

**U.S. Department of the Interior
U.S. Geological Survey**

Prepared in cooperation with the
FEDERAL HIGHWAY ADMINISTRATION

Chemical-Help Application for Classification and Identification of Stormwater Constituents

Open-File Report 00-468

A Contribution to the
NATIONAL HIGHWAY RUNOFF DATA AND METHODOLOGY SYNTHESIS



U.S. Department
of Transportation



U.S. Department of the Interior
U.S. Geological Survey

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By GREGORY E. GRANATO, TIMOTHY R. DRISKELL, and CATHERINE NUNES

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Northborough, Massachusetts
2000

U.S. DEPARTMENT OF THE INTERIOR
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PREFACE

Knowledge of the characteristics of highway runoff (concentrations and loads of constituents and the physical and chemical processes which produce this runoff) is important for decision makers, planners, and highway engineers to assess and mitigate possible adverse impacts of highway runoff on the Nation's receiving waters. In October 1996, the Federal Highway Administration and the U.S. Geological Survey began the National Highway Runoff Data and Methodology Synthesis to provide a catalog of the pertinent information available; to define the necessary documentation to determine if data are valid (useful for intended purposes), current, and technically supportable; and to evaluate available sources in terms of current and foreseeable information needs. This paper is one contribution to the National Highway Runoff Data and Methodology Synthesis and is being made available as a U.S. Geological Survey Open-File Report pending its inclusion in a volume or series to be published by the Federal Highway Administration. More information about this project is available on the World Wide Web at <http://ma.water.usgs.gov/fhwa/>

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| | | | | | | | |
|-------------------------------------|----------------------------|-------------------------|------------------------|-------------------|-------------------|------------------------|-------------------|
| in | inches | 25.4 | millimeters | mm | mm | millimeters | mm |
| ft | feet | 0.305 | meters | m | m | meters | m |
| yd | yards | 0.914 | meters | m | m | meters | m |
| mi | miles | 1.61 | kilometers | km | km | kilometers | km |
| AREA | | | | | | | |
| in ² | square inches | 645.2 | square millimeters | mm ² | mm ² | square millimeters | mm ² |
| ft ² | square feet | 0.093 | square meters | m ² | m ² | square meters | m ² |
| yd ² | square yards | 0.836 | square meters | m ² | m ² | square meters | m ² |
| ac | acres | 0.405 | hectares | ha | ha | hectares | ha |
| mi ² | square miles | 2.59 | square kilometers | km ² | km ² | square kilometers | km ² |
| VOLUME | | | | | | | |
| fl oz | fluid ounces | 29.57 | milliliters | mL | mL | milliliters | mL |
| gal | gallons | 3.785 | liters | L | L | liters | L |
| ft ³ | cubic feet | 0.028 | cubic meters | m ³ | m ³ | cubic meters | m ³ |
| yd ³ | cubic yards | 0.765 | cubic meters | m ³ | m ³ | cubic meters | m ³ |
| TEMPERATURE (exact) | | | | | | | |
| °F | Fahrenheit temperature | 5(F-32)/9 or (F-32)/1.8 | Celsius temperature | °C | °C | Celsius temperature | °C |
| ILLUMINATION | | | | | | | |
| fc | foot-candles | 10.76 | lux | lx | lx | lux | lx |
| fl | foot-Lamberts | 3.426 | candela/m ² | cd/m ² | cd/m ² | candela/m ² | cd/m ² |
| FORCE and PRESSURE or STRESS | | | | | | | |
| lbf | poundforce | 4.45 | newtons | N | N | newtons | N |
| lbf/in ² | poundforce per square inch | 6.89 | kilopascals | kPa | kPa | kilopascals | kPa |
| TEMPERATURE (exact) | | | | | | | |
| °F | Fahrenheit temperature | 1.8C + 32 | Fahrenheit temperature | °F | °F | Fahrenheit temperature | °F |
| ILLUMINATION | | | | | | | |
| fc | foot-candles | 0.0929 | foot-candles | fc | fc | foot-candles | fc |
| fl | foot-Lamberts | 0.2919 | foot-Lamberts | fl | fl | foot-Lamberts | fl |
| FORCE and PRESSURE or STRESS | | | | | | | |
| lbf | poundforce | 0.225 | newtons | N | N | newtons | N |
| lbf/in ² | poundforce per square inch | 0.145 | kilopascals | kPa | kPa | kilopascals | kPa |

NOTE: Volumes greater than 1000 l shall be shown in m³.

* SI is the symbol for the International System of Units. Appropriate rounding should be made to comply with Section 4 of ASTM E380.

Chemical-Help Application for Classification and Identification of Stormwater Constituents

By Gregory E. Granato, Timothy R. Driskell, and Catherine Nunes

Abstract

A computer application called Chemical Help was developed to facilitate review of reports for the National Highway Runoff Water-Quality Data and Methodology Synthesis (NDAMS). The application provides a tool to quickly find a proper classification for any constituent in the NDAMS review sheets. Chemical Help contents include the name of each water-quality property, constituent, or parameter, the section number within the NDAMS review sheet, the organizational levels within a classification hierarchy, the database number, and where appropriate, the chemical formula, the Chemical Abstract Service number, and a list of synonyms (for the organic chemicals). Therefore, Chemical Help provides information necessary to research available reference data for the water-quality properties and constituents of potential interest in stormwater studies. Chemical Help is implemented in the Microsoft help-system interface. (Computer files for the use and documentation of Chemical Help are included on an accompanying diskette.)

INTRODUCTION

A readily accessible archive of information that is valid, current, and technically defensible is needed to make informed planning, design, and management decisions (Granato and others, 1998; Dionne and others, 1999). The National Highway Runoff Water-Quality Data and Methodology Synthesis (NDAMS) is a cataloging and assessment of the documentation of information relevant to the quality of highway-runoff available in published reports. Results of a report

review process designed to provide information necessary to evaluate available reports is recorded on the NDAMS review sheets (Dionne and others, 1999).

One key factor in the review process is the availability of information about a number of water-quality properties and constituents that may be of interest to decision makers concerned with the quality of, and potential environmental effects of stormwater runoff. The U.S. Geological Survey (USGS) developed a preliminary list of water-quality properties and constituents of potential concern with input from the Federal Highway Administration (FHWA), State transportation agencies, and the regulatory community. This list was expanded throughout the review process as new properties and constituents were identified within reports that document results of stormwater-quality investigations (Dionne and others, 1999). The list ultimately included more than 450 constituents of interest that are classified by constituent type. Many of these constituents are organic chemicals with long and complex names that can be difficult to recognize, especially since many of these chemicals have a number of synonyms and naming conventions (Lopes and Dionne, 1998).

The report review process was hampered by the search for individual constituents among the NDAMS review sheets because the list of water-quality properties and constituents of potential concern represent 48 pages of the NDAMS report review sheet documented by Dionne and others (1999). It was difficult and time consuming to classify and define any given constituent and to find the appropriate review sheet to record the pertinent information. A computer-help application called Chemical Help was developed to facilitate the review process by providing a tool to quickly find the proper classification for any constituent in the review sheet or for identifying chemical names not yet in the review database.

This report provides basic instructions for use of Microsoft Windows Help Applications and describes the Chemical Help computer-help application. The computer-help application instructions describe basic operations, such as printing and the use of "index" or "find" features, and higher-level operations, such as bookmarks and annotations. Computer files for the use and documentation of the Chemical-Help application are included on an enclosed computer disk. The information in the Chemical Help product is described in relation to the NDAMS review process and for future use of this product. Future use may include investigations of the characteristics of water-quality properties and constituents and a reference for use of the NDAMS database, which is designed to document results of the review process.

COMPUTER-HELP APPLICATION INSTRUCTIONS

Help systems are computerized reference tools that allow users to have convenient access to information. Help systems are familiar to many computer users as the software documentation and reference manuals that are available in windows programs on the main menu under the heading "Help." While most help files are associated with a given application, help files can also be used as independent information systems. Help systems can be thought of as automated reference books. Help systems incorporate powerful search features (including index and find features) that can be used to find and view pertinent information. The Help file uses one or more "topics" (individually named pieces of information on a single subject) to organize and catalog information. The topics are individually identified so that the Windows Help can locate necessary information. A Help system is contained in a Help (HLP) file that runs under the standard Microsoft Windows Help program (WINHELP.EXE or WINHLP32.EXE) interface.

To use Chemical Help, simply find the file ChemHelp.hlp (usually identified by a book icon with a question mark on the cover) and double click to activate this help system. When Chemical Help is activated, the cover page and a menu of help options appear to facilitate the search for relevant information (fig. 1). The Windows Help Page Menu contains five

sub-menus (File, Edit, Bookmark, Options, and Help) and four toolbar buttons (Help Topics, Back, Print, <<, and >>). The menus and buttons provide functionality that can be customized by the user.

The drop-down menu can be used to modify the Chemical Help file. The "File" menu allows the user to open a different help file, print the displayed topic, or exit the help file. The "Edit" menu allows the user to copy or annotate topic information. The "Bookmark" menu allows quick access to selected topics. The "Options" menu includes "Keep Help on Top," "Display History Window," "Font," and "System Colors." The History Window will show a list of hyperlinks to all help topics recently visited during the current help session. The other features on the "Options" menu are window format options. In this help system, "Help" button provides relevant version information. The annotation and bookmark features are especially useful for customization of the help file by potential users.

The annotation feature is one of the interactive help-system features that allow users to customize information. To add annotations to any help topic, click on Edit/Annotate, and then enter the desired information in the annotation window. A paperclip symbol will appear next to the topic title when the topic is accessed, which is a hyperlink to the information entered into the annotation window by the user.

The Bookmark feature allows the user to save the location of selected topics under the bookmark submenu. Once a topic is book-marked, the user can jump directly to topic information from the bookmark menu. Existing bookmarks also can be deleted using the define feature. To bookmark the page you are viewing, click on Bookmark/Define, and then click OK to accept the default bookmark name, or enter your own string to give the bookmark a different name. To find bookmarked help topics, click on Bookmark, and then click again on the desired bookmark from the drop-down list.

The real functionality of the chemical help system is the options available from the four toolbar buttons (Help Topics, Back, Print, <<, and >>). The "Help Topics" toolbar button provides a pop-up action interface with the "Index" and "Find" features. These features are used to find the desired information in the chemical help system. The "Back" toolbar button

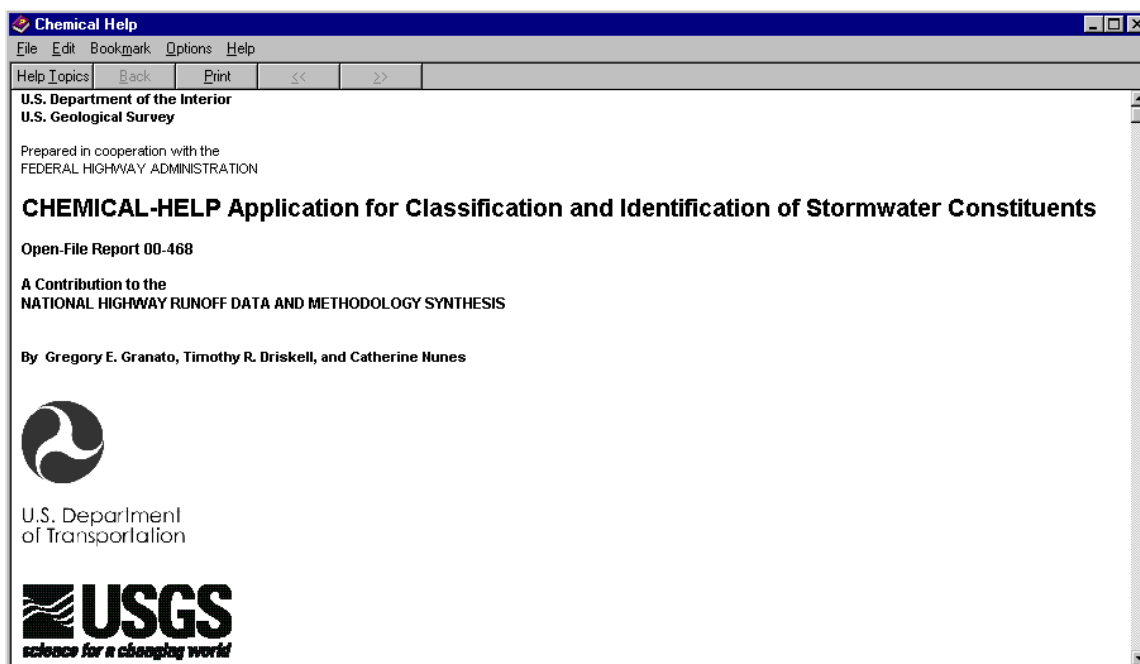


Figure 1. Chemical Help system cover page.

allows the user to move through the topics visited during a session in reverse chronological order. The "Print" toolbar button is designed as a shortcut to allow the user to print the topic being displayed on-screen. The "<<" and ">>" toolbar buttons allow the user to step through all the topics available in each section of the chemical-help system (in the order that they are stored in the help file).

The Index feature under the "Help Topics" toolbar button is used in Chemical Help as a table of contents, which relates to the NDAMS report-review sheet water-quality sections (fig. 2) as defined by Dionne and others (1999). To access information within each section, the user may enter the section name in the top window or click on the name in the lower window, and then click on the "Display" button (or hit the enter key). In Chemical Help, the index will lead to a specific menu for each section. For example, figure 3 shows the menu available for the deicers (deicing chemicals). Once the section-specific menu appears, the user may select the topic for the constituent of interest and this information will be displayed in the help

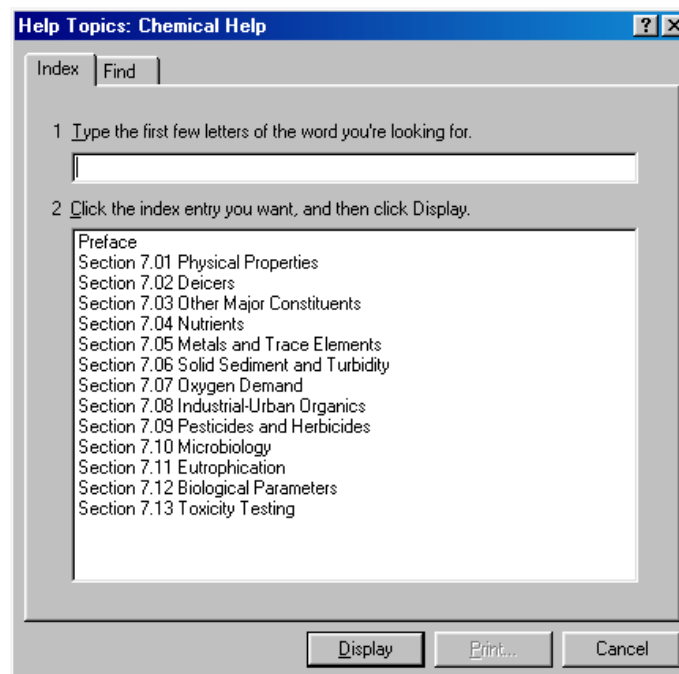


Figure 2. The index feature interface under the "Help Topics" toolbar button.

window. For example, figure 4 shows the chemical classification information defined by Dionne and others (1999), the NDAMS database-index number, and constituent-specific information for the chemical Benzene.

The "Find" feature under the "Help Topics" toolbar button is a fully searchable index of all the information recorded in Chemical Help (fig. 5). When the "Find" feature is first activated, a Microsoft Help Wizard program creates the "Find" interface. This process creates a file ChemHelp.FTS in the directory containing the help file. The top window in the "Find" interface is used to enter terms of interest. Each successive character entered in this window narrows the list of matching words displayed in the word list and the topic list. Once a word and(or) topic list is selected, the user may view topics of interest by clicking on the "Display" button (or hitting the enter key). Subjects that are commonly used to search by the Find tab are chemical name, chemical formula, database number, constituent type, Chemical Abstract Service (CAS) number, and for organic chemicals, any of the available synonyms.

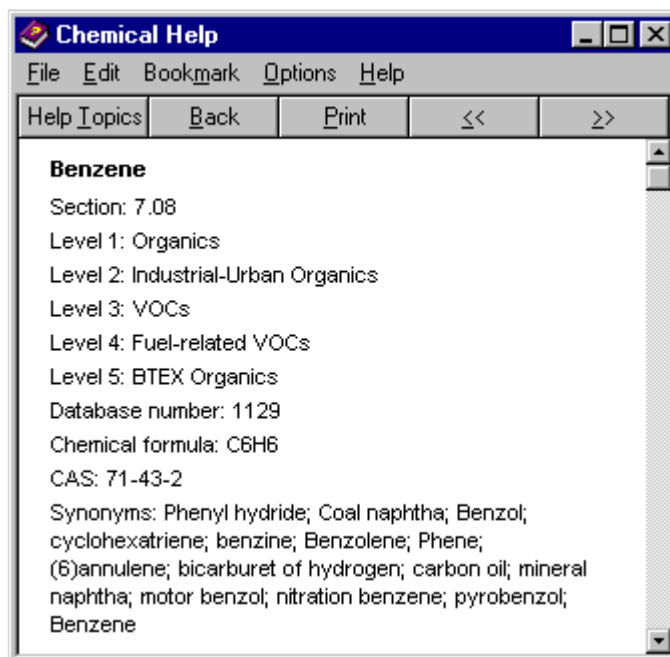


Figure 4. Example of the help-topic interface with Chemical Help contents for benzene.

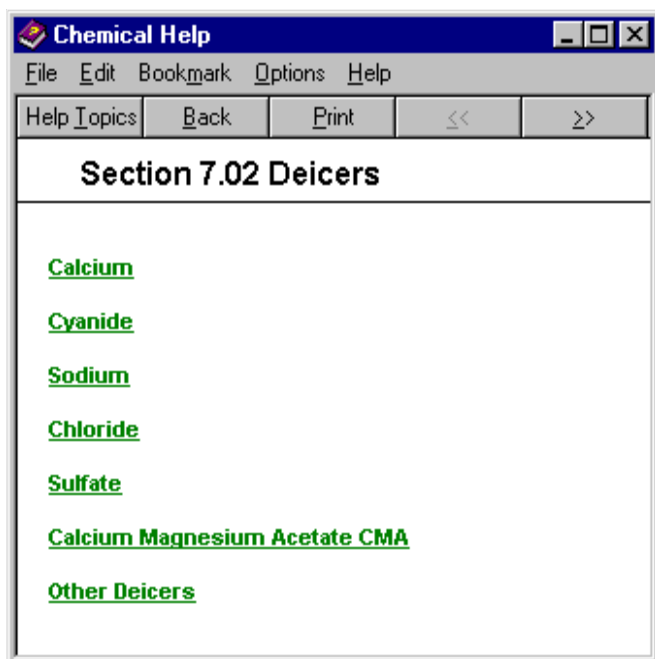


Figure 3. Example of the section-specific menu for deicers.

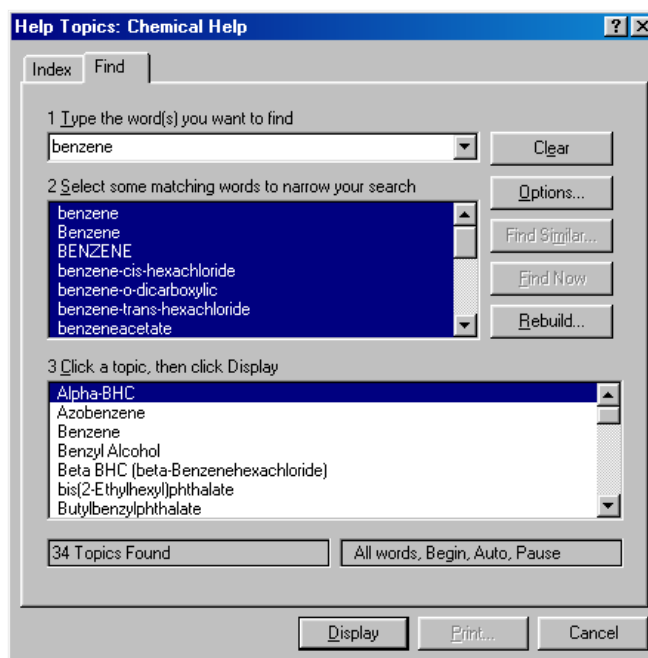


Figure 5. The find feature interface under the "Help Topics" toolbar button.

INFORMATION IN CHEMICAL HELP

The chemical help tool provides information about the water-quality properties and constituents of potential interest in stormwater studies that were documented during the NDAMS review process. Each of these water-quality properties and constituents is documented on a summary page—the help-system topic—designed to provide reference information that can be used to find that property, constituent or biological parameter in the NDAMS review sheet (Dionne and others, 1999) and in the NDAMS database. These help-system topics are also designed to provide information necessary to research the physical, chemical, and biological properties of the properties, constituents, and parameters of interest. Each topic includes the name of

each water-quality property, constituent, or parameter, the section number within the NDAMS review sheet (table 1), the organizational levels within a classification hierarchy, the database number, and where appropriate the chemical formula, the CAS number, and, for the organic chemicals, a list of synonyms (fig. 4).

Properties, constituents and other measures of water quality are classified in a hierarchical structure defined for the NDAMS review sheet. In general, constituents are classified as physical, inorganic, organic, ecological, or other (fig. 6). The properties, constituents, and measures of water quality that are commonly analyzed in comprehensive water-quality investigations of urban and highway runoff are classified into 14 categories (table 1) in the NDAMS review sheet.

Table 1. Organization of the National Highway Runoff Water Quality Data and Methodology Synthesis review sheet water-quality constituent subsections

[Water-quality constituent subsections as operationally defined by Dionne and others, 1999]

| Section number | Category title | Operational definition |
|----------------|---------------------------------|---|
| 7.01 | Properties | The physicochemical measures that indicate water quality and other parameters, such as weather, that are recorded on water-quality sampling field-record sheets as explanatory variables. |
| 7.02 | Deicers | The major inorganic constituents of road salts, other deicers, and cyanide (which is used as a component of anticaking compounds in road salts). |
| 7.03 | Major constituents | The class of inorganic constituents commonly present in natural waters at concentrations exceeding 1.0 milligram per liter. |
| 7.04 | Nutrients | The nitrogen and phosphorus species commonly measured as constituents in water-quality studies. |
| 7.05 | Metals and trace elements | The class of inorganic constituents commonly present in natural waters at concentrations less than about 1.0 milligram per liter. |
| 7.06 | Solids, sediment, and turbidity | Measures of the amount of solids in a hydrologic system that may be incorporated into stormwater runoff. |
| 7.07 | Oxygen demand | Measures of potentially biodegradable organic compounds in solution. |
| 7.08 | Organics | The carbon-based compounds that are identified as industrial/urban pollutants in stormwater investigations. |
| 7.09 | Pesticides and herbicides | The carbon-based compounds used for control of undesirable species in agriculture, landscaping, and right-of-way maintenance. |
| 7.10 | Microbiology | Measures of water quality in terms of the number of microorganisms of species commonly used to indicate impaired water quality. |
| 7.11 | Eutrophication | Measures of the trophic state of a water body receiving runoff. |
| 7.12 | Biological parameters | Measures of the effect of water-quality constituents on organisms present in the ecosystem at documented monitoring sites. |
| 7.13 | Toxicity testing | Direct measures of the effect of water-quality constituents on test organisms. |
| 7.14 | Other constituents | Measures of water quality that do not fit into one of the previous categories and(or) were not measured in more than one of the highway- and urban-runoff reports reviewed for this national synthesis. |

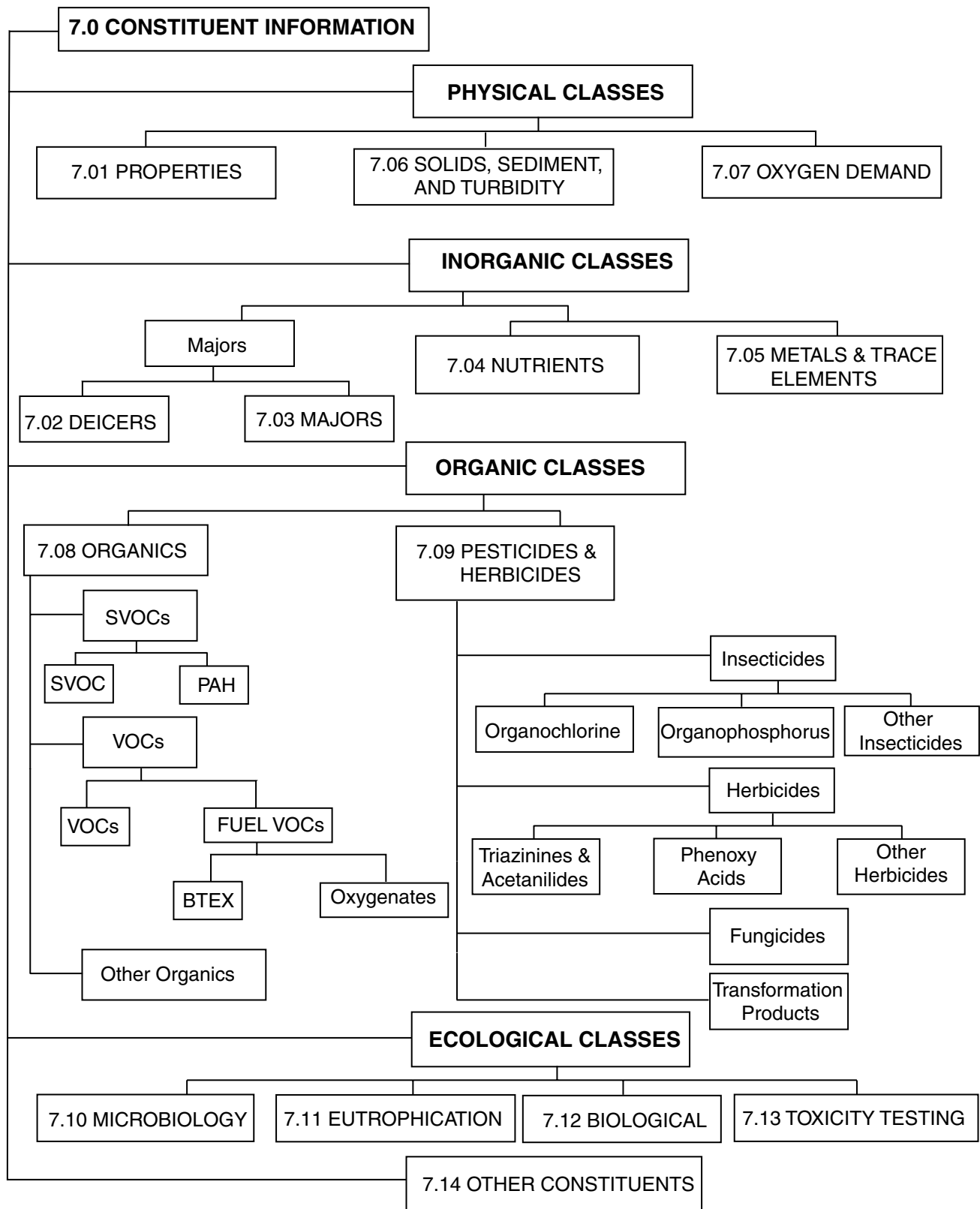


Figure 6. Classification of the water-quality constituent subsections among operational groups consistent with the focus of highway and urban runoff studies as operationally defined by Dionne and others (1999).

Dionne and others (1999) define these categories according to the operational definitions that are prevalent among reports of nonpoint-source contamination. The constituents within the physical class (fig. 6), which include properties; oxygen demand; and solids, sediment, and turbidity, were defined according to the chemical characteristics of natural water (Hem, 1992; Bricker, 1999) and water-quality criteria (U.S. Environmental Protection Agency, 1986; 1999). The inorganic classes (fig. 6), which include major constituents, nutrients, and trace elements, were also designated with respect to the chemical characteristics of natural water (Hem, 1992; Bricker, 1999). Some major constituents normally associated with deicing chemicals were identified within a category for deicers (Granato, 1996; Transportation Research Board, 1991). The third class comprises organic compounds in general. Within the organic compounds, Lopes and Dionne (1998) identified individual organic compounds (fig. 6) as either semivolatile organic compounds (SVOCs) or volatile organic compounds (VOCs). Within the SVOCs some constituents are identified as polycyclic aromatic hydrocarbons (PAHs). Within the VOCs some constituents are identified as fuel VOCs. These VOCs are further identified as BTEX (benzene, toluene, ethylbenzene, styrene and xylenes) or oxygenates. Within the organics class, pesticides and herbicides (fig. 6) are identified as insecticides (such as organochlorine, organophosphorus and other insecticides), herbicides (such as triazinines and acetanilides, phenoxy acids, and other herbicides), fungicides and transformation products as defined by the USGS National Water Quality Assessment (NAWQA) Program (Majewski and Capel, 1995; Barbash and Resek, 1996; Larson, and others, 1997). The ecological classes include microbiology, eutrophication, biological parameters and toxicity testing as discussed in highway (Gupta and others, 1981, Dupuis and others, 1985; Driscoll and others, 1990; Buckler and Granato, 1999) and urban studies (Athayde and others, 1983, Makepeace and others, 1995).

The CAS number is an index to a wealth of data about each substance of potential interest for stormwater studies. The Chemical Abstract Service

(CAS), a division of the American Chemical Society, has created a database of more than 25,000,000 substance records, including more than 16,000,000 organic and inorganic substances (Chemical Abstract Service, 2000). The CAS identifies each substance by a unique number within the CAS Registry System. Although the CAS Registry Numbers have no inherent chemical significance, they are an internationally recognized system for identification of different substances that unifies the many different systematic, generic, proprietary, and trivial names used to identify these substances. A number of extensive databases are available on the Internet to assist users in obtaining additional research data about water-quality properties and constituents of potential concern in stormwater studies (table 2). The CAS number, therefore, can be used as a keyword to find a wealth of information about individual water-quality constituents. The entries identified in table 2 as "searchable by CAS number" provide electronic search capabilities on this identifier (such as chemfinder.com), whereas the entries listed as "indexed by CAS number" provide information in tabular format where the CAS number is one identifier (such as the U.S. Environmental Protection Agency's water-quality criteria report; U.S. Environmental Protection Agency, 1999). Many of the sites are accessible to the public, but others are internal or subscriber-based service sites. The Internet addresses of the sites listed in table 2 are current as of August 2000.

Lopes and Dionne (1998) identify organic chemicals using the International Union of Pure and Applied Chemistry (IUPAC) conventions for the NDAMS project. Many common and brand names are often used for these chemicals, however, so these primary synonyms are provided in the Chemical Help system (fig. 6) for organic chemicals that are often identified as such in the literature. These synonyms are provided to facilitate search capabilities using the find feature within the chemical-help system.

Table 2. Sources of information about water-quality properties and constituents of potential concern in stormwater studies that are indexed by the Chemical Abstract Service number

[Internet addresses are current as of August 2000. Individual addresses may change, but this information should be useful in the search for more current information. CAS, Chemical Abstract Service; MSDS, Material Safety Data Sheets; NIST, National Institute of Science and Technology; NWQL, National Water Quality Laboratory; TRI, Toxics Release Inventory; USEPA, U.S. Environmental Protection Agency; USGS, U.S. Geological Survey]

| Description | Internet Address | Accessibility | Content |
|---|---|---------------|--|
| CAS website | http://www.cas.org/ | Members | Search for information about 25,000,000 substance records by CAS number. |
| Chemfinder.com | http://chemfinder.camsoft.com/ | Public | Provides physical, chemical, biochemical, health, MSDS, Regulatory, and structural information about chemicals. Searchable by CAS number. |
| Pennsylvania Department of Environmental Protection Chemical Web Site | http://www.dep.state.pa.us/physicalproperties/CASNUM_Search.htm | Public | Provides physical and chemical properties of chemicals referenced to standard publications under different environmental conditions as appropriate. Searchable by CAS number. |
| USEPA TRI database in Envirofacts | http://www.epa.gov/enviro/html/toxic_releases.html | Public | The TRI contains information about more than 650 toxic chemicals that are being used, manufactured, treated, transported, or released into the environment. Includes geographic information that tabulates air emissions, surface water discharges, releases to land, underground injections, and transfers to off-site locations. Searchable by CAS number. |
| USEPA Water Quality Criteria and Standards Program | http://www.epa.gov/OST/standards/ | Public | Ambient, aquatic life, drinking water, human health, and other information. Indexed by CAS number. |
| USGS NWQL, public laboratory schedules page | http://srvdwimdn.er.usgs.gov/nawqa/schedules.html | Public | This page lists the USGS National Water Quality Laboratory (NWQL) schedules used by the National Water Quality Assessment Program (NAWQA). |
| USGS NWQL, detection limit page | http://wwwnwql.cr.usgs.gov/Public/ltmdl/ltmdlplash.html | Public | Provides long-term method detection level and laboratory reporting level information. Indexed by CAS number. |
| US National Institute of Health, National Toxicity Program on-line database | http://ntp-server.niehs.nih.gov/Main_Pages/Chem-HS.html | Public | Chemical Health and Safety Data, Provides physical, chemical, toxicity, carcinogenicity, teratogenicity, and other information (including common synonyms). Searchable by CAS number. |
| US NIST, Chemistry WebBook | http://webbook.nist.gov/chemistry/ | Public | Provides thermochemical, thermophysical, and ion energetics data compiled by NIST under the Standard Reference Data Program. Searchable by CAS number. |
| U.S. Park Service Environmental Contaminants Encyclopedia | http://www1.nature.nps.gov/toxic/index.html | Public | Summary of information related to fish, wildlife, invertebrates, and other non-human living resources. Indexed by CAS number. |
| Webelements.com | http://www.webelements.com/webelements.html | Public | Provides a periodic table of the elements with physical, chemical, geological, and historical information about each element. Indexed by CAS number. |

SUMMARY

A computer application called Chemical Help was developed to facilitate review of reports for the NDAMS. NDAMS is a cataloging and assessment of the documentation of information relevant to highway-runoff water quality available in published reports. One key factor in the review process is the availability of information about a number of water quality properties and constituents that may be of interest to decision makers concerned with the quality of, and potential environmental effects of stormwater runoff. The list of water quality properties and constituents of potential concern developed by the U.S. Geological Survey, Federal Highway Administration and others includes more than 450 constituents of interest that are classified by constituent type. This list comprises over 48 pages of the NDAMS report review sheet documented by Dionne and others (1999), and this Chemical-Help application provided a simple and efficient interface that was used to identify individual constituents within the hierarchy defined for the review sheets.

This report provides basic instructions for use of Microsoft Windows Help Applications and describes the Chemical Help computer-help application. Computer files for the use and documentation of the Chemical Help computer-help application are included on an enclosed computer disk. The information in the chemical help product is described in relation to the NDAMS review process and future uses for this product to provide a resource for investigators who may wish to investigate water quality properties and constituents of potential concern, and (or) to use the NDAMS database, which is designed to document results of the review process. This application is also the key to access a wealth of available information because the topic covering each constituent provides the name of each water-quality property, constituent, or biological parameter, the section number within the NDAMS review sheet, the organizational levels within a classification hierarchy, the database number, and where appropriate the chemical formula, the CAS number, and a list of synonyms (for the organic chemicals). This information (especially the CAS number) can be used to locate pertinent information about the physical chemical and ecological properties of water-quality parameters of interest.

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