cancer rating[1]	Cancer risk E-5 level (µg/L)	DWEL (µg/L)	Taste or odor threshold (µg/L)	MCL (µg/L)	MCLG (µg/L)	Lifetime health advisory (µg/L)
	Halogenated alkenes—Continued							
1,1-dichloroethene	Cancer, liver and kidney effects[2]	C	--	400	[6]1,500	7	7	7
cis-1,2-dichloroethene	Liver, kidney, nervous, circulatory system effects[2]	D	--	400	--	70	70	70
trans-1,2-dichloroethene	Liver, kidney, nervous, circulatory system effects[2]	D	--	600	[7]4.3	100	100	100
cis-1,3-dichloropropene	Cancer[5]	B_2	2	10	--	--	0	--
trans-1,3-dichloropropene	--	B_2	2	10	--	--	0	--
hexachlorobutadiene	--	C	1	70	[7]6	--	1	1
tetrachloroethene	Cancer[2]	--	7	500	[6]190	5	0	--
trichloroethene	Cancer[2]	B_2	30	300	[6]310	5	0	--
	Aromatic hydrocarbons							
benzene	Cancer[2]	A	10	--	[6]170	5	0	--
naphthalene	Liver, reproductive system effects[2]	D	--	100	[8]2.5	--	--	20
styrene	Liver, nervous system effects[2]	C	--	7,000	[6]11	100	100	100
	Alkyl benzenes							
n-butylbenzene	--	--	--	--	--	--	--	--
1,2-dimethylbenzene	Liver, kidney, nervous system effects[2]	D	--	60,000	--	10,000	10,000	10,000
1,3-dimethylbenzene	Liver, kidney, nervous system effects[2]	D	--	60,000	[6]17	10,000	10,000	10,000
1,4-dimethylbenzene	Liver, kidney, nervous system effects[2]	D	--	60,000	--	10,000	10,000	10,000
ethylbenzene	Liver, kidney, nervous system effects[2]	D	--	3,000	[6]29	700	700	700
methylbenzene	Liver, kidney, nervous, circulatory effects[2]	D	--	7,000	[6]42	1,000	1,000	1,000
iso-propylbenzene	Nervous system effect, eye and skin irritant[4]	--	23.3	--	[6].80	--	--	--
n-propylbenzene	--	--	--	--	--	--	--	--
1,2,4-trimethylbenzene	Respiratory, nervous system effects[5]	--	--	--	[7]500	--	--	--
	Halogenated aromatics							
chlorobenzene	Nervous system effects[3]	D	--	700	[6]50	100	100	100
1,2-dichlorobenzene	Liver, kidney, respiratory, nervous system effects[4]	D	--	3,000	[6]24	600	600	600
1,3-dichlorobenzene	Liver, kidney, blood cell damage[2]	D	600	3,000	[8]77	--	--	600

Table 4. Human-health and aesthetic concerns, and drinking-water regulations, goals, and advisories (U.S. Environmental Protection Agency, 1994, 1996a) for NAWQA volatile organic compound target analytes—Continued

IUPAC name	Human-health concern	Cancer rating[1]	Cancer risk E-5 level (µg/L)	DWEL (µg/L)	Taste or odor threshold (µg/L)	MCL (µg/L)	MCLG (µg/L)	Lifetime health advisory (µg/L)
		Halogenated aromatics—Continued						
1,4-dichlorobenzene	Cancer[2]	C	--	4,000	[8]4.5	75	75	75
1,2,3-trichlorobenzene	--	--	--	--	[7]10	--	--	--
1,2,4-trichlorobenzene	Liver, kidney effects[2]	D	--	40	[7]5	70	70	70
		Ethers						
tert-amyl methyl ether	--	--	--	--	--	--	--	--
diisopropyl ether	Strong irritant[4]	--	--	--	--	--	--	--
ethyl *tert*-butyl ether	--	--	--	--	--	--	--	--
methyl *tert*-butyl ether	--	C (tentative)	70	1,000	[8]15	--	--	[9, 10]20-40
		Others (aldehydes and nitriles)						
2-propenal	Respiratory system effects, eye and skin irritant[5]	C	--	--	[6]110	--	--	--
2-propenenitrile	Cancer[5]	B_1	.6	--	[6]9,100	--	0	--

[1]Carcinogen rating as determined by U.S. Environmental Protection Agency (1996a).
- A, Human carcinogen—sufficient evidence in epidemiologic studies to support causal association between exposure and cancer;
- B_1, Probable human carcinogen—limited evidence in epidemiological studies;
- B_2, Probable human carcinogen—sufficient evidence from animal studies;
- C, Possible human carcinogen—limited or equivocal evidence from animal studies and inadequate or no data from human studies;
- D, Not classified—inadequate or no human and animal evidence of carcinogenicity; and
- E, No evidence of carcinogenicity for humans. No evidence of carcinogenicity in at least two adequate animal tests in different species or in adequate epidemilogic and animal studies
- --, Information not available

[2]U.S. Environmental Protection Agency, 1994.
[3]Total for THMs is 100 µg/L.
[4]Prager, 1995.
[5]Lewis, 1997.
[6]Ammore and Hautala, 1983.
[7]Verschueren, 1983.
[8]Young and others, 1996.
[9]This advisory is based on aesthetic reasons (taste and/or odor properties).
[10]U.S. Environmental Protection Agency, 1997.

The USEPA has established Maximum Contaminant Level Goals (MCLGs) for 33 of the VOC target analytes. The MCLG is a nonenforceable concentration of a drinking-water contaminant that is protective of adverse human-health effects and allows an adequate margin of safety. Most of the compounds classified as known or probable carcinogens have an MCLG set at zero; that is, the goal is that these compounds are not present in drinking water.

The USEPA has also established lifetime health advisories for drinking water, and 26 of the VOC target analytes have such an advisory. One additional VOC target analyte, methyl *tert*-butyl ether, has an aesthetic advisory for taste and odor concerns. Drinking-water health advisories are provided for various exposure durations including 1-day, 10-day, long-term (approximately 7 years), and lifetime (U.S. Environmental Protection Agency, 1996a). Lifetime health advisories for the VOC target analytes are given in the last column of table 4. This advisory is defined by the USEPA as the concentration of a chemical in drinking water that is not expected to cause any adverse noncarcinogenic effect over a lifetime of exposure within a specified margin of safety. Health advisories serve as informal technical guidance to the States and water utilities for protecting public health when contamination situations occur in drinking-water supplies.

Aquatic Toxicity and Water-Quality Guidelines

Detailed information on the aquatic toxicity of the VOC target analytes and other VOCs has been reported recently by Rowe and others (1997). That publication provides a comprehensive listing of aquatic toxicity data for each VOC target analyte for each aquatic organism tested to date. Select information for aquatic toxicity adapted from Rowe and others (1997) is given in table 5 including the lowest concentration and associated effect for the most sensitive species. Freshwater, water-quality guidelines established by the USEPA and Environment Canada are also listed in table 5.

The lowest concentration and effect information listed in table 5 were derived from USEPA's AQUIRE data base (U.S. Environmental Protection Agency, 1996b). AQUIRE, a centralized international source for toxic effects information, has been updated periodically for the past 17 years. To be included in table 5, toxicity studies listed in AQUIRE had to meet the following criteria: (1) studies must have been conducted in freshwater, and (2) studies must have complete or moderately complete documentation of test procedures. Toxicity information listed in table 5 is based on information retrieved from AQUIRE in 1997.

Aquatic toxicity tests typically are conducted by exposing organisms to a range of contaminant concentrations under controlled conditions and measuring the response of the organisms (Rand and Petrocelli, 1985). Acute toxicity tests are used to determine if solutions are toxic to species during short-duration exposures (typically 96 hours or less), and species mortality is the most common endpoint. Chronic toxicity tests use a longer duration of exposure (typically 7 days or more). Responses other than species mortality typically are measured during chronic tests and may include changes in reproduction, growth, and behavior. No exact duration or response, however, distinguishes acute nor chronic toxicity tests.

The majority of published toxicity information for VOCs are median lethal concentration (LC_{50}) values, the estimated concentrations at which 50 percent of the organisms died during the toxicity test. The median effective concentration (EC_{50}) is the estimated concentration that affects 50 percent of the organisms; however, the endpoint of the test is an effect other than mortality. Other toxicity information for VOCs include: (1) no observed effective concentration (NOEC), the highest concentration at which effects are not found or are not statistically significant; (2) lowest observed effective concentration (LOEC), the lowest concentration producing a statistically significant effect; and (3) maximum acceptable toxicant concentration (MATC), the chronic value representing the hypothetical threshold concentration that is the geometric mean between the NOEC and LOEC concentrations.

Some aquatic species are more sensitive to certain contaminants than others and are affected at lower concentrations. Furthermore, some compounds are acutely toxic to a species over a relatively narrow concentration range. When this occurs, the lowest concentration that affects the species is reported in table 5 as a range rather than a single value. Four measures of aquatic toxicity were reviewed for each VOC target analyte to determine the lowest concentration and associated effect. In order of precedence, these include the MATC, LOEC, EC_{50}, and LC_{50}. The lowest concentrations, measured in micrograms per liter, were available for 42 of the 55 VOC target analytes, and the lowest concentrations ranged from 6.5 to 13 µg/L for hexachlorobutadiene to 672,000 µg/L for methyl *tert*-butyl ether.

Table 5. Lowest concentrations of volatile organic compound target analytes that affect the most sensitive aquatic species, and water-quality guidelines (adapted from Rowe and others, 1997)

[Values in micrograms per liter unless otherwise indicated; IUPAC, International Union of Pure and Applied Chemistry; when available, the lowest concentration is given in the following order of precedence: MATC, maximum acceptable toxicant concentration; LOEC, lowest observed effective concentration; EC_{50}, median effective concentration; LC_{50}, median lethal concentration; --, not reported; nv, no value; <, less than; >, greater than]

IUPAC name	Taxonomic classification	*Genus, species*/ Common name	Lowest concentration and effect					Duration of test (hours)	USEPA freshwater acute guidelines[2]	USEPA freshwater chronic guidelines[2]	Canadian water-quality guidelines[3]
			MATC	LOEC	EC_{50}	LC_{50}	End-point effect[1]				
Halogenated alkanes											
bromodichloromethane	--	--	--	--	--	--	--	--	11,000	--	--
bromomethane	fish	*Oryzias latipes*/ Medaka, high eyes	nv	nv	400	--	BEH	96	11,000	--	--
chlorodibromomethane	fish	*Cyprinus carpio*/ Common, mirror, colored carp	nv	nv	nv	34,000	MOR	72-120	11,000	--	--
chloroethane	--	--	--	--	--	--	--	--	[4]860,000	[5]230,000	--
chloromethane	fish	*Lepomis macrochirus*/ Bluegill	nv	nv	nv	550,000	MOR	96	--	--	--
1,2-dibromo-3-chloro-propane	fish	*Lepomis macrochirus*/ Bluegill	nv	nv	nv	20,000	MOR	48	--	--	--
1,2-dibromoethane	fish	*Micropterus salmoides*/ Largemouth bass	nv	nv	nv	15,000	MOR	24	--	--	--
dichlorodifluoromethane	--	--	--	--	--	--	--	--	11,000	--	--
1,1-dichloroethane	--	--	--	--	--	--	--	--	--	--	--
1,2-dichloroethane	fish	*Pimephales promelas*/ Fathead minnow	29,000-59,000	--	--	--	GRO	768	118,000	20,000	100
dichloromethane	amphibian	*Rana catesbeiana*/ Bullfrog	nv	nv	17,780	--	TER	192	11,000	--	98
1,2-dichloropropane	fish	*Pimephales promelas*/ Fathead minnow	6,000-11,000	--	--	--	GRO	768	--	--	--
hexachloroethane	fish	*Oncorhynchus mykiss*/ Rainbow trout, donaldson trout	67-207	--	--	--	GRO	768	980	540	--

Table 5. Lowest concentrations of volatile organic compound target analytes that affect aquatic species and water-quality guidelines—Continued

IUPAC name	Taxonomic classification	*Genus, species*/ Common name	Lowest concentration and effect					Duration of test (hours)	USEPA freshwater acute guidelines[2]	USEPA freshwater chronic guidelines[2]	Canadian water-quality guidelines[3]
			MATC	LOEC	EC_{50}	LC_{50}	End-point effect[1]				
Halogenated alkanes—Continued											
tetrachloromethane	fish	*Pimephales promelas*/ Fathead minnow	52,100	--	--	--	MOR	168	35,200	--	13
tribromomethane	plant	*Selenastrum capricornutum*/ Green algae	nv	nv	38,600	--	CLR	96	11,000	--	--
trichloromethane	amphibian	*Hyla crucifer*/ Spring peeper	nv	nv	270	--	TER	168	28,900	1,240	2
1,1,1-trichloroethane	fish	*Pimephales promelas*/ Fathead minnow	nv	nv	11,100	--	IMM	72	18,000	--	--
1,1,2-trichloroethane	fish	*Oncorhynchus mykiss*/ Rainbow trout, donaldson trout	6,000-14,800	--	--	--	GRO	768	18,000	9,400	--
trichlorofluoromethane	--	--	--	--	--	--	--	--	11,000	--	--
1,2,3-trichloropropane	fish	*Pimephales promelas*/ Fathead minnow	nv	nv	nv	66,500	MOR	96	--	--	--
1,1,2-trichloro-1,2,2-trifluoroethane	--	--	--	--	--	--	--	--	--	--	--
Halogenated alkenes											
bromoethene	--	--	--	--	--	--	--	--	--	--	--
chloroethene	--	--	--	--	--	--	--	--	--	--	--
1,1-dichloroethene	plant	*Scenedesmus abundans*/ Green algae	nv	nv	410,000	--	GRO	96	11,600	--	--
cis-1,2-dichloroethene	--	--	--	--	--	--	--	--	11,600	--	--
trans-1,2-dichloroethene	insect	*Daphnia magna*/ Water flea	nv	nv	nv	220,000	MOR	48	11,600	--	--

Table 5. Lowest concentrations of volatile organic compound target analytes that affect aquatic species and water-quality guidelines—Continued

IUPAC name	Taxonomic classification	*Genus, species*/ Common name	Lowest concentration and effect					Duration of test (hours)	USEPA freshwater acute guidelines[2]	USEPA freshwater chronic guidelines[2]	Canadian water-quality guidelines[3]
			MATC	LOEC	EC_{50}	LC_{50}	End-point effect[1]				
Halogenated alkenes—Continued											
cis-1,3-dichloropropene	--	--	--	--	--	--	--	--	6,600	244	--
trans-1,3-dichloropropene	--	--	--	--	--	--	--	--	6,600	244	--
hexachlorobutadiene	fish	*Pimephales promelas*/ Fathead minnow	6.5-13	--	--	--	GRO	768	90	9.3	0.1
tetrachloroethene	fish	*Oncorhynchus mykiss*/ Rainbow trout, donaldson trout	500-1,400	--	--	--	GRO	768	5,280	840	110
trichloroethene	fish	*Jordanella floridae*/ Flagfish	nv	11,000	--	--	MOR	240	45,000	21,900	20
Aromatic hydrocarbons											
benzene	fish	*Pimephales promelas*/ Fathead minnow	nv	17,200	--	--	GRO	168	5,300	--	300
naphthalene	insect	*Daphnia magna*/ Water flea	nv	nv	690	--	PTR	2	2,300	620	--
styrene	fish	*Oncorhynchus mykiss*/ Rainbow trout, donaldson trout	nv	nv	nv	2,500	MOR	24	--	--	--
Alkyl benzenes											
n-butylbenzene	insect	*Daphnia magna*/ Water flea	490	--	--	--	IMM	48	--	--	--
1,2-dimethylbenzene	fish	*Oncorhynchus kisutch*/ Coho salmon, silver salmon	nv	nv	600	--	AVO	1	--	--	--
1,3-dimethylbenzene	plant	*Selenastrum capricornutum*/ Green algae	nv	nv	3,900	--	GRO	192	--	--	--

Table 5. Lowest concentrations of volatile organic compound target analytes that affect aquatic species and water-quality guidelines—Continued

IUPAC name	Taxonomic classification	*Genus, species*/ Common name	Lowest concentration and effect					Duration of test (hours)	USEPA freshwater acute guidelines[2]	USEPA freshwater chronic guidelines[2]	Canadian water-quality guidelines[3]
			MATC	LOEC	EC_{50}	LC_{50}	End-point effect[1]				
Alkyl benzenes—Continued											
1,4-dimethylbenzene	plant	*Selenastrum capricornutum*/ Green algae	nv	nv	3,200	--	GRO	72	--	--	--
ethylbenzene	insect	*Daphnia magna*/ Water flea	nv	nv	1,810	--	IMM	24	32,000	--	90
methylbenzene	fish	*Pimephales promelas*/ Fathead minnow	nv	6,000	--	--	GRO	768	17,500	--	2
iso-propylbenzene	insect	*Daphnia magna*/ Water flea	nv	nv	601	--	IMM	48	--	--	--
n-propylbenzene	plant	*Selenastrum capricornutum*/ Green algae	nv	nv	1,800	--	GRO	72	--	--	--
1,2,4-trimethylbenzene	insect	*Daphnia magna*/ Water flea	nv	nv	3,600	--	IMM	48	--	--	--
Halogenated aromatics											
chlorobenzene	insect	*Daphnia magna*/ Water flea	nv	nv	585	--	IMM	48	250	50	15
1,2-dichlorobenzene	insect	*Daphnia magna*/ Water flea	nv	nv	550	--	REP	336	1,120	763	2.5
1,3-dichlorobenzene	fish	*Oncorhynchus mykiss*/ Rainbow trout, donaldson trout	555-1,040	--	--	--	GRO	768	1,120	763	2.5
1,4-dichlorobenzene	fish	*Oncorhynchus mykiss*/ Rainbow trout, donaldson trout	565-1,040	--	--	--	GRO	768	1,120	763	4
1,2,3-trichlorobenzene	insect	*Daphnia magna*/ Water flea	nv	nv	200	--	REP	336	--	--	0 .9

Table 5. Lowest concentrations of volatile organic compound target analytes that affect aquatic species and water-quality guidelines—Continued

IUPAC name	Taxonomic classification	*Genus, species*/ Common name	Lowest concentration and effect					Duration of test (hours)	USEPA freshwater acute guidelines[2]	USEPA freshwater chronic guidelines[2]	Canadian water-quality guidelines[3]
			MATC	LOEC	EC_{50}	LC_{50}	End-point effect[1]				
Halogenated aromatics—Continued											
1,2,4-trichlorobenzene	fish	*Oncorhynchus mykiss*/ Rainbow trout, donaldson trout	406	--	--	--	GRO	1,080	250	50	0.5
Ethers											
tert-amyl methyl ether	--	--	--	--	--	--	--	--	--	--	--
diisopropyl ether	fish	*Pimephales promelas*/ Fathead minnow	nv	nv	nv	91,700	MOR	96	--	--	--
ethyl *tert*-butyl ether	--	--	--	--	--	--	--	--	--	--	--
methyl *tert*-butyl ether	fish	*Pimephales promelas*/ Fathead minnow	nv	nv	nv	672,000	MOR	96	--	--	--
Others (aldehydes and nitriles)											
2-propenal	insect	*Daphnia magna*/ Water flea	nv	nv	51	--	IMM	48	68	21	1,000
2-propenenitrile	insect	*Daphnia magna*/ Water flea	nv	nv	10,950	--	IMM	48	7,550	2,600	--

[1]Endpoint effect: AVO, avoidance; BEH, behavior; BMS, biomass; CLR, chlorophyll; GRO, growth; IMM, immobilization; MOR, mortality; PTR, phototactic response; REP, reproduction; TER, teratogenesis.

[2]U.S. Environmental Protection Agency, 1996c.

[3]Canadian Council of Resource and Environmental Ministers, 1991.

[4]1-hour average, freshwater acute water-quality guidelines.

[5]4-day average, freshwater chronic water-quality guidelines.

Water-quality guidelines published by the USEPA for protection of freshwater biota are available for 33 of the 55 VOC target analytes, and 17 have water-quality guidelines established by Environment Canada (table 5). Information concerning these guidelines was obtained from USEPA's Integrated Risk Information System (IRIS) (U.S. Environmental Protection Agency, 1996c) and from Environment Canada (Canadian Council of Resource and Environment Ministers, 1991). When toxicity information is insufficient to develop criteria, the USEPA uses values equal to the LOEC as a guideline. The acute and chronic criteria are based on the highest concentration of a pollutant that freshwater aquatic organisms can be exposed to for an established period of time without deleterious effects. Nonenforceable Canadian guidelines are based on short-term toxicity data (96-hour LC_{50}) of the most sensitive species multiplied by application factors of 0.05 for nonpersistent effects and 0.01 for persistent effects (Canadian Council of Resource and Environment Ministers, 1991).

Physical, Chemical, and Biological Properties

Transport, behavior, and fate of VOCs are determined by a combination of various physical, chemical, and biological properties (Rathbun, 1998). The most important physical, chemical, and biological properties of the VOC target analytes used to predict their aquatic behavior and fate include: aqueous solubility, vapor pressure, Henry's law constant, octanol-water partitioning coefficient, sorption coefficient, half-life (hydrolysis, photolysis, chemical oxidation, and aerobic and anaerobic biodegradation), and bioconcentration factors. Definitions for these properties are given in appendix 2.

Several references have already compiled a vast majority of the physical, chemical, and biological properties for the VOC target analytes. Especially noteworthy are the comprehensive compilations reported by Rathbun (1998), Howard (1990, 1991a, 1991b, 1993, 1997), Howard and others (1991), and Mackay and others (1992a, 1992b, 1993, 1995). Other reference texts and several journals have additional physical, chemical, and biological data for the VOC target analytes.

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APPENDIXES

Appendix 1. Volatile organic compounds (VOCs) considered as candidate target analytes and results of Phase 1 of screening procedure

[IUPAC, International Union of Pure and Applied Chemistry; DWEL, drinking-water equivalent level; CWQC, chronic water-quality criteria; ≤, less than or equal to; µg/L, micrograms per liter; NWQL, U.S. Geological Survey National Water Quality Laboratory; SH, National Water Quality Laboratory analysis schedule; --, information not available]

Candidate target analyte		Information used in the Phase 1 screening procedure to identify compounds as candidate target analytes						Compound on NWQL SH 2090
Compound number	IUPAC name	Physical properties typical of VOCs	Human carcinogen rating[1]	DWEL (µg/L)	CWQC or aquatic toxicity (µg/L)	Occurs frequently in water samples	Other national concerns	
1	acrylamide	Yes	B_2	7	--	--	--	No
2	benzene	Yes	A	--	--	--	--	Yes
3	bromodichloromethane	Yes	B_2	700	--	--	--	Yes
4	bromoethene	Yes	A	--	--	--	--	No
5	chloroethane	Yes	B	--	230,000	--	--	Yes
6	chloroethene	Yes	A	--	--	--	--	Yes
7	*bis*-(2-chloroethyl) ether	Yes	B_2	--	--	--	--	No
8	*bis*-(2-chloroethyl) sulfide	Yes	A	--	--	--	--	No
9	*bis*-(chloromethyl) ether	Yes	A	8	--	--	--	No
10	chloromethyl methyl ether	Yes	A	--	--	--	--	No
11	1,2-dibromo-3-chloropropane	Yes	B_2	--	--	--	--	Yes
12	1,2-dibromoethane	Yes	B_2	--	--	--	--	Yes
13	1,2-dichloroethane	Yes	B_2	--	20,000	--	--	Yes
14	dichloromethane	Yes	B_2	2,000	--	--	--	Yes
15	1,2-dichloropropane	Yes	B_2	--	--	--	--	Yes
16	*cis*-1,3-dichloropropene	Yes	B_2	10	244	--	--	Yes
17	*trans*-1,3-dichloropropene	Yes	B_2	10	244	--	--	Yes
18	1,4-dioxane	Yes	B_2	--	--	--	--	No
19	formaldehyde	Yes	B_1	5,000	--	--	--	No
20	2-propenenitrile	Yes	B_1	--	2,600	--	--	No
21	tetrachloromethane	Yes	B_2	30	--	--	--	Yes

Appendix 1. Volatile organic compounds (VOCs) considered as candidate target analytes and results of Phase 1 of screening procedure—Continued

Candidate target analyte		Information used in the Phase 1 screening procedure to identify compounds as candidate target analytes						Compound on NWQL SH 2090
Compound number	IUPAC name	Physical properties typical of VOCs	Human carcinogen rating[1]	DWEL (µg/L)	CWQC or aquatic toxicity (µg/L)	Occurs frequently in water samples	Other national concerns	
22	tribromomethane	Yes	B_2	700	--	--	--	Yes
23	trichloroethene	Yes	B_2	300	21,900	--	--	Yes
24	trichloromethane	Yes	B_2	400	1,240	--	--	Yes
25	1,2,3-trichloropropane	Yes	B_2	200	--	--	--	Yes
26	bromomethane	Yes	D	50	--	--	--	Yes
27	chloromethane	Yes	C	100	--	--	--	Yes
28	hexachlorobutadiene	Yes	C	70	9.3	--	--	Yes
29	hexachloroethane	Yes	C	40	540	--	--	No
30	naphthalene	Yes	D	100	620	--	--	Yes
31	pentachlorobenzene	Yes	--	28	50	--	--	No
32	1,2,4-trichlorobenzene	Yes	D	40	50	--	--	Yes
33	1,1,2-trichloroethane	Yes	C	100	9,400	--	--	Yes
34	*n*-butylbenzene	Yes	--	--	[2]490	--	--	Yes
35	chlorobenzene	Yes	D	700	50	--	--	Yes
36	hexachlorocyclopentadiene	Yes	D	200	5.2	--	--	No
37	2-propenal	Yes	--	--	21	--	--	No
38	*iso*-propylbenzene	Yes	--	--	[2]610	--	--	Yes
39	*n*-propylbenzene	Yes	--	--	[2]1,800	--	--	Yes
40	chlorodibromomethane	Yes	C	700	--	Yes	--	Yes
41	1,2-dichlorobenzene	Yes	D	3,000	763	Yes	--	Yes
42	1,3-dichlorobenzene	Yes	D	3,000	763	Yes	--	Yes
43	1,4-dichlorobenzene	Yes	C	4,000	763	Yes	--	Yes
44	1,1-dichloroethane	Yes	--	--	--	Yes	--	Yes

Appendix 1. Volatile organic compounds (VOCs) considered as candidate target analytes and results of Phase 1 of screening procedure—Continued

Candidate target analyte		Information used in the Phase 1 screening procedure to identify compounds as candidate target analytes						Compound on NWQL SH 2090
Compound number	IUPAC name	Physical properties typical of VOCs	Human carcinogen rating[1]	DWEL (μg/L)	CWQC or aquatic toxicity (μg/L)	Occurs frequently in water samples	Other national concerns	
45	1,1-dichloroethene	Yes	C	400	20,000	Yes	--	Yes
46	*cis*-1,2-dichloroethene	Yes	D	400	--	Yes	--	Yes
47	*trans*-1,2-dichloroethene	Yes	D	600	--	Yes	--	Yes
48	dichlorodifluoromethane	Yes	D	5,000	--	Yes	--	Yes
49	1,2-dimethylbenzene	Yes	D	60,000	--	Yes	--	Yes
50	1,3-dimethylbenzene	Yes	D	60,000	--	Yes	--	Yes
51	1,4-dimethylbenzene	Yes	D	60,000	--	Yes	--	Yes
52	ethylbenzene	Yes	D	3,000	--	Yes	--	Yes
53	methylbenzene	Yes	D	7,000	--	Yes	--	Yes
54	methyl *tert*-butyl ether	Yes	C(tentative)	1,000	--	Yes	--	Yes
55	styrene	Yes	C	7,000	--	Yes	--	Yes
56	tetrachloroethene	Yes	--	500	840	Yes	--	Yes
57	1,1,1-trichloroethane	Yes	D	1,000	--	Yes	--	Yes
58	trichlorofluoromethane	Yes	D	10,000	--	Yes	--	Yes
59	1,2,4-trimethylbenzene	Yes	--	--	--	Yes	--	Yes
60	1,1,2-trichloro-1,2,2-trifluoroethane	Yes	--	--	--	--	Yes	Yes
61	1,2,3-trichlorobenzene	Yes	--	--	--	--	Yes	Yes
62	*tert*-amyl methyl ether	Yes	--	--	--	--	Yes	No
63	diisopropyl ether	Yes	--	--	--	--	Yes	No
64	ethyl *tert*-butyl ether	Yes	--	--	--	--	Yes	No
65	bromobenzene	Yes	--	--	--	--	--	Yes
66	bromochloromethane	Yes	--	50	--	--	--	Yes
67	2-butanone	Yes	--	--	--	--	--	No

Appendix 1. Volatile organic compounds (VOCs) considered as candidate target analytes and results of Phase 1 of screening procedure—Continued

Candidate target analyte		Information used in the Phase 1 screening procedure to identify compounds as candidate target analytes						Compound on NWQL SH 2090
Compound number	IUPAC name	Physical properties typical of VOCs	Human carcinogen rating[1]	DWEL (μg/L)	CWQC or aquatic toxicity (μg/L)	Occurs frequently in water samples	Other national concerns	
68	*tert*-butylbenzene	Yes	--	--	--	--	--	Yes
69	*tert*-butyl formate	Yes	--	--	--	--	--	No
70	*bis*-(2-chloroisopropyl) ether	Yes	D	1,000	--	--	--	No
71	1-chloro-2-methylbenzene	Yes	D	700	--	--	--	Yes
72	1-chloro-4-methylbenzene	Yes	D	700	--	--	--	Yes
73	dibromomethane	Yes	D	--	--	--	--	Yes
74	dichloroacetonitrile	Yes	C	300	--	--	--	No
75	1,1-dichloropropane	Yes	--	--	5,700	--	--	No
76	1,3-dichloropropane	Yes	--	--	5,700	--	--	Yes
77	2,2-dichloropropane	Yes	--	--	5,700	--	--	Yes
78	1,1-dichloropropene	Yes	--	--	244	--	--	Yes
79	*n*-hexane	Yes	D	--	--	--	--	No
80	isophorone	Yes	C	7,000	--	--	--	No
81	1-isopropyl-4-methylbenzene	Yes	--	--	--	--	--	Yes
82	(1-methylpropyl)benzene	Yes	--	--	--	--	--	Yes
83	pentachloroethane	Yes	--	--	1,200	--	--	No
84	phenol	Yes	D	20,000	2,560	--	--	No
85	1,1,1,2-tetrachloroethane	Yes	C	1,000	--	--	--	Yes
86	1,1,2,2-tetrachloroethane	Yes	--	--	2,400	--	--	Yes
87	trichloroacetonitrile	Yes	--	--	--	--	--	No
88	1,3,5-trichlorobenzene	Yes	D	200	--	--	--	No
89	1,3,5-trimethylbenzene	Yes	--	--	--	--	--	Yes
90	benzidine	No	--	--	--	--	--	No

Appendix 1. Volatile organic compounds (VOCs) considered as candidate target analytes and results of Phase 1 of screening procedure—Continued

Candidate target analyte		Information used in the Phase 1 screening procedure to identify compounds as candidate target analytes						Compound on NWQL SH 2090
Compound number	IUPAC name	Physical properties typical of VOCs	Human carcinogen rating[1]	DWEL (μg/L)	CWQC or aquatic toxicity (μg/L)	Occurs frequently in water samples	Other national concerns	
91	bromochloroacetonitrile	No	--	--	--	--	--	No
92	chloroacetic acid	No	--	--	--	--	--	No
93	4-chloro-3-methylphenol	No	--	--	--	--	--	No
94	(chloromethyl) oxirane	No	B_2	70	--	--	--	No
95	2-chlorophenol	No	D	200	--	--	--	No
96	4-chlorophenol	No	--	--	--	--	--	No
97	chloropicrin	No	--	--	--	--	--	No
98	dichloroacetic acid	No	B_2	100	--	--	--	No
99	dichloroacetylaldehyde	No	--	--	--	--	--	No
100	3,3-dichlorobenzidine	No	--	--	--	--	--	No
101	2,4-dichlorophenol	No	D	100	--	--	--	No
102	2,4-dimethylphenol	No	--	--	--	--	--	No
103	1,3-dinitrobenzene	No	D	5	--	--	--	No
104	2,4-dinitro-o-cresol	No	--	--	--	--	--	No
105	2,4-dinitrotoluene	No	B_2	100	--	--	--	No
106	2,6-dinitrotoluene	No	B_2	40	--	--	--	No
107	diphenylamine	No	D	1,000	--	--	--	No
108	diphenylhydrazine	No	--	--	--	--	--	No
109	ethylene glycol	No	D	40,000	--	--	--	No
110	ethylene thiourea	No	B_2	3	--	--	--	No
111	hexachlorobenzene	No	B_2	30	--	--	--	No
112	maleic hydrazide	No	D	20,000	--	--	--	No
113	nitrobenzene	No	--	--	--	--	--	No

Appendix 1. Volatile organic compounds (VOCs) considered as candidate target analytes and results of Phase 1 of screening procedure—Continued

Candidate target analyte		Information used in the Phase 1 screening procedure to identify compounds as candidate target analytes						Compound on NWQL SH 2090
Compound number	IUPAC name	Physical properties typical of VOCs	Human carcinogen rating[1]	DWEL (μg/L)	CWQC or aquatic toxicity (μg/L)	Occurs frequently in water samples	Other national concerns	
114	4-nitrophenol	No	D	300	--	--	--	No
115	nitroquanidine	No	D	4,000	--	--	--	No
116	*n*-nitrosodibutylamine	No	--	--	--	--	--	No
117	*n*-nitrosodiethylamine	No	--	--	--	--	--	No
118	*n*-nitrosodimethylamine	No	--	--	--	--	--	No
119	*n*-nitrosodiphenylamine	No	--	--	--	--	--	No
120	nitrosodi-n-propylamine	No	--	--	--	--	--	No
121	*n*-nitrosopyrrolidine	No	--	--	--	--	--	No
122	pentachlorophenol	No	B_2	1,000	--	--	--	No
123	picloram	No	D	2,000	--	--	--	No
124	1,2,4,5-tetrachlorobenzene	No	--	--	--	--	--	No
125	2,3,5,6-tetrachlorophenol	No	--	--	--	--	--	No
126	trichloroacetic acid	No	C	4,000	--	--	--	No
127	trichloroethanol	No	--	--	--	--	--	No
128	2,4,5-trichlorophenol	No	--	--	--	--	--	No
129	2,4,6-trichlorophenol	No	B_2	--	--	--	--	No
130	toxaphene	No	B_2	--	--	--	--	No

[1]Carcinogen rating as determined by U.S. Environmental Protection Agency (1996a).

A, Human carcinogen—sufficient evidence in epidemiologic studies to support causal association between exposure and cancer;
B_1, Probable human carcinogen—limited evidence in epidemiological studies;
B_2, Probable human carcinogen—sufficient evidence from animal studies;
C, Possible human carcinogen—limited or equivocal evidence from animal studies and inadequate or no data from human studies;
D, Not classified—inadequate or no human and animal evidence of carcinogenicity; and
E, No evidence of carcinogenicity for humans. No evidence of carcinogenicity in at least two adequate animal tests in different species or in adequate epidemilogic and animal studies
--, Information not available

[2]Selected from USEPA's AQUIRE (USEPA, 1996b) database because of low toxicity. A safety factor of 100 was applied to this value for selection because of aquatic toxicity.

Appendix 2. Definitions for physical, chemical, and biological properties

Aqueous solubility	A measure of the pure compound's abundance by volume in the aqueous phase when the solution is in equilibrium with the pure compound in its actual aggregation state (gas, liquid, solid) at a specified temperature and pressure (Schwarzenbach and others, 1993).
Vapor pressure	The pressure of the vapor of a compound at equilibrium with its pure condensed phase, be it liquid or solid (Schwarzenbach and others, 1993).
Henry's law constant	The ratio of a compound's abundance in the gas phase to the abundance in the aqueous phase at equilibrium at a specific temperature and pressure (Schwarzenbach and others, 1993).
Octanol-water partitioning coefficient	The subdivision of a population of molecules between the octanol and water phases (Schwarzenbach and others, 1993).
Sorption coefficient	The subdivision of a population of molecules between the organic carbon and water phases (Schwarzenbach and others, 1993).
Half-life	A measure of the time in which the concentration of the compound is lowered by a factor of 2 (Schwarzenbach and others, 1993).
Bioconcentration factor	A measure of the uptake from water of the compound by organisms within an aquatic system (Rathbun, 1998).