

CHEMICAL AQUATIC FATE AND EFFECTS (CAFE) DATABASE:

USER'S MANUAL, VERSION 1.2

May 2016



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National Oceanic and Atmospheric Administration

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List of Acronyms and Abbreviations

CAFE	Chemical Aquatic Fate and Effects database
CAS	Chemical Abstracts Service registry numbers
CAMEO [®]	Computer-Aided Management of Emergency Operations
CEFIC	European Chemical Industry Council (translated from French)
DOT	Department of Transportation
DTox	Dispersant and Chemically Dispersed Oil Toxicity Database
EAT	ECETOC Aquatic Toxicity database
EC ₅₀	Median effects concentration
ECETOC	European Centre for Ecotoxicology and Toxicology of Chemicals
ECOTOX	ECOTOXicology database
EPI	Estimation Program Interface Suite (EPI Suite™)
GNOME	General NOAA Operational Modeling Environment
h	hour
HC	Hazard Concentration
HC1	1 st percentile Hazard Concentration
HC5	5 th percentile Hazard Concentration
HSDB	Hazardous Substances Data Bank
K _{OC}	Organic carbon-water partitioning coefficient
K _{OW}	Octanol-water partitioning coefficient
LC ₅₀	Median lethal concentration
LOEC	Lowest Observed Effect Concentration
MW	Molecular weight
NIST	National Institute of Standards and Technology
NOEC	No Observed Effect Concentration
NR	Not Reported
PHYSPROP	SRC, Inc.'s Physical Properties Database
psu	practical salinity units
QA/QC	Quality Assurance/Quality Control
SRC	SRC, Inc., formerly Syracuse Research Corporation
SSD	Species Sensitivity Distribution
Web-ICE	Web-based Interspecies Correlation Estimation
95%CI	95% confidence interval



1.0 Abstract

In response to increasing need of rapid and accurate environmental assessments of chemical spills, the Emergency Response Division (ERD) of NOAA's Office of Response and Restoration developed the Chemical Aquatic Fate and Effects (CAFE) Database. This user-friendly computer software system serves as a tool to aid responders in their assessment of the environmental impacts that may arise from chemical spills in situations where critical decisions need to be made within a few hours after a spill occurs. CAFE provides ready access to aquatic fate data (e.g., chemical properties, partitioning, and degradation) for more than 30,000 chemicals; over 140,000 toxicity records (24h to 96h- LC₅₀) for more than 4,600 chemicals and 200 aquatic species (e.g., fish, crustaceans); as well as toxicity data for more than 140 crude oils and 130 dispersants.

Current capabilities of CAFE include four data selection modes (i.e., Chemical, Oil, Dispersant, and Dispersant and oil scenarios). One of these modes, the Chemical scenario, includes chemical property data that can be useful in understanding and predicting chemical behavior in aquatic environments (**Aquatic Fate Module**). All scenarios include aquatic toxicity data to aid in the characterization of potential risks to aquatic communities via Species Sensitivity Distribution curves (SSDs; **Aquatic Effects Module**). CAFE also includes Short Exposure Risk Reports for a select number of chemicals. In addition, CAFE's flexible import options allow users to enter their own data, providing additional information that enhances risk analyses for specific chemicals. CAFE Version 1.2 offers a user-friendly platform allowing for an intuitive query layout, quick display of fate and toxicity data, and easy data report generation. CAFE 1.2. now offers an import/export feature of user-added data. Every effort was made to ensure that the interface complied with requirements needed to address concerns about individuals with color blindness.

The purpose of this manual is to provide general guidance on the use of all the features of CAFE. Specific emphasis is made on the use and application of data in the **Aquatic Effects Module**. In addition, documentation is provided on the Quality Control/Quality Assurance (QA/QC) developed and implemented during the development of CAFE (see Appendix A).



2.0 Introduction

Several hundred potentially toxic chemicals are transported in the U.S. at volumes high enough to pose significant risks to localized ecosystems in the event of an accidental spill. The Emergency Response Division (ERD) of NOAA's Office of Response and Restoration responds annually to chemical spills in aquatic environments on behalf of the United States Coast Guard. In response to the increasing need of rapid and accurate environmental assessments of chemical spills, ERD developed and continues to update the Chemical Aquatic Fate and Effects (CAFE) database. This database serves as a tool to aid responders in their assessment of the environmental impacts from chemical spills into aquatic environments in situations where critical decisions need to be made within a few hours after a spill occurs (Bejarano et al., 2016). CAFE is used by the NOAA Scientific Support Coordinators (SSCs) and ERD scientists in their understanding of the fate of spilled chemicals, and the potential effects on aquatic receptors. CAFE has also been made available to the larger scientific community and the public, facilitating access to data and assisting scientists with their data needs.

Key features of CAFE are displayed in **Figure 2.1**. Data in CAFE are sorted into four scenarios: **Chemical, Oil Only, Dispersant Only, and Dispersant and Oil**. Further, data are summarized into two modules which provide complementary information to the users: the **Aquatic Fate Module** (Chemical scenario only), and the **Aquatic Effects Module** (all scenarios).

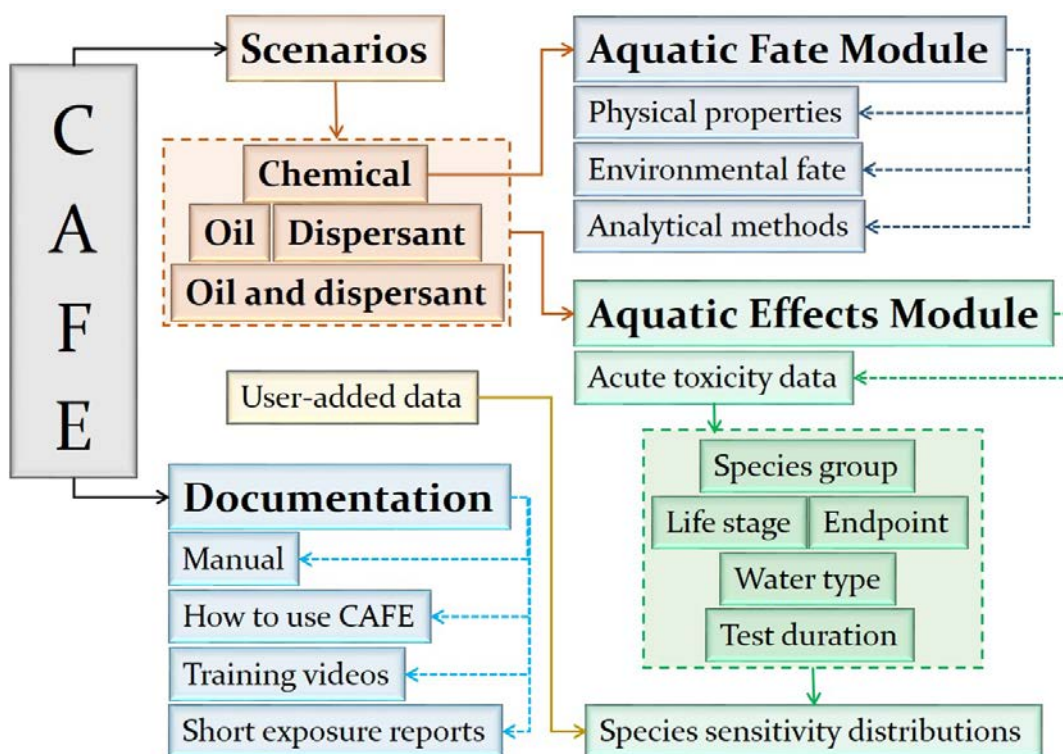


Figure 2.1. Diagram summarizing key features of CAFE.



The **Aquatic Fate Module** contains chemical specific information helpful in assessing the fate of chemicals in aquatic environments. Some of the data currently within this module include:

- Physical properties (e.g., boiling point, water solubility, molecular weight, molecular structure) of more than 30,000 chemicals.
- Environmental fate properties (e.g., estimated K_{OC} , biodegradation timeframes, volatilization, environmental partitioning) including explanations of individual properties.
- Analytical methods used in the quantification of chemicals in different media, as well as details on the intended use of specific chemicals.
- Citations of the original data sources.

The information available in the **Aquatic Fate Module**, combined with site-specific information, can be used by environmental modelers in their estimation of the concentrations of the spilled chemical in water, as well as its fate in the environment. This module also helps answer basic operational questions such as what medium to sample for the spilled chemical.

The **Aquatic Effects Module** contains chemical, oil, dispersant, and oil and dispersant specific toxicity information helpful in assessing the potential effects of the spilled chemical on aquatic receptors. Some of the data currently within this module include:

- Acute toxicity (i.e., LC_{50} , EC_{50} , LOEC, NOEC) data for a variety of aquatic receptors under different exposure durations (i.e., 24, 48, 72, and 96 hours [h]).
- A graphic display of toxicity data in the form of Species Sensitivity Distributions (SSD) based on exposure duration (24, 48, 72, and 96 h).
- SSDs based on user-defined features (e.g., water type, exposure duration).

The information available in the Aquatic Effects Module, and specifically the easily generated SSD curves, can be used to derive an estimated concentration of the spilled chemical in water that may pose adverse risks to aquatic receptors. Such estimates can be derived directly from the SSD curve for any given chemical where toxicity data exist. A user-added feature of CAFE also allows the user to add their own data and plot it in conjunction with data from CAFE.

In addition to the two large modules of CAFE and this document, several additional documents are available including a copy of this document, as well as Short Exposure Risk Reports for selected chemicals. These reports were developed for high priority chemicals with sufficient acute toxicity data in CAFE that followed one or more of the following criteria:

- Involved in accidents by the Department of Transportation.
- Potentially toxic to humans and biological resources.
- Reasonably water soluble.
- Shipped in bulk and have a reasonable risk of being spilled in large quantities.



CAFE is designed to allow the user to navigate through a series of screens where data selections can be made, narrowing the type and amount of information used in data plotting. Throughout the development of CAFE, special attention was given to address users with disabilities (Section 508 29 U.S.C. '749d) particularly by selecting color palettes (whenever possible) designed to be readable by individuals with color blindness.

Prior to the official release of the first version of CAFE a beta-version was extensively tested both internally and externally by a number of individuals (testers). This step was critical to ensure that CAFE met the requirements expected of an interactive tool. During the testing window, recommendations were made to improve the appearance and functionality of the tool, and a series of software bugs and technical issues were identified and addressed.

Key attributes of CAFE include:

- Easy to follow layouts, appearance, and functionality.
- Four data selection modes (i.e., chemical, oil, dispersant, and oil and dispersant scenarios).
- Query screens to allow for user-specific data inclusion/exclusion.
- Interactive standard navigation buttons containing common search attributes.
- Help buttons providing descriptions of specific attributes.
- Search results displayed in tables and graphics.
- A user-added section allowing CAFE users to add their own data to CAFE's plots.
- Short Exposure Risk Reports for a select number of chemicals.
- A "How To" document detailing how to perform data queries.
- Relevant documentation including CAFE's user manual and a complete Quality Assurance/Quality Control Plan.

New Features in CAFE version 1.2 are as follows:

- Updated CAFE's Effects Module with 2015 ECOTOX data
- Updated short exposure risk estimate reports for a new total of 46 chemicals
- Enable import/export of user-added data
- Updated CAFE's Fate Module with new EPI Suite data
- 5 CAFE training videos on how to use CAFE



3.0 Database Development and Quality Assurance

Several data types were compiled and incorporated into CAFE from different sources and data providers. This process required a comprehensive review and standardization of data to ensure their quality during the development of CAFE (for a detailed description, see the **Quality Assurance, Quality Control Plan [QA/QC Plan]** specifically developed for CAFE, **Appendix A**).

Briefly, the QA/QC Plan for CAFE is intended to meet the following goals:

- Summarize data management procedures and manipulations used during the development of CAFE.
- Provide a means by which the quality of information can be maintained in future updates.
- Provide a sound basis for documenting, evaluating, and verifying the accuracy of the data compilation process.
- Provide guidelines for the preparation and review of reports emerging from CAFE.
- Provide the means that would allow the user to assess the quality of data compilation efforts.

In addition, CAFE was extensively tested by the CAFE development team, as well as by several external reviewers. Testing of beta-versions was a necessary step to ensure that major issues with the interactive tool were identified and addressed prior to its public release. The CAFE development team selected many environmental scientists as beta testers in an attempt not only to assure the quality of the computer software, but also to assure that high scientific standards were being met. Beta testers were encouraged to provide suggestions on opportunities for improvement of the current version, which were carefully considered and addressed in the current version or future versions of CAFE.



4.0 Using and Querying CAFE

The sections below provide a general overview on how to use this interactive tool. For detailed and simplified guidance on how to use CAFE, please refer to the “**How to Use CAFE**” document.

4.1 Disclaimer

The CAFE development team took several steps to ensure that the interactive tool contained data of high value for the user. While every effort was made to address data inconsistencies and potential issues, the use of CAFE comes without warranties. A “**Disclaimer**” window (**Figure 4.2**) is provided to acknowledge that any data interpretations are the sole responsibility of the user, and that mention of any commercial products does not constitute any endorsement by the US government.

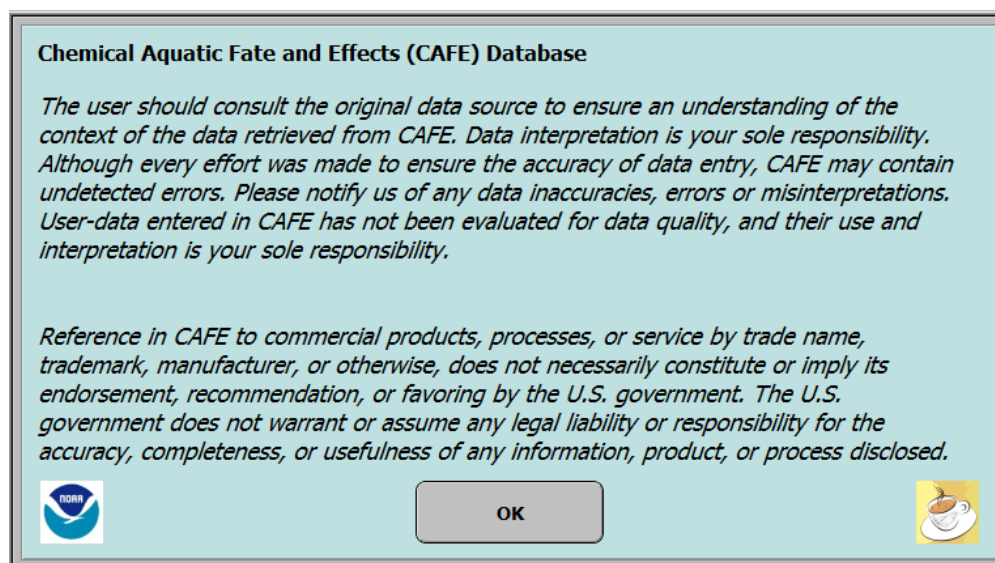


Figure 4.2. CAFE's disclaimer. Accepting acknowledgment of this disclaimer is needed before accessing and querying the database.

4.2 Chemical Searches

Data in CAFE are divided into four sub-databases (**Specific Scenario**) (**Figure 4.3**) where the user would be able to query chemicals, oils, or dispersants by chemical name, or by Chemical Abstracts Service (CAS) registry numbers (Chemical Scenario only).



1. Home	2. Chemical	3. Species	4. Life Stage	5. Endpoint	6. Water Type	7. Test Duration	Plot Graph	Clear All Selections
----------------	-------------	------------	---------------	-------------	---------------	------------------	------------	----------------------

1. Specify Scenario

Select a scenario from the options listed below, then click the Next button to continue

Chemical
Select this scenario to predict the fate and effects of a chemical (e.g. benzene, ammonia, etc.) in a chemical spill. (does not include oil, dispersants, and chemically dispersed oil).

Oil only
Select this scenario to predict the effects of oil (e.g. Alaska North Slope crude) in an oil spill. Fate data are available in ADIOS.

Dispersant only
Select this scenario to predict the effects of a dispersant (e.g. Corexit 9500). No fate data are available for dispersants.

Dispersant and oil
Select this scenario to predict the effects of a particular oil mixed with a particular dispersant or chemically dispersed oil. No fate data are available for chemically dispersed oil.

Warning: User should read the User Manual/Quality Assurance Plan to understand all known limitations inherent in the CAFE Software Program.

<p>User-Added Data</p> <p><input type="button" value="View User-Added Toxicity Data"/></p> <p><input type="button" value="User-Added Data Entry Screen"/></p>	<p>Documents</p> <p><input type="button" value="User Manual"/></p> <p><input type="button" value="How to Use CAFE"/></p> <p><input type="button" value="View Short Exposure Risk Reports"/></p>
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CAFE Training Videos

NOAA/ERD, 2016. Chemical Aquatic Fate and Effects (CAFE) Database. Version 1.2 [Computer Software]. National Oceanic and Atmospheric Administration, Office of Response and Restoration, Emergency Response Division. Seattle, WA.

	Chemical Name	CAS #	Species Name Common	Group	Life Stage	End Point	Water Type	Time Duration (hrs)	
--	---------------	-------	------------------------	-------	------------	-----------	------------	---------------------	--

Figure 4.3. CAFE's Specific Scenario. Selecting the appropriate sub-database is needed before chemical-specific queries are performed.

The user can perform queries of chemicals, oil, or dispersants by either entering a complete or partial chemical name, or by entering the CAS number. In both cases, the user is responsible for entering the correct spelling or appropriate CAS number (Chemical Scenario only).

Under the Chemical Scenario, if a chemical name is entered, the user has the option of searching the database by “**exactly matching**,” “**starts with**,” “**ends with**,” or “**anywhere in**” (Figures 4.4). The **exactly matching** option searches the database for a match of the *exact* chemical name. For instance, if the user searches for “benzene,” benzene is the *only* chemical name that appears on the search results. The **starts with** option searches the database for chemicals that *start with* the *exact* chemical name. For example, if the user searches for “benzene,” the names that appear on the search results would include “benzene,” “benzenesulfonic acid,” “benzenesulfonyl chloride,” etc. The **ends with** option searches the database for chemicals that *end with* the *exact* chemical name. For example, if the user searches for “benzene,” the names that appear on the search results would include “benzene,” “1,2-Dichloro-2-(dichloromethyl)benzene,” “1-Bromo-2-Fluorobenzene,” etc. The **anywhere in** option searches the database for chemicals that contain the search term *anywhere in* the chemical name. For example, if the user searches for “benzene,” the names that appear on the search results would include “benzene,” “benzenesulfonyl chloride,” “1,2-Dichloro-2-(dichloromethyl)benzene,” etc.



The figure displays four screenshots of the CAFE software interface, arranged in a 2x2 grid. Each screenshot shows the 'Chemical' scenario and search results for the chemical name 'benzene'. The search mode is indicated at the top of each screenshot.

Top-Left Screenshot: Search Mode: exactly matching

Number of matches for Name exactly matching "benzene": 1

Chemical or Dispersant Name	CAS Number	# of records	View
BENZENE	71432	237	Fate Effects

Top-Right Screenshot: Search Mode: starts with

Number of matches for Name starts with "benzene": 1294

Chemical or Dispersant Name	CAS Number	# of records	View
BENZENE	71432	237	Fate Effects
BENZENE METHANOL, 4-[2-(DIAMINO-5-PYRIMIDINYL)METHYL]	55687564		Fate Effects
BENZENE-1,2-DITHIOL	17534155		Fate Effects
BENZENE, (3-METHYLBUTOXY)METHYL -	122736		Fate Effects
BENZENE, (METHYLTHIO)METHYL -	766927		Fate Effects
BENZENE, 2-(1-PROPOXYETHOXY)ETHYL -	7493574		Fate Effects
BENZENE, 2-(DIMETHOXYMETHYL)-1-HEPTENYL -	91872		Fate Effects
BENZENE, (1-BUTYLDECYL)-	4534569		Fate Effects
BENZENE, (1-BUTYLHEPTYL)-	4537159		Fate Effects
BENZENE, (1-BUTYLHEXYL)-	4537115		Fate Effects
BENZENE, (1-BUTYLNONYL)-	4534503		Fate Effects
BENZENE, (1-BUTYLOCTYL)-	2719633		Fate Effects

Bottom-Left Screenshot: Search Mode: ends with

Number of matches where a word in Chemical Name ends with "benzene": 472

Chemical or Dispersant Name	CAS Number	# of records	View
1-(1,1-DIMETHYLETHYL)-4-METHYLBENZENE	98511	3	Fate Effects
1-(4-CHLOROPHENOXY)-2-NITROBENZENE	39145476	3	Fate Effects
1-(CHLOROMETHYL)-3-METHOXYBENZENE	824986	5	Fate Effects
1-(CHLOROMETHYL)-4-NITROBENZENE	100141	5	Fate Effects
1-(DICHLOROMETHYL)-2,3,4-TRICHLOROBENZENE	56961821		Fate Effects
1-[[[OBDOMETHYL]SULFONYL]-4-METHYLBENZENE	20018091	6	Fate Effects
1-[[[2-(4-ETHOXYPHENYL)-2-METHYLPROPOXY]METHYL]-3-	80844071	76	Fate Effects
1-AZIDO-4-CHLORO-BENZENE	3296057		Fate Effects
1-BROMO-2-CHLORO-4-NITROBENZENE	29682391		Fate Effects
1-BROMO-2-ETHYLBENZENE	1973224		Fate Effects
1-BROMO-2-FLUOROBENZENE	1072851		Fate Effects
1-BROMO-2-METHOXYBENZENE	578574		Fate Effects

Bottom-Right Screenshot: Search Mode: anywhere in

Number of matches where "benzene" is anywhere in Chemical Name: 2426

Chemical or Dispersant Name	CAS Number	# of records	View
1-(1,1-DIMETHYLETHYL)-4-METHYLBENZENE	98511	3	Fate Effects
1-(4-CHLOROPHENOXY)-2-NITROBENZENE	39145476	3	Fate Effects
1-(CHLOROMETHYL)-3-METHOXYBENZENE	824986	5	Fate Effects
1-(CHLOROMETHYL)-4-NITROBENZENE	100141	5	Fate Effects
1-(DICHLOROMETHYL)-2,3,4-TRICHLOROBENZENE	56961821		Fate Effects
1-[[[OBDOMETHYL]SULFONYL]-4-METHYLBENZENE	20018091	6	Fate Effects
1-[[[2-(4-ETHOXYPHENYL)-2-METHYLPROPOXY]METHYL]-3-	80844071	76	Fate Effects
1-AZIDO-4-CHLORO-BENZENE	3296057		Fate Effects
1-BENZENESULFONYL-S-ETHYL-5-PHENYLHYDANTOIN	21413252		Fate Effects
1-BROMO-2-CHLORO-4-NITROBENZENE	29682391		Fate Effects
1-BROMO-2-ETHYLBENZENE	1973224		Fate Effects
1-BROMO-2-FLUOROBENZENE	1072851		Fate Effects

Figure 4.4. CAFE's search options for chemical names under the Chemical Scenario. From left to right, top to bottom: options for searches by "exactly matching," "starts with," "ends with," or "anywhere in."



Since CAFE combines data from multiple data sources, the only unique identifier of chemical names is the CAS number. The CAS Number query allows only for entries of numeric values *without dashes*, with queries performed by **exact matching numbers** (Figure 4.5). If multiple chemical names within the database have the same CAS numbers, all other synonyms will be displayed. The user should be aware that because chemical names are not unique identifiers, the “Chemical Name” search is riskier in guaranteeing that the user has identified the correct chemical. Therefore it is preferable for searches to be based on CAS numbers.

Under the Chemical Scenario, if there is a matching record in the database with either chemical name or CAS number searches, highlighted buttons for the **Aquatic Fate** or **Aquatic Effects Modules** will be available. If one of the modules does not contain data, the module button will not be highlighted (see sections below).

The screenshot shows the CAFE search interface. At the top, there are navigation tabs: 1. Home, 2. Chemical (highlighted), 3. Species, 4. Life Stage, 5. End Point, 6. Water Type, 7. Test Duration. There are also buttons for 'Plot Graph' and 'Clear All Selections'. Below the tabs, the search mode is set to 'exactly matching'. The search criteria are: '1. Search for Chemical (by Name or CAS Number)'. The 'Name (not case sensitive)' field is empty, and the 'CAS Number' field contains '50000'. Below the search fields, it says '2. View Fate or Toxic Effects for Chemical or Dispersant' and 'Number of matches for CAS is exactly 50000: 2'. There are two tables of results. The first table is titled 'Preferred Name for Chemicals with CAS #: 50000' and has one row: 'FORMALIN' with CAS Number 50000 and 222 records. The second table is titled 'Other Chemicals Having the Same CAS #: 50000' and has one row: 'FORMALDEHYDE' with CAS Number 50000 and 222 records. At the bottom, there is a legend for the data columns: Chemical Name, CAS #/ID, Species Name, Group, Life Stage, End Point, Water Type, Time Duration (hrs).

Figure 4.5. CAFE’s search options for CAS numbers. Note that the search mode does not apply to searches based on CAS.

For the other scenarios (Oil, Dispersant, and Dispersant and oil), chemical names can also be searched by “**exactly matching**,” “**starts with**,” “**ends with**,” or “**anywhere in**.” (Figures 4.6). In addition, the main scenario page offers additional query options before accessing the **Aquatic Effects Module**. Note that these three scenarios do not contain an **Aquatic Fate Module**. The users are encouraged to refer to NOAA’s Automated Data Inquiry for Oil Spills (ADIOS) (<http://response.restoration.noaa.gov/ADIOS>), for fate information on specific oils.



The figure displays three sequential screenshots of the CAFE software interface, illustrating search options for chemical names under different scenarios. Each screenshot includes a navigation bar at the top with tabs for Home, Oil, Dispersant, Species, Life Stage, End Point, Water Type, Test Duration, Plot Graph, and Clear All Selections. Below the navigation bar is a search mode selector (exactly matching, starts with, ends with, anywhere in) and a Proceed to button.

Oil only scenario: The interface is titled "Oil only". It features four main selection sections:

- 1. Select Oil:** Includes a search criteria field, a "Search" button, and a table with columns for "Oil Name" and "# of records".
- 2. Select Analytical Method:** Offers checkboxes for Chromatography, Spectroscopy, Gravimetry, and NR.
- 3. Select Analyte(s):** Offers checkboxes for VOC, TPH, PAH, OL, and NAM.
- 4. Select Exposure Condition(s):** Offers checkboxes for Constant static, Spiked, flow-through, Continuous, flow-through, Field enclosure, Static renewal, Spiked, and NR.

Dispersant only scenario: The interface is titled "Dispersant only". It features three main selection sections:

- 1. Select Dispersant:** Includes a search criteria field, a "Search" button, and a table with columns for "Dispersant Name" and "# of records".
- 2. Select Analytical Method:** Offers checkboxes for Chromatography, Spectroscopy, Gravimetry, and NR.
- 3. Select Exposure Condition(s):** Offers checkboxes for Constant static, Spiked, flow-through, Continuous, flow-through, Field enclosure, Static renewal, Spiked, and NR.

Dispersant and oil scenario: The interface is titled "Dispersant and oil". It features six main selection sections:

- 1. Select Oil:** Includes a search criteria field, a "Search" button, and a table with columns for "Oil Name" and "# of records".
- 2. Select Dispersant:** Includes a search criteria field, a "Search" button, and a table with columns for "Dispersant Name" and "# of records".
- 3. Select Dispersant/Oil Ratio:** Includes a text input field and "Select All" and "Clear All" buttons.
- 4. Select Analytical Method(s):** Offers checkboxes for Chromatography, Spectroscopy, Gravimetry, and NR.
- 5. Select Analyte(s):** Offers checkboxes for VOC, TPH, PAH, OL, and NAM.
- 6. Select Exposure Condition(s):** Offers checkboxes for Constant static, Spiked, flow-through, Continuous, flow-through, Field enclosure, Static renewal, Spiked, and NR.

At the bottom of each screenshot is a table header with columns: Dispersant/Oil Name, CAS #/ID, Species Name (Common/Latin), Group, Life Stage, End Point, Water Type, Time Duration (hrs), and Show Selection Summary.

Figure 4.6. CAFE's search options for chemical names under the Oil, Dispersant only, and Dispersant and oil Scenarios (top to bottom).



Additional query options include:

- Selection of analytical methods used in the quantification of reported effects concentrations (e.g., chromatography, spectroscopy, gravimetry, not reported [NR]).
- Selection of chemical analytes targeted for reporting effects concentrations (e.g., volatile organic compounds [VOC], Total Petroleum Hydrocarbons [TPH], Polycyclic Aromatic Hydrocarbons [PAH], Oil Loading [OL], No Analytes Measured [NAM]) (Oil, and Dispersant and oil Scenarios only).
- Selection of exposure conditions used to generate effects concentrations (e.g., Constant static; Spiked, flow-through; Static renewal; Spiked; Continuous, flow-through, NR).
- Selection of dispersant-to-oil ratio used to prepare the aqueous exposure media (Dispersant and oil Scenario only).

Any of these additional query options allow the user to make individual selection of specific attributes, or the selection of all possible attributes. It is assumed that the user understands the nuances associated with combining data across the types of data selection displayed in CAFE (e.g., combining PAH and TPH data). Once all selections are made, the user will proceed to the remaining screens within the **Aquatic Fate Module**, which are identical to those displayed under the Chemical Scenario.

4.3 Aquatic Fate Module

Only under the Chemical Scenario option, the user would be prompted to the **Aquatic Fate Module**. This module was compiled for more than 30,000 chemicals from the following sources:

- SRC, Inc., formerly Syracuse Research Corporation (PHYSPROP) (<http://www.srcinc.com/what-we-do/environmental/scientific-databases.html>).
- Hazardous Substances Data Bank (HSDB) (<http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB>).
- National Institute of Standards and Technology Standard Reference Database (NIST) (<http://www.nist.gov/srd/>).
- US EPA Office of Pollution Prevention and Toxics, Estimation Program Interface (EPI) Suite (EPI Suite™, formerly EPIWIN) (<http://www.epa.gov/opptintr/exposure/pubs/episuite.htm>).

The Aquatic Fate Module contains three sub-modules (**Figure 4.7**):

Structure and Physical Properties. This sub-module includes:

- A graphic representation of the molecular structure.
- Physical description of individual chemicals: odor, color and form, and human exposure (e.g., skin, eye, respiratory irritation).
- Physical properties important in modeling the environmental fate of individual chemicals: boiling, melting and flash points, density, vapor pressure, water solubility, octanol-water



partitioning coefficient ($\log K_{OW}$) (see Glossary for definitions of the physical properties).

- Help windows, which provide definitions for physical properties of interest.

Environmental Fate. This sub-module displays fate information (from various US EPA models¹) and environmental explanations on important characteristics that determine the fate of a particular chemical, including:

- Soil adsorption, biodegradation half-life, estimates of volatilization from water, hydrolysis, photooxidation and media partitioning.
- Detailed environmental explanations on the fate and behavior of individual chemicals in different media (air, water, soil, other).
- Help windows, which provide definitions for the environmental properties of interest.

Analytical Methods and Uses. This sub-module includes:

- A complete description of the different methods used to quantify individual chemicals (e.g., specific method numbers in specific media), including the complete citation of the original source. For each available “Media,” a complete description of the analytical method is provided under “Media,” which includes:
 - Method number and name
 - Contact information of the organization that developed the method
 - Scope application
 - Application concentration range
 - Summary of the analytical method
 - Contamination and inferences
 - Maximum holding time
 - Sample handling
 - Quality control requirements
 - References
- Description of the current and intended use of individual chemicals, including the complete citation and the original source of this information.

¹ Fugacity Model estimates environmental partitioning; River Model estimates the volatilization rate from rivers and lakes; Aqueous Hydrolysis Rate Program (HYDROWIN) estimates the hydrolysis half-life; Atmospheric Oxidation Program (AOPWIN) estimates the atmospheric photooxidation half-life; Sewage Treatment Model estimates the method of removal by biodegradation, sludge adsorption, and volatilization; Biodegradation Probability Program (BIOWIN™) estimates the biodegradation timeframe (source: EPI Suite™ V4.11, <http://www.epa.gov/oppt/exposure/pubs/episuite.htm>).



Home Return **Physical Properties** Environmental Fate Analytic Methods Print

Fate Data - Physical Properties Chemical Name **Formaldehyde** CAS Number **50000**

Odor Pungent, suffocating odor Structure

Color/Form Clear, water-white, very slightly acid, gas or liquid
Formaldehyde solution is a clear, colorless or nearly colorless liquid ...
Nearly colorless gas (often used in an aqueous solution)

Skin, Eye, and Respiratory Irritation: Contact with the skin causes irritation, tanning effect, and allergic sensitization. Contact with eyes causes irritation, itching, and lacrimation. Vapor: Mucous membrane irritant.

Boiling Point (°C) -19.1° C (Experimental) Flash Point 181°F (83°C) (Closed Cup), 37% Aqueous

Melting Point (°C) -92° C (Experimental) Ionization Potential (eV) 10.88 eV

Density Hvp (cal/g)

Autoignition Temp. 795°F (424°C) (formaldehyde gas) HLC (atm-m3/mol) .000000337 (Experimental)

Vapor Density Log Kow .35 at 25°C (Experimental)

Viscosity Vapor Pressure (mmHg) 3886 mm Hg at 25°C (Extrapolated)

Explosive/Flammable Limits Lower 7.0%; Upper 73.0% A moderate explosion hazard when exposed to heat or flame. When aqueous formaldehyde solutions are heated above their flash points, a potential for an explosion hazard exists. Water Solubility (mg/L) 400000 at 20°C (Experimental)

Home Return Physical Properties **Environmental Fate** Analytic Methods Print

Fate Data - Environmental Properties Chemical Name **Formaldehyde** CAS Number **50000**
EPI Suite v4.11

Soil Adsorption Estimated Koc 1 Environmental Explanations
If released to the environment, Formaldehyde is expected to be found predominantly in soil (53.6%). It is also expected to be found in water (44.1%), air (2.13%) and sediment (0.0826%).

Primary Biodegradation Estimated Biodegradation Timeframe days SOIL
- In soil, Formaldehyde is expected to have very high mobility based upon a KOC of 1 (Estimated).

Estimated Volatilization from Water
- Formaldehyde may volatilize from dry soil surfaces based upon a vapor pressure of 3886 mm Hg (Extrapolated).
- Formaldehyde may volatilize from moist soil surfaces based upon a Henry's Law constant of 3.37E-07 atm-cu m/mole (Experimental).

Estimated Hydrolysis at pH=7
- Formaldehyde may volatilize slowly from water surfaces based upon a Henry's Law constant of 3.37E-07 atm-cu m/mole (Experimental).
- Estimated volatilization half-lives for a model river and model lake are 952.6 hours and 10440 hours, respectively.

Estimated Atmospheric
- In water, Formaldehyde is not expected to adsorb to suspended solids and sediment based upon a KOC of 1 (Estimated).
The Aqueous Hydrolysis Rate Program (HYDROWIN) estimates aqueous hydrolysis rate constants for only certain chemical classes: esters, carbamates, epoxides, isocyanates and selected alkyl halides. HYDROWIN estimates acid- and base-catalyzed rate constants; it does not estimate neutral hydrolysis rate constants.
HYDROWIN could not estimate a hydrolysis half-life for Formaldehyde. This chemical may be stable with respect to hydrolysis. However, the inability of HYDROWIN to estimate a hydrolysis half-life does not necessarily mean that Formaldehyde is hydrolytically stable; it may contain functional group(s) for which HYDROWIN cannot estimate a hydrolysis rate constant.

Estimated Environmental Partitioning
Percent to air 2.13
Percent to water 44.1
Percent to soil 53.6
Percent to sediment 0.0826

Estimated Wastewater Removal (%)
Total Removed 1.87
Due to Biodegradation 0.09
Due to Sludge Adsorption 1.76
Due to Volatilization 0.02

AIR
The Atmospheric Oxidation Program for Microsoft Windows (ADPOWIN) estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. It should be noted that if a compound does not exist in the vapor phase in the environment (VP < 1E-8 mm Hg), reaction with photochemically generated hydroxyl radicals will not be an important fate process.
- Formaldehyde will exist solely as a vapor in the atmosphere based upon a vapor pressure of 3886 mm Hg (Extrapolated).
- The half-life for the reaction of Formaldehyde with photochemically generated hydroxyl radicals is 1.316 days, assuming a hydroxyl radical concentration of 1.3E+6 OH/cm3 and a 12-hour day.

Home Return Physical Properties Environmental Fate **Analytic Methods** Print

Fate Data - Analytic Methods Chemical Name **Formaldehyde** CAS Number **50000**

Method #	Media
1	556 Water
2	556.1 Water
3	D6303 Water
4	2016 Air
5	2539 Air
6	2941 Air
7	3500 Air
8	3900 Air
9	5700 Dust (Textile or
10	52 Air
11	ID-205 Air

Method 556
Determination of Carbonyl Compounds in Drinking Water by Pentafuorbenzylhydroxylamine Derivatization and Capillary Gas Chromatography with Electron Capture Detection
Revision 1.0, June 1998
U.S. EPA Office of Ground Water and Drinking Water Technical Support Center 26 West Martin Luther King Drive Cincinnati, OH 45268-1320; U.S.EPA National Exposure Research Laboratory (NERL) 26 West Martin Luther King Drive Cincinnati, OH, 45268-0001 Phone: 513-569-7931 Fax: 513-569-7757
Scope Application:
This method determines certain carbonyl compounds in finished drinking water and raw source water.
Application Concentration Range
2-40 ug/L
Summary of Method
A 20-ml sample is adjusted to slight acid pH, and the compounds of interest are derivatized by reacting them with PFBEHA reagent for 2 hours with heat. The osime derivatives are extracted from the sample using hexane. The extract is processed through an acid wash step. The concentrations of osime derivatives (converted from compounds of interest) are measured using a gas chromatograph with an electron capture detector.
Uses
1 In the manufacture of amino and phenolic resins
2 Use to make 1,4-butanediol, polyols, acetals
3 Used as a corrosion inhibitor, hydrogen
4 Chemical intermediate for phenolic
5 Soil sterilant in mushroom houses before
6 Veterinary medication
7 Pesticide registered for use in the U.S.
Citation
Kirk-Othmer Encyclopedia of Chemical Technology, 4th ed. Volumes 1 to present. New York, NY: John Wiley and Sons, 1991 -

Figure 4.7. Components of the Aquatic Fate Module: physical properties, environmental fate, analytic methods (top to bottom).



The information presented in this module can be used by modelers which, combined with site-specific information (e.g., river flow, water volume, salinity) can be useful in generating plume behavior models, 3-D and forecast trajectories, and predicted environmental concentrations. The information in the **Aquatic Fate Module** can be printed from user-customized reports.

4.4 Aquatic Effects Module

Under all scenarios, the user would be prompted to the Aquatic Effects Module. This module contains acute toxicity data (24, 48, 72, and 96 h exposures) for over 4,600 chemicals and over 200 aquatic species (fish, crustaceans, and others) amounting to more than 140,000 toxicity records. This module was compiled from the following sources:

- Environmental Protection Agency (ECOTOX) (<http://cfpub.epa.gov/ecotox/>)².
- European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC) (<http://www.ecetoc.org>)³.
- An oil and dispersant database (DTox) (<http://www.researchplanning.com/projects/dtox-worldwide-quantitative-database-toxicity-dispersants-chemically-dispersed-oil/>).
- Expert consultations.
- Peer-reviewed publications, and other open literature.

A detailed description of the criteria used for data inclusion from each of these sources is provided in CAFE's QA/QC Plan (see Appendix A). Briefly, criteria included:

- Those criteria used for data inclusion in the original data sources (US EPA ECOTOX, ECETOC, and DTox).
- Studies with reported chemical name or CAS registry numbers (Chemical Scenario only).
- Studies including only one chemical per test (mixture data were not included under the Chemical Scenario).
- Laboratory testing only (monitoring studies were not included).
- Toxicological endpoints on live, whole organisms.
- Toxicity data using aquatic plant or animal species.
- Data sources reporting environmental chemical concentration/dose or application rate.
- Toxicity data associated with an explicitly reported exposure duration.
- Documents and articles publicly available.
- Full articles published in English, except when information in another language could be accurately translated.

² The large majority of toxicity data in CAFE (95%) comes from ECOTOX.

³ ECETOC kindly provided their ECETOC Aquatic Toxicity (EAT3) database for inclusion in CAFE.



Information compiled from these sources includes:

- Acute toxicity data for a variety of aquatic receptors grouped into corals, crustaceans, fish, mollusks, and other (e.g., algae, echinoderms).
- Life stage information on the species tested (e.g., embryo, larva, juvenile, adult, unknown).
- Acute toxicity data (i.e., median lethal concentration [LC₅₀], median effects concentration [EC₅₀], lowest observed effect concentration [LOEC], and no observed effect concentration [NOEC]).
- The water type used in toxicity testing (i.e., fresh, salt water).
- The exposure duration associated with individual toxicity data (i.e., 24, 48, 72, and 96 h).

All of these attributes are displayed in CAFE across several windows where data selection options are given to facilitate the customization of queries (**Figure 4.8**). The user should note that not all chemicals in CAFE have the same amount of toxicity data. Both the degree of query customization and the amount of data available for the chemical of interest may influence the speed of CAFE's performance. For example, cadmium chloride, which has several thousand individual toxicity test values, may take minutes to sort, whereas substances with only a few data points would be processed nearly instantaneously.

When query selections are made, a summary of the resulting data is displayed in the form of tables, which are automatically updated as the user makes data selections across the different windows. In the summary table, a green dot indicates that data are available for the specified query. The user should be aware that the number of toxicity records decreases as more parameters are selected. In all windows, options are given to select all, or clear all selections.

Prior to the graphic display of data, the user must select a single test exposure duration (bottom window, **Figure 4.8**). Here, the option is given to select data based on applicability. The applicability scores (High, Moderate, or Low) are based on the relevance of these data to spill response, and not on the overall scientific merit of individual records. The criteria used to assign applicability scores to each record within the database were as follows:

High

- Toxicity data with reported concentrations on the basis of measured concentrations.
- Toxicity data from laboratory setting performed under flow-through conditions.
- Reported $\geq 90\%$ active ingredient purity (Chemical Scenario only).

Moderate

- Toxicity data with reported concentrations on the basis of measured concentrations.
- Toxicity data from laboratory setting performed under static or static renewal conditions.
- Reported 75-<90% active ingredient purity (Chemical Scenario only).



Low

- Toxicity data with reported concentrations on the basis of nominal or unmeasured concentrations.
- Toxicity data not clearly stating if the reported concentration are nominal, unmeasured, or measured.
- Toxicity data not clearly stating the laboratory conditions used during testing.
- Reported <75% active ingredient purity (Chemical Scenario only).

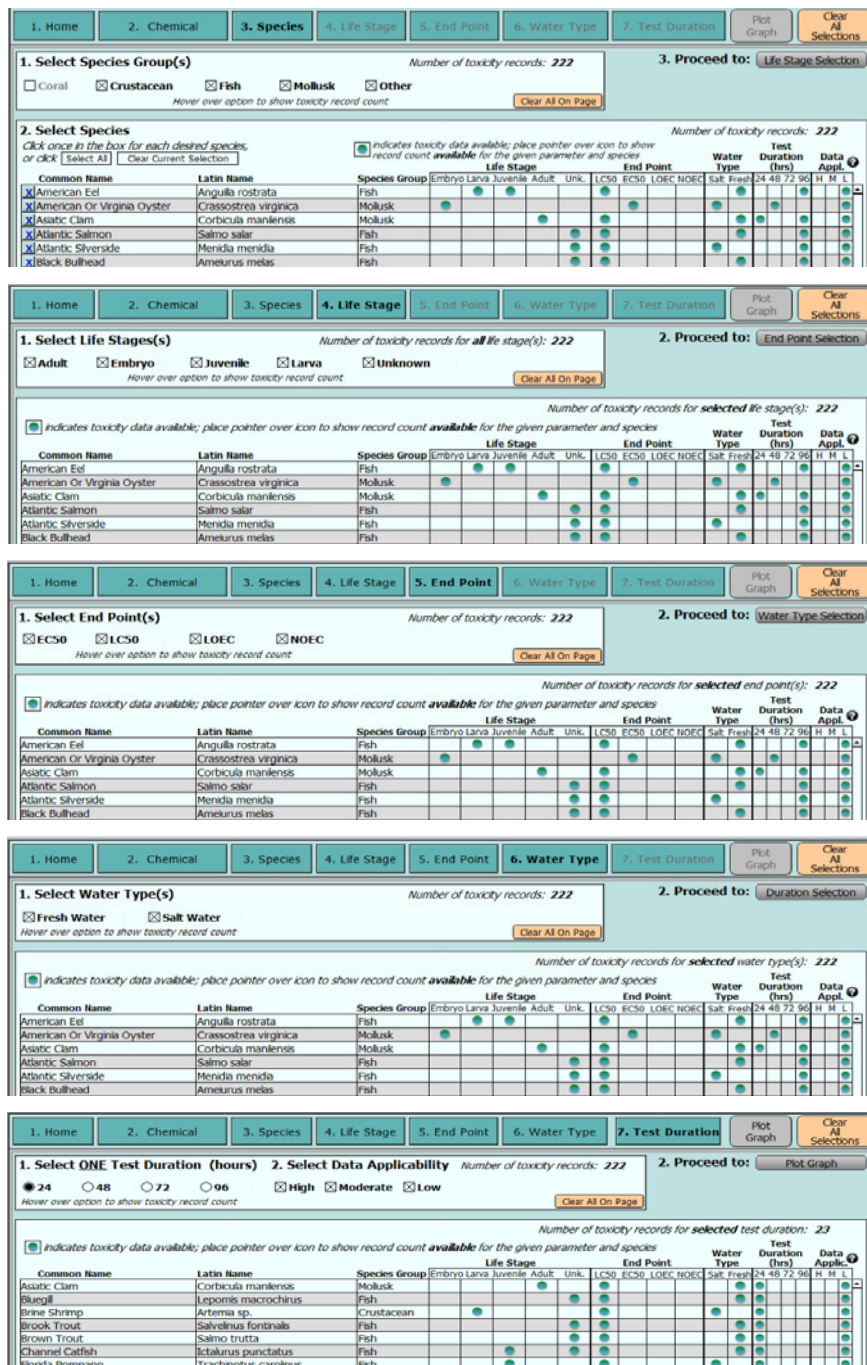


Figure 4.8. Windows of the Aquatic Effects Module where selections can be made based on species, life stages, endpoints, water type, and exposure duration (top to bottom). Only the top portion of each individual window is shown.

Once the user makes data selections, the resulting toxicity data are plotted with standardized concentration units ($\mu\text{g/L}$; see CAFE's QA/QC Plan, Appendix A) in the form of Species Sensitivity Distributions (SSDs) (Box 4.1; Figure 4.9).

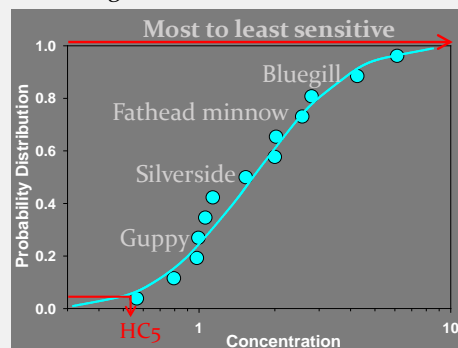


Species Sensitivity Distributions

- ❑ SSDs are probabilistic models generated by ranking the relative sensitivity of individual species from the most sensitive to the least sensitive
- ❑ SSDs were generated using laboratory toxicity test results (e.g., LC50 data) for individual species and chemicals by fitting a distribution function to the ranked species as a function of exposure concentration
- ❑ Specific percentiles, or hazard concentrations (e.g., HC5) could be used as threshold concentrations of concern
- ❑ SSDs can be used to estimate the proportion of species adversely affected at a given chemical concentration

Important considerations

- ❑ SSDs may not be appropriate if they include a small number of species, or if various taxonomic or functional groups are not appropriately represented
- ❑ Species tested under laboratory conditions are a small number of the aquatic species and they may not represent all species
- ❑ Highly sensitive or insensitive species could strongly influence SSDs
- ❑ Several types of distributions could be used to fit the empirical data (e.g., normal-, log-normal, logistic) leading to slightly different HC estimates



Because of the inherent uncertainties of SSDs, assessments should be supplemented with additional data sources and information

Box 4.1. Overview of Species Sensitivity Distributions. For additional and more detailed information, refer to related peer-reviewed literature (e.g., Posthuma et al., 2002).

In CAFE, SSDs are generated for datasets with a minimum of 5 species by fitting the empirical toxicity data to a logistic function defined by $F(x) = \frac{L}{(1+c*e^{(a*x)})}$, $x \in R$, where L is the curve's maximum value, and a and c the regression coefficients. For each individual species and by scientific name, the geometric mean of all reported concentrations is calculated and used to generate SSDs. These curves are plotted over a colored background representing a common scale of relative toxicity for aquatic organisms.

Scale
Very highly toxic (<100 µg/L)
Highly toxic (100-1,000 µg/L)
Moderately toxic (1,000-10,000 µg/L)
Slightly toxic (10,000-100,000 µg/L)
Practically nontoxic (>100,000 µg/L)

This color code scheme was adopted from the US EPA Office of Pesticide Programs⁴. SSDs are useful in that a protection threshold or a hazard level (hazard concentration, HC) can be derived as a measure of chemical risk. Two hazard concentrations (HC1 and HC5, equivalent to the

⁴ Source: <https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/technical-overview-ecological-risk-assessment-0>



concentrations at which 1% and 5%, respectively, of the species in the SSD may not be protected⁵) are automatically estimated with each SSD.

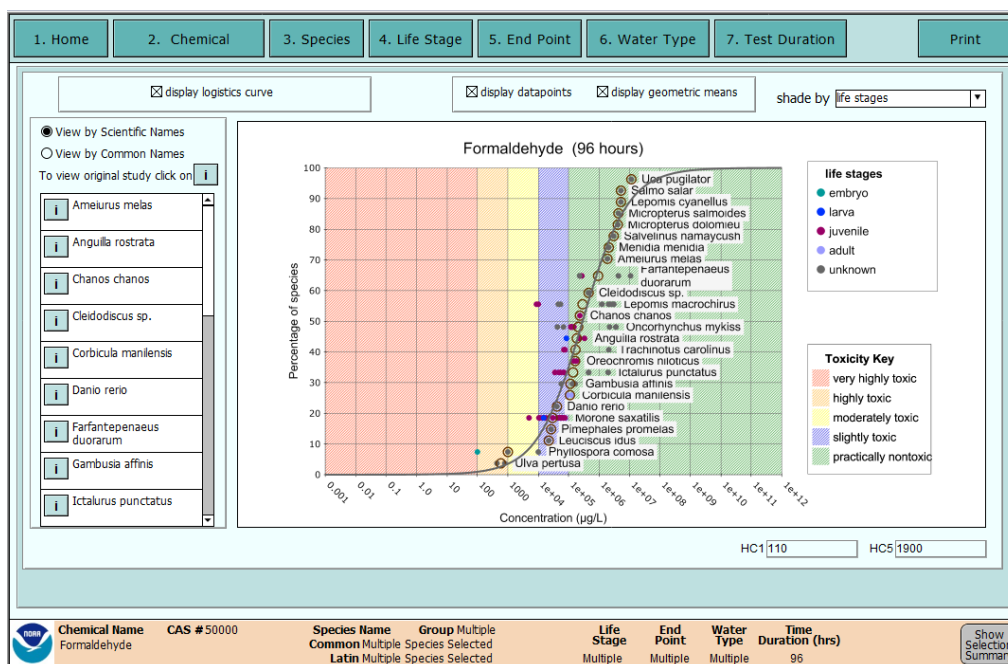


Figure 4.9. CAFE's graphic display of toxicity data in the form of Species Sensitivity Distributions.

There are several features in the graphic display of SSDs:

- All SSDs display the name of the chemical and the selected exposure duration at the top of the plot.
- All concentrations are plotted on a log scale and standardized to $\mu\text{g/L}$.
- The estimated HC1 and HC5 ($\mu\text{g/L}$) are displayed for each curve and updated with every individual query.
- A toxicity key is always displayed, showing the scale of relative risk over which SSDs are plotted.
- The user has the option of showing or hiding each individual point, the geometric mean for individual species, or both, as well as the fitted curve.
- Each point on the SSD can be shaded by specific features: applicability, endpoints, life stage, data sources, species taxonomic group, and water type. Additional shading options are also available under other sub-modules of CAFE. The color key is automatically updated, displaying the colors associated with each point in the SSD.

⁵ While there is debate in the scientific literature regarding the appropriateness of one versus another HC percentile, the HC5 selected here was chosen because this is the most commonly used percentile, while a lower percentile (HC1) would offer an additional safety factor preferable when dealing with very highly toxic chemicals. It is important to note that uncertainty increases towards the tail ends of the curve, and therefore, the use and interpretation of HC1s should be made with caution.



- In a few cases where further data manipulations were needed to improve curve fitting, the Display Geometric Means option shows shaded geometric means identified as minor or major outliers (refer to CAFE's QA/QC Plan in Appendix A for details).
- A list of all species used to generate a SSD (scientific or common name) is also shown (see below).
- A selection summary shows a comprehensive list of query choices made by the user.
- All of these features are consistent, regardless of the user-specified scenario.

With regards to SSDs, the user should be aware that:

- The current version of CAFE does not contain confidence intervals associated with the mean response of the SSD curve, and consequently, the HC1 and HC5 values are only point estimates taken at the 1% and 5% y-axis intersection of the logistic curve. Because of the uncertainties in estimated values, the user is encouraged to support these values by reviewing additional data sources external to CAFE.
- The current version of CAFE does not contain a goodness-of-fit test that evaluates how well the logistic curve fits the empirical data. Partially to address this limitation, a 5 species minimum was imposed for curve fitting. However the user is encouraged to be critical of the fitted curve. Visual inspection of the curve fitting is mandatory in assuring the user's data and resulting HC1 and HC5 estimates seem reasonable and defensible.
- CAFE only uses one family distribution (logistic) to estimate the mean response and estimated HC1 and HC5s. Other fitting approaches, which may lead to slightly different results, have not been implemented.
- While the use of SSDs is an improvement over the application of safety factors (e.g., LC₅₀/1000), SSDs are not intended to address species interactions, or population, community, or ecosystem level impacts. The user is assumed to understand the strengths and limitations of SSDs and their associated HC estimates.
- The user is entirely responsible for interpreting the plotted SSD. Several peer-reviewed literature (e.g., Posthuma et al., 2002) and online sources are available detailing how these curves are derived, how they are interpreted, and some of their strengths and limitations.

Each individual species plotted on the SSD has an associated report displaying important details from the original data source (**Figure 4.10**). Useful information includes chemical characteristics (e.g., grade, purity), test conditions (e.g., water type, exposure duration), species (e.g., scientific name, life stage tested), publication (e.g., reference number), test concentration (e.g., analytical method, concentration units), effects results (e.g., reported effect) and endpoint (e.g., reported metric).

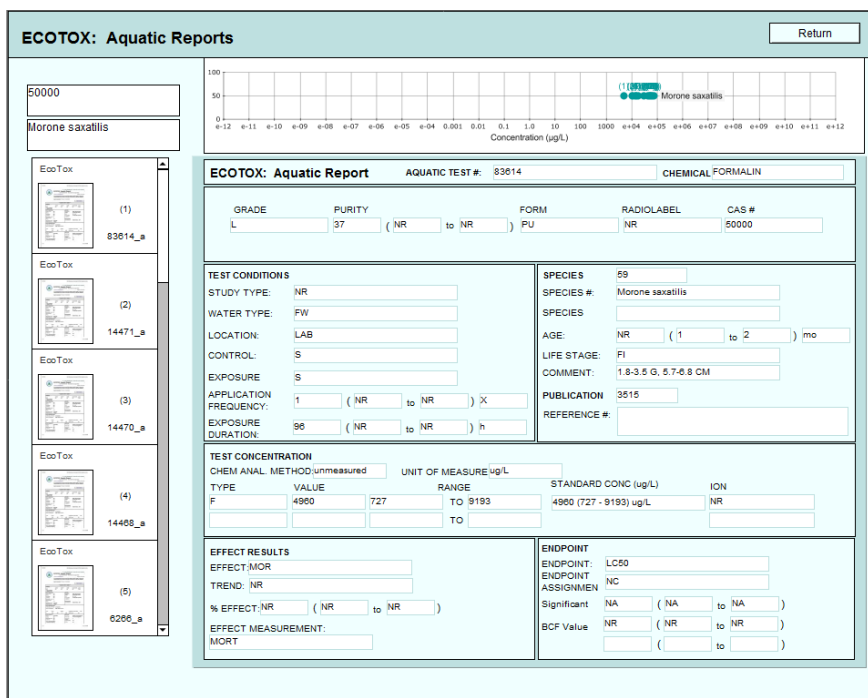


Figure 4.10. Display of the reports for individual records used to generate SSDs based on user-specific queries. All codes displayed are those of the original database. For example, within the Effect Measurement window, MORT is equivalent to mortality in ECOTOX.

4.5 User-Added Toxicity Data

In CAFE, the Home tab allows users to enter their own aquatic toxicity data, which are used to augment that dataset used to build SSDs. Once a specific scenario is selected (Chemical, Dispersant only, Oil only, or Dispersant and oil), the user will be able to view the data entry form (**Figure 4.11**) and add their data.

4.5.1 User-Added Data Entry

To complete user-added data entry, all steps must be completed and submitted before clicking the final submit button. Within the data entry form, users can:

- Search and select the chemical/oil/dispersant name associated with the user's data by searching CAFE's collection of names via a name search mode (“**exactly matching**,” “**starts with**,” “**ends with**,” or “**anywhere in**”).
- Under the chemical scenario only, search and select the CAS number associated with the user's data by searching CAFE's collection of CAS numbers.
- The user will be given option to submit the name of a new chemical, if chemical or CAS searches do not match those associated with the user's data.
- If a chemical is added without an associated CAS number, CAFE will enter CAS number as defaults (e.g., User/1).



- Search and select the species' common name or scientific names associated with the user's data by searching CAFE's collection of species names.
- The user will be given the option to submit the species' common name or scientific name, if common or scientific names do not match those associated with the user's data.
- Dropdown menus allow the user to select specific life stages, endpoints, water type, test duration, and applicability. Additional dropdown selections are available under the dispersant, oil, and dispersant and oil scenarios.
- A data entry space is available for the entry of the effects concentration ($\mu\text{g/L}$).
- For the Dispersant and Oil scenario, the user can only input five dispersant and oil ratios per test duration
- The user will be given option to submit the name of a new dispersant or oil, if dispersant or oil searches do not match those associated with the user's data.
- Certain oil and dispersant combinations cannot be located through the search feature in the Dispersant and Oil scenario—even though the individual products may be available in the database. Only a limited number of oils are associated with dispersants in the combination scenario. For example, the user can search for and locate the oil/dispersant combination, Alaska North Slope and Corexit 9527; however, the user can't locate the oil/dispersant combination, Agha Jari Iran and Actusol (even though both these products are available independently in the Oil scenario and the Dispersant scenario). If the user want to add an oil/dispersant record for Agha Jari Iran and Actusol, the user need to add "Agha Jari Iran" as a *new* oil and "Actusol" as a *new* dispersant. That combination will then be available in the Dispersant and Oil scenario.
- CAFE is an aquatic database, but data from terrestrial species may still be present. For example, the search for "rat" produces several results. Future QA/QC efforts are needed to identify and remove all terrestrial records from this database

Note that there are slight differences in the data entry forms depending on the scenario selected by the user.

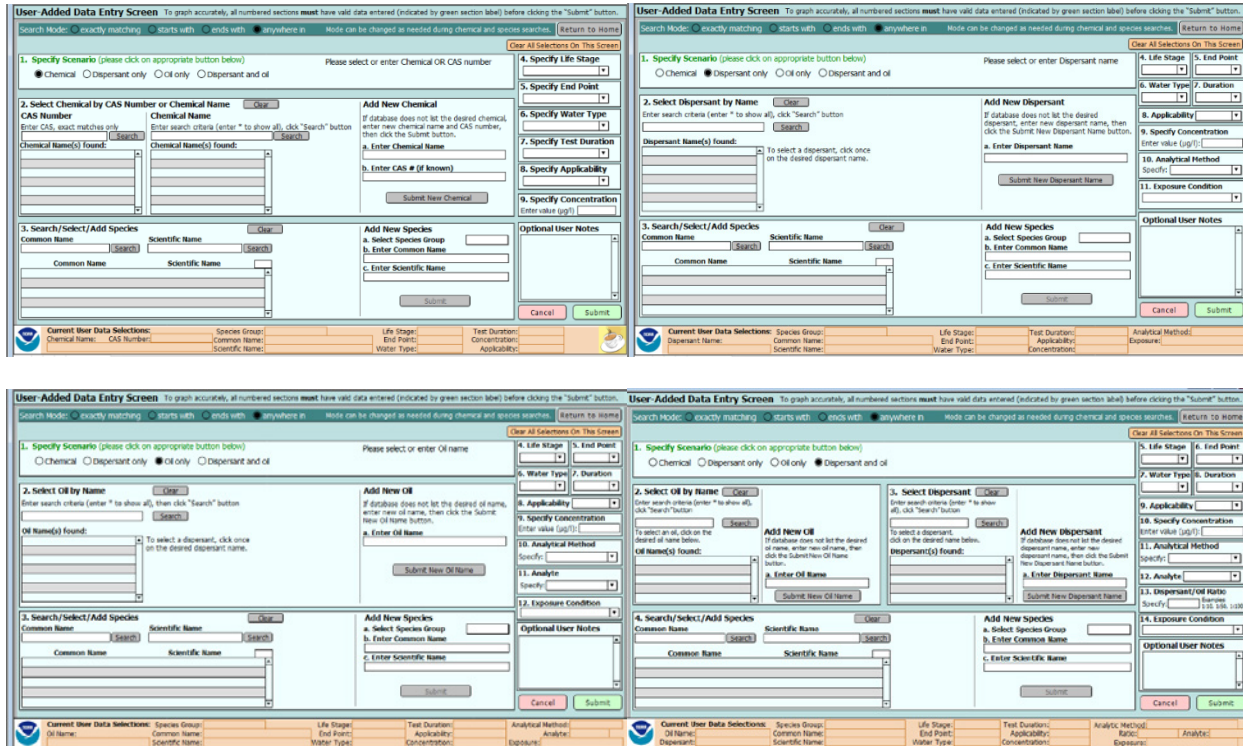


Figure 4.11. User-added data entry screen by Specific Scenario within CAFE (left-right, top-bottom: chemical, dispersant only, oil only, and dispersant and oil scenarios).

Once data are added by the user and the entry form is completely filled in, an alert box will guide the user through the next steps, which include viewing the added data, adding more data points, or continuing to the home page where the chemical of interest would need to be selected before user-added data are shown on the SSD. The user could also refer to the “**View User-Added Toxicity Data**” screen on the Home tab to view, edit or delete each individual submission (**Figure 4.12**).

Home

User-Added Toxicity Data By default, CAFE has a comprehensive database of chemical, dispersant, and oil toxicity effects on various organisms. Additionally, CAFE allows users to add toxicity data. It is the user's responsibility to verify the accuracy and completeness of all user-added data.

Chemicals/Oils/Dispersants

Names cannot be edited, they can be deleted only when they are not attached to any records.

Category	Chemical Name	# of records	
Chemical	Val Chemical	1	Delete
Disp & Oil	Value Dispersant	2	Delete
Disp & Oil	Value Oil	2	Delete

Species Names

Names cannot be edited, they can be deleted if they are not attached to any

Common Name	Latin Name	Species Group	# of records
Green Coral	Lisa corales	Coral	1
Value Crab	Valus Crabby	Crustacean	1
Value Fish	Valus fishes	Fish	1

To Edit : Click on pencil icon; an editable screen with the data for that entry will appear. To Delete: Click once on red X, then confirm delete request.

Data Code	Chemical/ Dispersant	CAS # / ID	Oil Name	Species Group	Species Name	Scientific Name	Life Stage	End Point	Water Type	Test Dur.	Analyte	Analytical Method	Disp/Oil Ratio	Conc. (ug/l)	Exposure Conditions
1	Benzene	71432		Fish	Atlantic Salmon	Salmo salar	Adult	LC50	Fresh	48				1111	✕
1	Val Chemical	3453467		Coral	Green Coral	Lisa corales	Unknown	LC50	Fresh	48				234243	✕
4	Value Dispersant	User - Value Oil	Value Oil	Fish	Value Fish	Valus fishes	Unknown	LC50	Fresh	48	NAM	Spectroscopy	1:10	4545	Constant static
4	Value Dispersant	User - Value Oil	Value Oil	Crustacean	Value Crab	Valus Crabby	Adult	NOEC	Salt	72	TPH	Chromatograph	1:10	1112	Static renewal

Figure 4.12. Summary of the user-added data allowing the user to review, edit or delete any data additions.



4.5.2 View User-Added Toxicity Data

Once data selections are made through CAFE's interactive screens and the data are plotted in the form of SSDs, the shade by "Sources" option allows the user to visualize the user-added data relative to data available in CAFE (Figure 4.13). User-added data can also be viewed within the aquatic reports associated with individual species on the SSD. The user should be aware that the outlier detection methods used within data that are part of CAFE (see CAFE's QA/QC plan) are not implemented for user-added data. Consequently, and as stated previously, SSD and HC interpretations are the sole responsibility of the user.

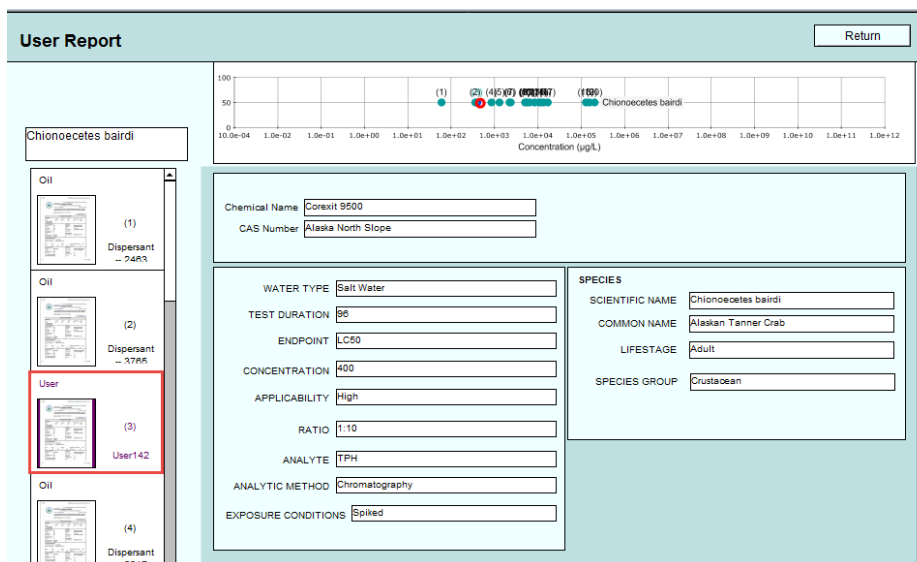
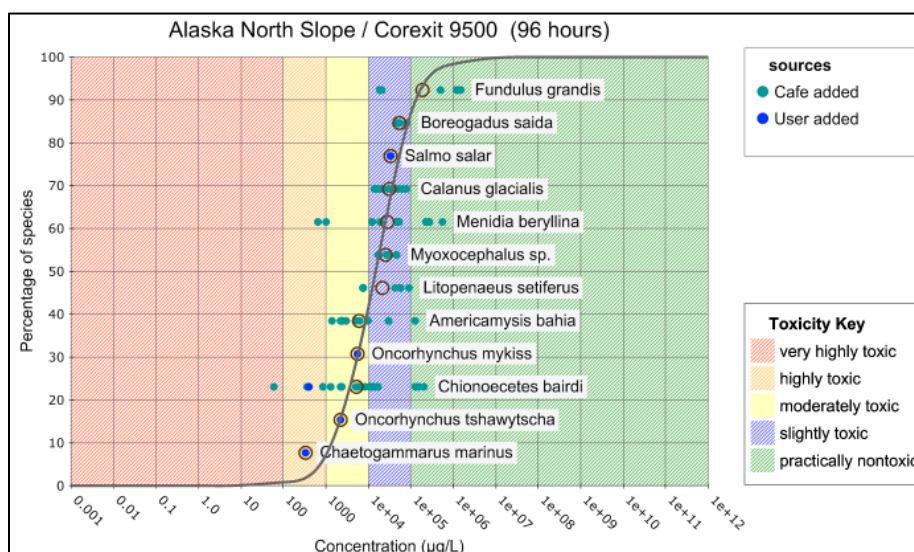


Figure 4.13. Example of an SSD shading by data sources (top) and the associated report displaying the details of the user-added data (bottom).



4.5.3 Import and Export User-Added Toxicity Data

CAFE version 1.2 has a new feature that allows the user to import and export their user-added data (**Figure 4.14**). The user will not be able to import their user added data from CAFE version 1.1 using this feature. The UserData folder, used to import and export user-added data, is found in the directory where CAFE's runtime has been saved on the user's computer.

Within this new feature, users can:

- Export user-added data created in the user-added data feature with three files (main_data.mer, chemical_names.mer and species_data.mer) contained in a UserData folder.
- Import user-added data with the exported UserData folder.
- Confirm export or import with a text summary.

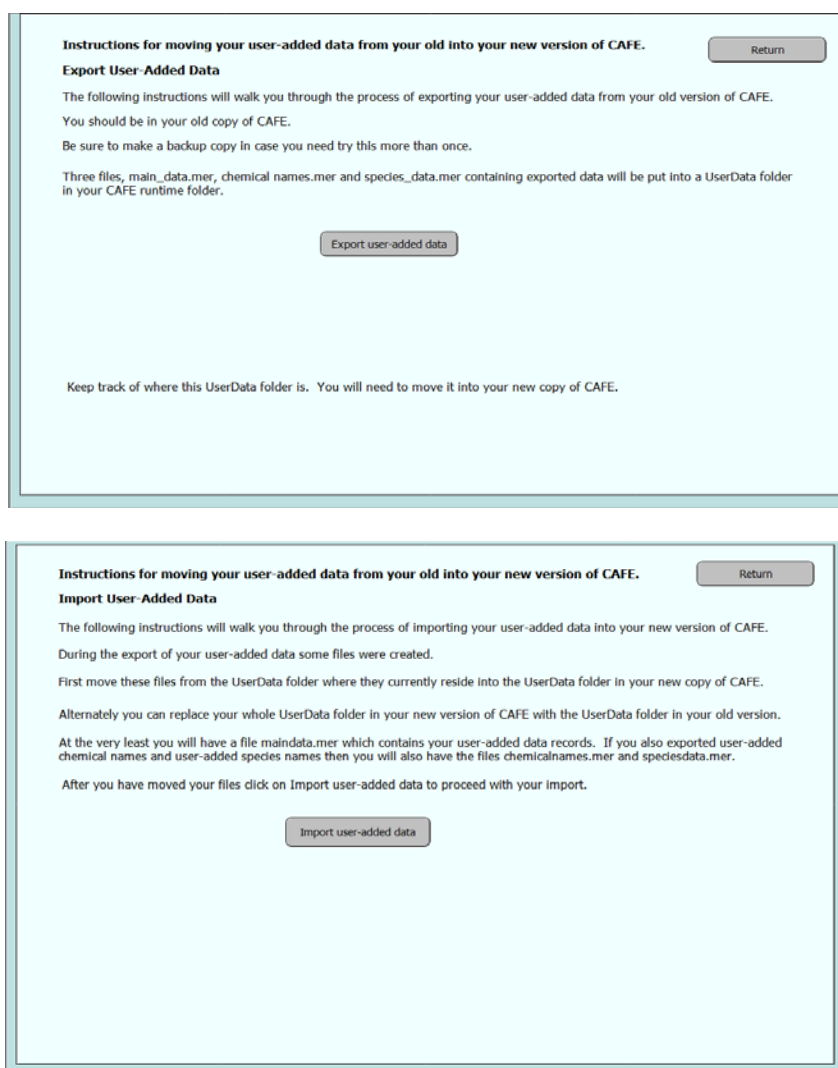


Figure 4.14 Example export (top) and import (bottom) user-added data feature.



4.6 Short Exposure Risk Reports

In CAFE, the Home tab allows the user to view reports for 46 individual chemicals (**Figure 4.15**).

Chemical Name	CAS Number	View:
1,1-Dimethylhydrazine	57147	Short Exposure Risk
1,1,2-Trichloroethane	79005	Short Exposure Risk
1,2,3,4,5,5-Hexachloro-1,3-cyclopentadiene	77474	Short Exposure Risk
2-Chloroethanol	107073	Short Exposure Risk
2-Furancarboxaldehyde	98011	Short Exposure Risk
2-Propanol	67630	Short Exposure Risk
2-Propanone	67641	Short Exposure Risk
2-Propenal	107028	Short Exposure Risk
2-Propenenitrile	107131	Short Exposure Risk
2,4-Diisocyanate-1-methylbenzene	584849	Short Exposure Risk
Acetic acid ethyl ester	141786	Short Exposure Risk
Ammonia	7664417	Short Exposure Risk
Benzene	71432	Short Exposure Risk
Bromine	7726956	Short Exposure Risk
Bromine chloride	13863417	Short Exposure Risk
Bromomethane	74839	Short Exposure Risk
Butyl benzyl phthalate	85687	Short Exposure Risk
Butyl ester, Acetic acid	123864	Short Exposure Risk
Cadmium	7440439	Short Exposure Risk
Cadmium Chloride	10108642	Short Exposure Risk
Chlorine	7782505	Short Exposure Risk
Chlorobenzene	108907	Short Exposure Risk
Chloromethyl benzene	100447	Short Exposure Risk
Chloromethyl oxirane	106898	Short Exposure Risk
[(Dimethoxyphosphinothioyl)thio]butanedioic acid, Diethyl ester	121755	Short Exposure Risk
Ethanol	64175	Short Exposure Risk
Ethylbenzene	100414	Short Exposure Risk

Figure 4.15. List of Short Exposure Risk Reports available in CAFE.

These reports were developed following the methodology described in Bejarano and Farr (2013) and covered in detail in **Appendix B**. Briefly, for each individual chemical of interest:

- Data were queried from the extended CAFE database, and supplemented with data in the US EPA ECOTOX database. A few additional data points were also generated through online searches or peer-reviewed literature and reports, or were provided by colleagues.
- SSDs by exposure duration (typically 24, 48, 72, and 96 h) with a minimum of 5 species were constructed, assuming a log-normal family distribution form.



- Individual SSD curves for all available “longer exposure durations” (typically 24, 48, 72, and 96 h) were bootstrapped 2,000 times and the mean HC5 with its associated 95% confidence interval (95%CI) estimated (**Figure 4.16**, left).
- HC5s and 95%CI for all SSD curves were plotted on a log-log scale versus the original exposure duration, and regressions linear bootstrap analysis used to estimate concentrations for short exposure durations (1, 2, 4, 8, 24 h) (**Figure 4.16**, right).
- All data manipulations and data processing steps were considered when assessing the level of reliability associated with the estimated concentrations of concern for individual analyses within each chemical-specific report.

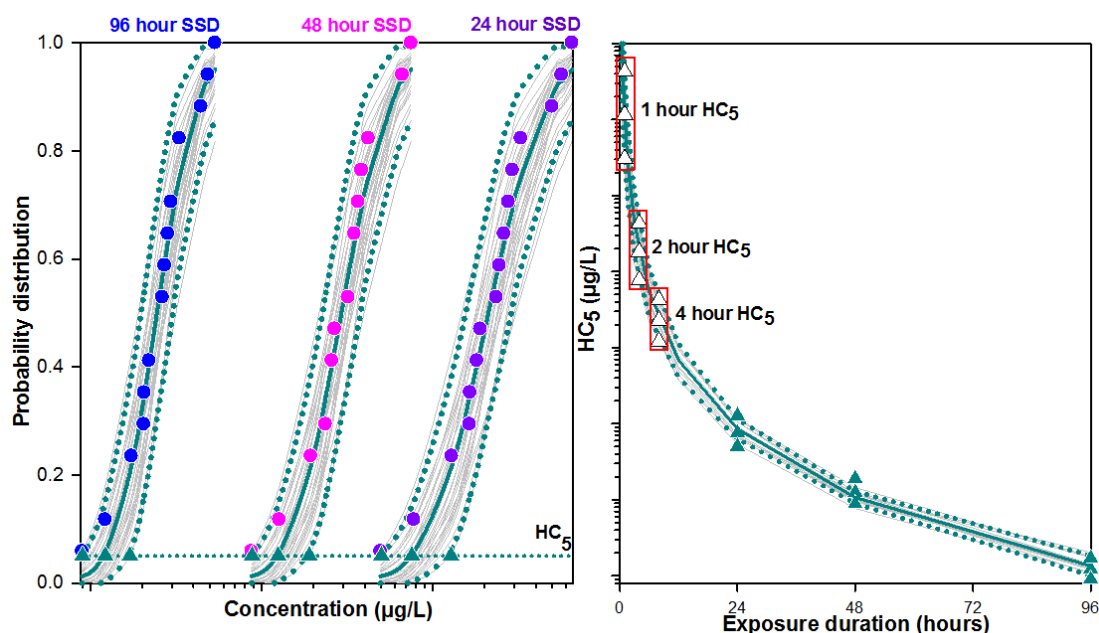


Figure 4.16. Schematic representation of the method used to derive HC5s for short exposure durations (≤ 24 h). Left plot: data from several longer-exposure durations (24, 48, 96 h; circles) were used to generate SSDs (gray lines) and their estimated mean and 95% confidence interval (95%CI) HC5 values (triangles). Right plot: HC5 values were used to estimate HC5 values for short exposure durations (white triangles).

Each of these individual reports (**Figure 4.17**) contains the following information:

- Information on the relative toxicity of the selected chemical.
- A summary of the reliability of risk estimates.
- Information on the amount of data used to estimate risk values (e.g., by exposure duration, taxonomic group, etc.).
- General observations regarding the chemical of interest.
- Graphics depicting concentrations at shorter exposure durations (≤ 24 h).



- Tables listing the selected short exposure durations (1, 2, 4, 8, 24 h), the estimated HC and 95% CIs for each exposure duration, and the overall reliability of the estimated values. When available, these are reported by taxonomic group (e.g., fish, crustaceans).
- A list of considerations that are chemical-specific.

The user can copy each individual page report (right-click), which creates a Windows metafile saved to the clipboard that can then be pasted into an external document.

Note: HC5 estimates from individual reports may not necessarily be identical to those obtained from the Effects Module of CAFE. These differences are the result of data manipulations (e.g., data inclusions and exclusions) and data processing (i.e., the use of a different family distribution to generate HC5s).

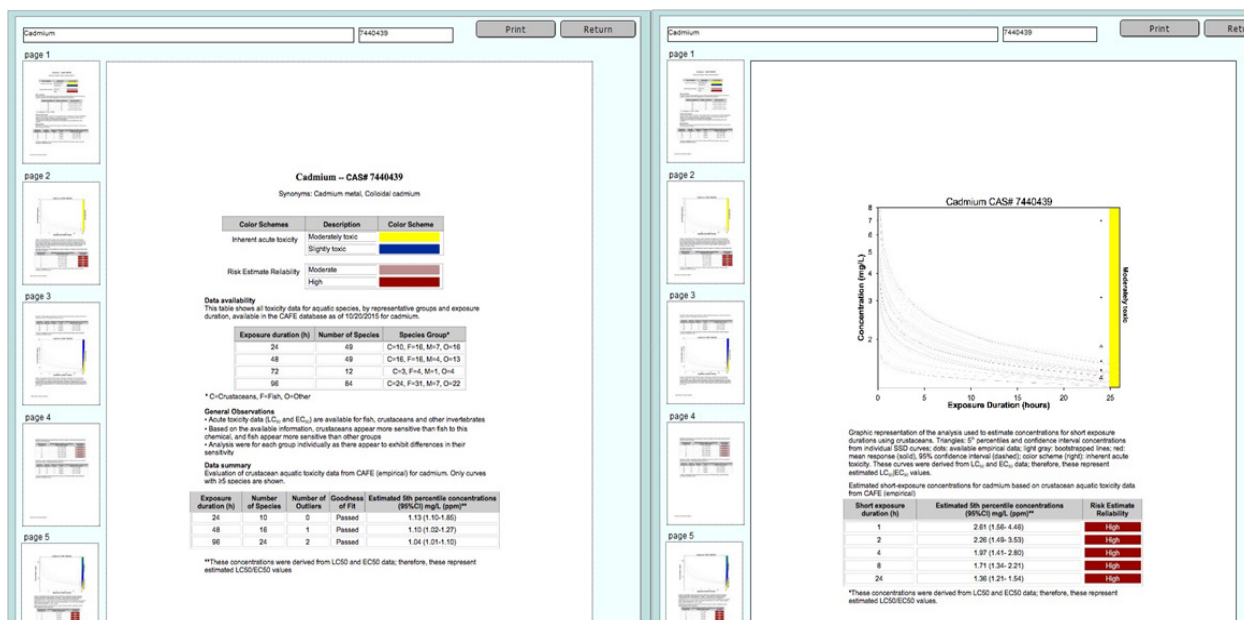


Figure 4.17. Representative example of a Short Exposure Risk Report.

Information, including the figures and tables, summarized in these individual risk estimate reports could be used to assess the potential acute effects resulting from exposure to the spilled chemical by means of comparisons with modeled or measured environmental concentrations. All risk estimates are based on the SSD's HC5s (derived from EC₅₀ and LC₅₀ data). A series of "Considerations" are also included at the end of each report to point out the relative protectiveness of risk estimate concentrations based on the known information for a particular chemical. The user is encouraged not to rely solely on the data presented in these reports. Please refer to NOAA/EPA's Computer-Aided Management of Emergency Operations (CAMEO[®]) software suite (<http://response.restoration.noaa.gov/cameo>) and the **Aquatic Fate Module** of CAFE for additional pertinent fate information; to the **Aquatic Effects Module** of CAFE for information on the most sensitive species; and to other sources of information for additional toxicological details.



4.7 Documentation

In CAFE, the Home tab allows the user to access documents relevant to CAFE. These include:

- A complete copy of this User's Manual, which includes as Appendix A the CAFE QA/QC plan, plus the technical document describing the procedure used to develop Short Exposure Risk Reports (Appendix B).
- A "How to Use CAFE" document, to help the user navigate the different screens of CAFE by providing specific and detailed guidance.
- Access to each individual Short Exposure Risk Reports.

4.8 Practical Use of CAFE: an Example with a Hypothetical Spill of Ethanol

This section briefly shows how users can use information from CAFE, including the 2-pager reports (available for selected chemicals), to make informed decisions regarding a spilled chemical. Following a chemical spill, responders need to have information to answer key questions, such as: Which chemical is involved? How hazardous is it? Is the chemical released or contained? What are the resources at risk? What recovery actions are in place?

CAFE provides easy-to-access data that provide information to help answer questions regarding environmental concerns, while also providing estimates on the relative sensitivity of aquatic organisms to the chemical of interest. This exercise is based on a *drill* involving the release of denatured ethanol.

4.8.1 Background Information

Determine what types of data are available in CAFE for the chemical of concern

Denatured ethanol is a mixture of ethanol (92-98%) with either gasoline (fuel grade ethanol, FGE/E85) or other hazardous additives. Additives often present in denatured ethanol include (in order of decreasing proportion): methanol (4%), methyl isobutyl ketone (2%), and ethyl acetate (1%). The main chemical of concern is ethanol (CAS# 64175), but other chemicals of interest include methanol (CAS# 67561), methyl isobutyl ketone (CAS# 108101), and ethyl acetate (CAS# 141786).

Establish the environmental concentration of concern

4.8.2 Spill Source Information

At 0800 hours on 26 September 2012, a barge containing 100,000 gallons of ethanol exploded and caught fire, releasing 50,000 barrels of denatured ethanol into Arthur Kill, NY (Gulfport Reach). NOAA's General NOAA Operational Modeling Environment, GNOME, (<http://response.restoration.noaa.gov/gnome>), estimated a maximum concentration at the point of release ranging from 20,000 to ~32,000 mg/L 1-2 hours post-release (**Figure 4.18** top), under the assumption of an instantaneous release (worst-case scenario), and concentrations <1,000 mg/L



over the course of 24 hours (**Figure 4.18** bottom), under the assumption of a 24-hour release (realistic scenario).

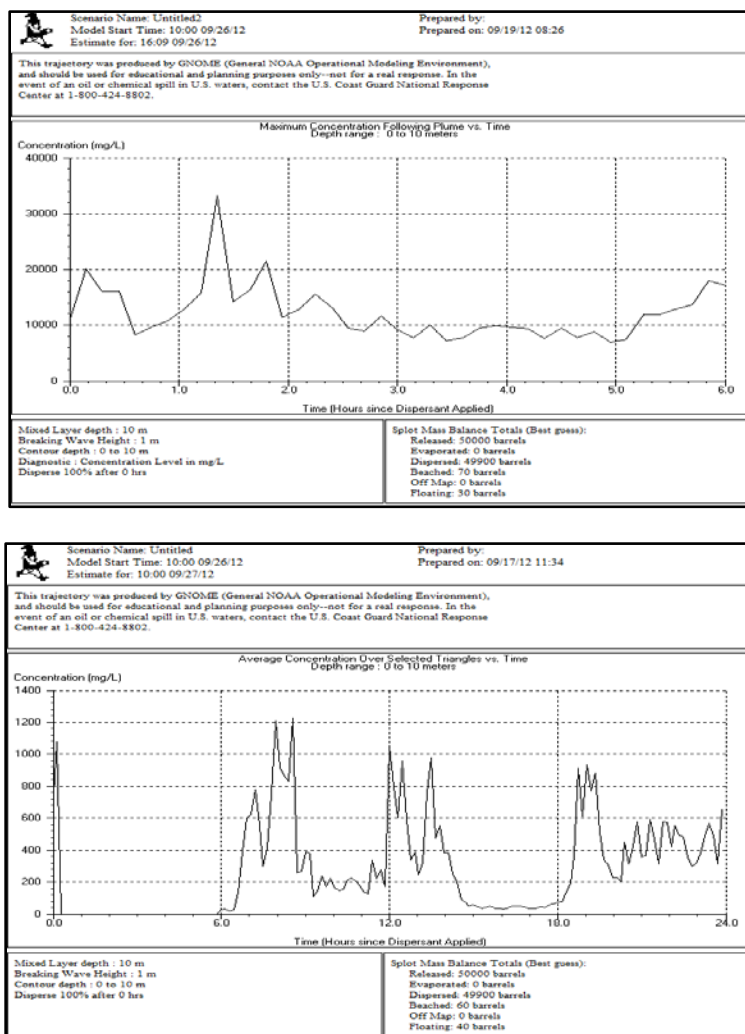


Figure 4.18. Model output from GNOME on the release (drill) of 50,000 barrels of denatured ethanol into Arthur Kill, NY. Scenario: Top: instantaneous release (worst-case scenario); Bottom: 24-hour release (realistic scenario).

4.8.3 Aquatic Fate

Gather FATE information from CAFE or other sources

Denatured ethanol is miscible in water (water solubility of 1,000,000 mg/L), and impacts related to ethanol spills are generally of short duration (Shaw, 2011⁶). However, the behavior of FGE/E85 will depend on mixing energy, and size/depth (dilution volume) of the receiving body (NRT, 2010⁷). In marine environments, salinity is

⁶ Shaw, 2011. Large Volume Ethanol Spills – Environmental Impacts and Response Options. 72 pp + Appx (<http://www.mass.gov/eopss/docs/dfs/emergencyresponse/special-ops/ethanol-spill-impacts-and-response-7-11.pdf>).

⁷ NRT, 2010. National Response Center Quick Reference Guide: Fuel Grade Ethanol Spills (including E85). 2010. 2 pp.



expected to have minor effects on the fate and transport of the ethanol and FGE/85 (NRT, 2010). Fate information for all the chemicals of interest is available in CAFE and displayed in **Figure 4.19** for ethanol.

The screenshot displays the CAFE software interface for Ethanol (CAS Number 64175). The interface is divided into two main sections: Physical Properties and Environmental Fate.

Physical Properties Section:

- Chemical Name:** Ethanol
- CAS Number:** 64175
- Odor:** Mkd, rather pleasant; like wine or whiskey; Weak, ethereal, vinous odor
- Color/Form:** Clear, colorless, very mobile liquid
- Structure:** CCO
- Skin, Eye, and Respiratory Irritation:** Exposure to vapor at sufficiently high concentrations may cause prompt stinging and watering of the eyes, but there appears to be no reports of eye injury from industrial exposure to alcohol vapors.
- Boiling Point (°C):** 78.2° C (Experimental)
- Melting Point (°C):** -114.1° C (Experimental)
- Density:** (blank)
- Autoignition Temp.:** 685°F (363°C)
- Vapor Density:** 1.59 (Air= 1)
- Viscosity:** 1.17 cP at 20°C
- Explosive/Flammable Limits:** Lower 3.3%; Upper 19% Vapor may explode if ignited in an enclosed area.
- Flash Point:** 55°F (13°C) (Closed Cup) (Experimental)
- Ionization Potential (eV):** 10.48 eV
- Hvap (cal/g):** (blank)
- HLC (atm-cu/mole):** .000005 at 25°C (Experimental)
- Log Kow:** -.31 (Experimental)
- Vapor Pressure (mmHg):** 59.26 mm Hg at 25°C (Experimental)
- Water Solubility (mg/L):** 1000000 at 25°C (Experimental)

Environmental Fate Section:

- Chemical Name:** Ethanol
- EPI Suite v4.11**
- CAS Number:** 64175
- Soil Adsorption:** Estimated Koc: 1.045
- Primary Biodegradation:** Estimated Biodegradation Timeframe: days
- Estimated Volatilization from Water:**
 - Half-life from Model River (hours): 80.17
 - Half-life from Model Lake (hours): 931.5
- Estimated Hydrolysis at pH=7:** Half-life (days): (blank)
- Estimated Atmospheric:** Half-life (days): 2.991
- Estimated Environmental Partitioning:**
 - Percent to air: 7.4
 - Percent to water: 40.6
 - Percent to soil: 51.9
 - Percent to sediment: 0.0718
- Estimated Wastewater Removal (%):**
 - Total Removed: 2.13
 - Due to Biodegradation: 0.09
 - Due to Sludge Adsorption: 1.75
 - Due to Volatilization: 0.28
- Environmental Explanations:**
 - SOIL:** If released to the environment, Ethanol is expected to be found predominantly in soil (51.9%). It is also expected to be found in water (40.6%), air (7.4%) and sediment (0.0718%).
 - In soil, Ethanol is expected to have very high mobility based upon a KOC of 1.045 (Estimated).
 - Ethanol may volatilize from dry soil surfaces based upon a vapor pressure of 59.3 mm Hg (Experimental).
 - Ethanol may volatilize from moist soil surfaces based upon a Henry's Law constant of 5.00E-06 atm-cu m/mole (Experimental).
 - WATER:** Ethanol may volatilize slowly from water surfaces based on a Henry's Law constant of 5.00E-06 atm-cu m/mole (Experimental).
 - Estimated volatilization half-lives for a model river and model lake are 80.17 hours and 931.5 hours, respectively.
 - In water, Ethanol is not expected to adsorb to suspended solids and sediment based upon a KOC of 1.045 (Estimated).
 - AIR:** The Atmospheric Oxidation Program for Microsoft Windows (AOPWIN) estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. It should be noted that if a compound does not exist in the vapor phase in the environment (VP < 1E-8 mm Hg), reaction with photochemically generated hydroxyl radicals will not be an important fate process.
 - Ethanol will exist solely as a vapor in the atmosphere based upon a vapor pressure of 59.3 mm Hg (Experimental).
 - The half-life for the reaction of Ethanol with photochemically generated hydroxyl radicals is 2.991 days, assuming a hydroxyl radical concentration of 1.5E+6 OH/cm3 and a 12-hour day.

Figure 4.19. Physical properties and environmental fate information for ethanol.

The environmental fate and partitioning of chemicals in denatured ethanol is shown in **Table 4.1**. Based on a Henry's Law Constant of less than 0.000134 atm-cu m/mole for ethyl acetate, these chemicals volatilize slowly from water surfaces. These chemicals will also not adhere to sediments and will likely remain at the top of the water column. Ethanol, methanol, and ethyl acetate are expected to biodegrade within days, while the biodegradation of methyl isobutyl ketone may require days to weeks (Aquatic Fate Module). Ethanol biodegradation in soil,



groundwater, and surface water have predicted half-lives ranging from 0.1 to 10 days. Biodegradation is the main pathway for elimination from the environment once ethanol is dissolved into water, and can happen rapidly as long as the water is warmer than 10 °C/50 °F. In colder temperatures, elevated ethanol concentrations can persist for several months (Shaw, 2011). Given information on partitioning, aquatic resources will likely be exposed to these chemicals via contaminated water.

Table 4.1. Environmental fate and partitioning of chemicals in denatured ethanol extracted from the Aquatic Fate Module of CAFE.

Chemical (CAS#)	Estimated Environmental Partitioning (%)			
	Air	Water	Soil	Sediment
Ethanol (64175)	8	41	51	<0.1
Methanol (67561)	10	40	50	<0.1
Methyl isobutyl ketone (108101)	5	43	52	<0.1
Ethyl acetate (141786)	16	44	40	<0.1

4.8.4 Aquatic Toxicity

Gather TOXICITY information from CAFE and other sources

Spills of ethanol/ethanol-gasoline blends in surface waters are expected to cause acute toxicity, potentially leading to fish kills. Effects on reptiles and mammals exposed to high blend concentrations can be expected, especially on delicate tissues (eyes). Based on the acute toxicity data available, ethanol concentrations of 1 part per thousand (g/L) for 24 h may injure most crustaceans (Figure 4.20). In addition, gasoline fractions in denatured ethanol are partitioned and transported into the water column by ethanol, making the more volatile and toxic fractions (e.g., benzene, toluene, ethylbenzene, and xylenes, BTEX) available to biological resources. The most significant impact of ethanol spills in surface water is oxygen depletion due to increased activity of biodegrading bacteria. The resulting hypoxia can lead to fish kills several days after a spill.

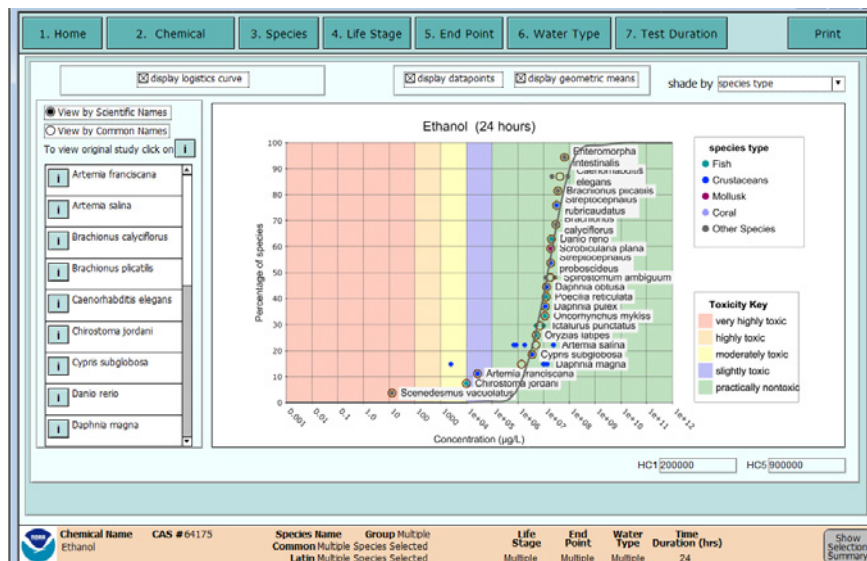


Figure 4.20. 24h-SSD for ethanol, shading data by species type.

4.8.4.1 Short Exposure Risk Reports

Determine if a 2-pager report is available for the chemical of concern

Ethanol is one of the 4 chemicals for which a Short Exposure Risk Report is available (Figure 4.21). Risk estimates for short exposures to ethanol (Table 4.2) are based on the fifth percentile concentration (derived from EC₅₀ and LC₅₀ data) of SSDs, assumed to be protective of 95% of the species tested for ethanol toxicity.

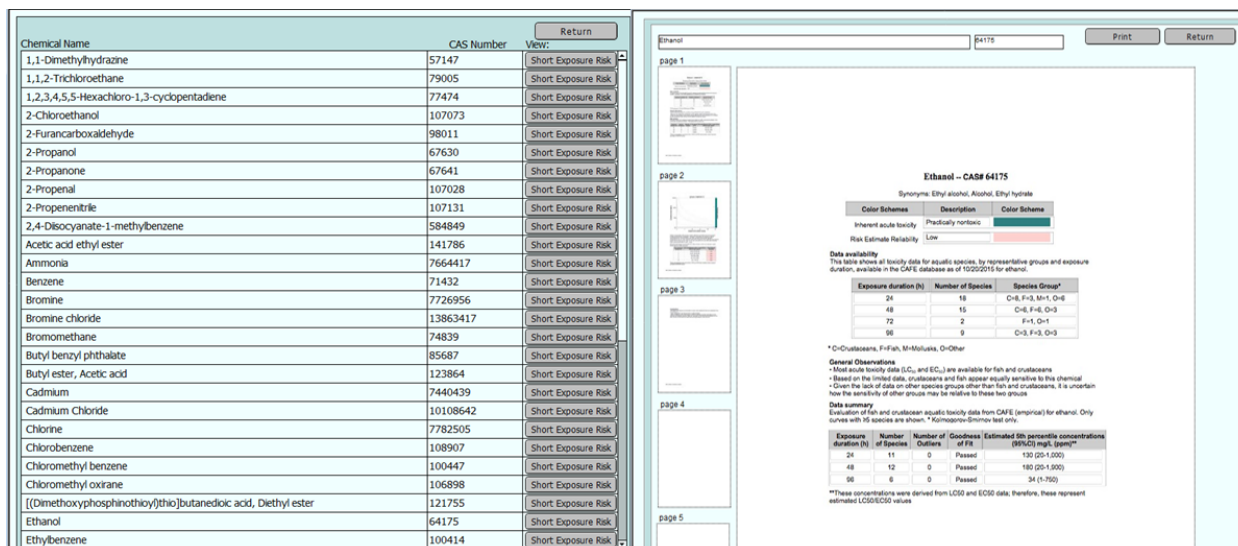


Figure 4.21. Screenshot of the Short Exposure Risk Reports (left), which includes ethanol, along with an excerpt of the report for ethanol (right).



Table 4.2. Information extracted from the “2-pager,” Short Exposure Risk Report for ethanol.

Estimated short-exposure concentrations for ethanol based on fish and crustacean aquatic toxicity data from CAFE (empirical)

Short exposure duration (h)	Estimated 5th percentile concentrations (95%CI) mg/L (ppm)*	Risk Estimate Reliability
1	3,500 (219-92,000)	Low
2	2,000 (189-28,500)	Low
4	970 (162-9,000)	Low
8	507 (140-3,000)	Low
24	181 (110-430)	Low

*These concentrations were derived from LC50 and EC50 data; therefore, these represent estimated LC50/EC50 values.

Considerations

- Estimated short-exposure concentrations may be more protective of fish and crustaceans than any other group
- These assessment may change based on data availability
- Refer to CAMEO and the Fate module of CAFE for additional pertinent information on this chemical, to the Effects module of CAFE for information on the most sensitive species, and to other sources of information for additional toxicological details on this chemical

4.8.5 Environmental Assessment

Comparison of the expected environmental concentrations of denatured ethanol under worst-case spill conditions are one order of magnitude higher than the mean values predicted to cause adverse effects to 95% of the exposed aquatic organisms for exposures lasting a few hours (1-4 h). Comparison of the expected environmental concentrations under realistic spill conditions are within the same order of magnitude of the mean values predicted to cause adverse effects to aquatic organisms exposed between 8 and 24 h. Under both exposure scenarios, adverse effects to fish and crustaceans may be observed (refer to Bejarano et al., 2016 for additional examples).



5.0 Data Limitations

While the CAFE development team made every effort possible to address data inaccuracies, errors may have been inadvertently introduced or missed. It is highly advisable that CAFE users consult the original scientific data source to supplement and confirm the data queried from CAFE.

As indicated previously, the large majority of aquatic toxicity data comes from the US EPA's ECOTOX database and consequently the same data limitations of ECOTOX apply to CAFE. Specifically, aquatic toxicity data have not been extracted from all available and relevant literature, and data are likely missing from chemicals that are not US EPA priority chemicals. In addition, aquatic toxicity updates in CAFE depend not only on continuing funding support, but also on the data updates (i.e., literature searches, data source acquisition, extraction and encoding) of ECOTOX, which are usually undertaken every six months. For this reason, CAFE users are encouraged to augment their data by conducting searches of the most recent publications to ensure that data not yet available in CAFE are identified and used in user-specific analyses.

Additional data limitations include:

- Data included in CAFE span several decades in which toxicity testing and analytical methods have likely changed, evolved, and improved. The effects of these changes on data quality are unknown.
- CAFE includes many aquatic species, but this number is relatively small, considering the diversity of species in freshwater and marine habitats.
- Data for taxonomic groups known to be sensitive (e.g., corals) are lacking in the database.
- CAFE is a data repository that is not intended to be used as the only source of information or as a substitute for the state of knowledge on the fate and effects of a particular chemical.
- Fate properties and molecular structures are not available for all chemicals, and fate data may be out of date for some chemicals.
- Toxicity data are limited for many chemicals, oils, and dispersants.
- Logistic curves do not correctly fit data that are too linear, and therefore HC1 or HC5 values cannot be estimated for all cases.
- SSDs can be exported by copying the entire screen and cropping the edges. In addition, SSDs can be printed with a toxicity data selection summary.
- Data loading can be slow for chemicals with large amounts of data (e.g., CAS 7758987 with over 6,000 toxicity records).



- SSDs and estimated HC values are used to aid in data interpretation. The current version of CAFE only uses one type of family distribution and does not include confidence intervals around the fitted curve.
- Some curves required identification and removal of outliers to enhance curve fitting (see CAFE's QA/QC plan). Outliers targeted for removal are displayed on SSDs that required such data manipulation (**Figure 5.22**).
- Too many labels associated with data points can make the graph unreadable (**Figure 5.22**), but query refinements and graph display options are available to improve readability.

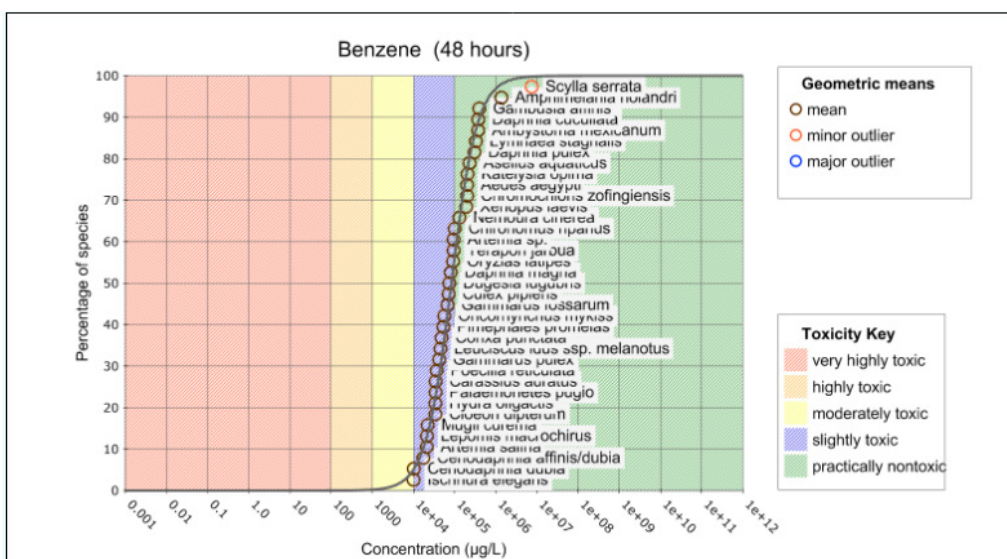


Figure 5.22. SSDs displaying some of the current limitations of CAFE: Curves with outliers (e.g., orange shading of least sensitive species) and plots with too many labels.

- Because the number of records and unique species used to develop SSDs varies widely across exposure durations, even within the same chemical, the expected trend of decreasing HC values with increasing exposure duration may not be apparent (see example in **Figure 5.23**). The user should exercise all the cautions highlighted in this manual in their interpretation of HC values.

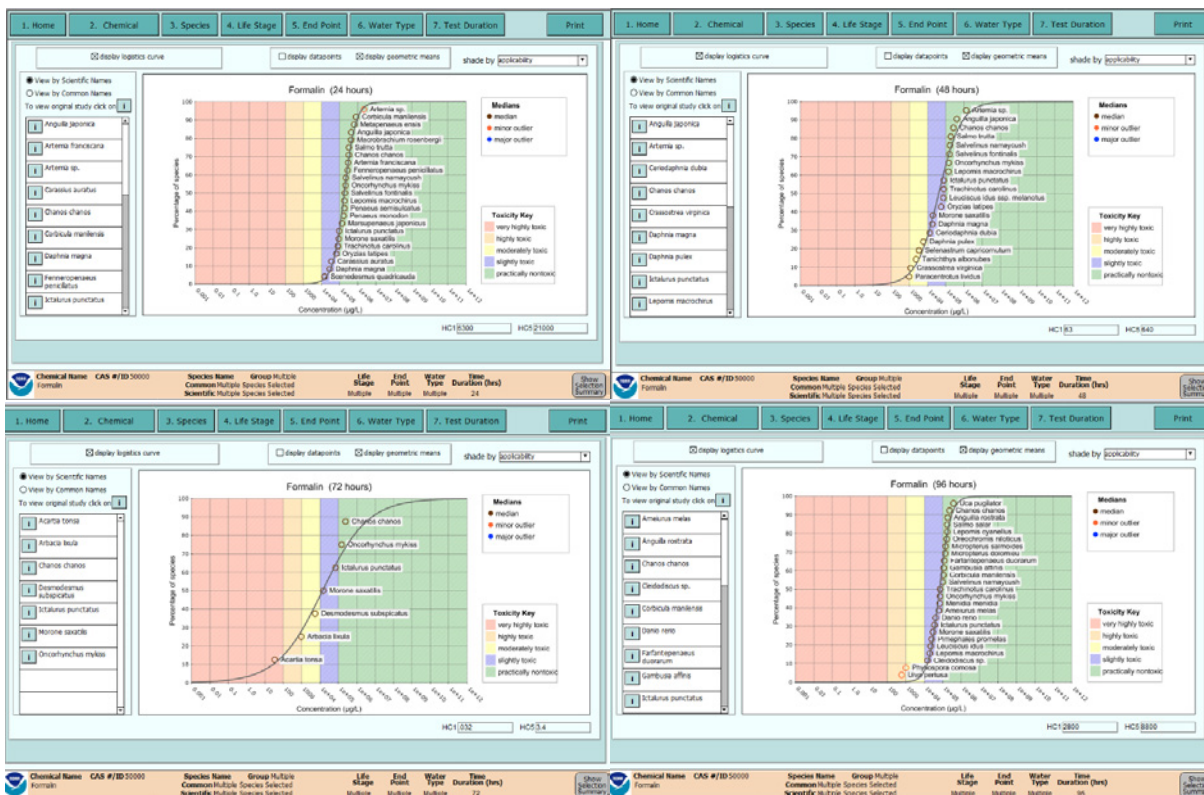


Figure 5.23. Example of non-decreasing HC values with increased exposure duration.

- As stated previously, CAFE is intended to be a centralized repository of data. Since new information is constantly generated, CAFE users should perform up-to-date literature searches and retrieve all pertinent data to supplement the data available in CAFE.
- CAFE users must apply their own data quality objectives to determine which data may be more useful to meet the expected goals.

As CAFE continues to be used in chemical spill response and gains a wider applicability by the larger scientific community, the CAFE development team will continue to identify opportunities for improvement of the current version of the tool. To the extent practical, many of these improvements will be addressed in future versions of CAFE.



6.0 Acknowledgements

The CAFE development team thanks data contributors and as well as an extensive number of individuals for their continuing support during the development of this tool.

We are extremely thankful to the following data contributors:

- European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC)
- Kenneth Doe, Environment Canada
- Christine Russom, Environmental Protection Agency (ECOTOX)
- Tony Gray, Syracuse Research Corporation (PHYSPROP)
- Hazardous Substances Data Bank (HSDB)
- National Institute of Standards and Technology (NIST)
- Estimation Program Interface (EPI) Suite (EPI Suite™, formerly EPIWIN)

We extend our gratitude to those “testers” who provided valuable input during the testing window of a beta version of CAFE. Their input was important in helping us identify opportunities for improvements in the current and future versions of CAFE.

List of Testers:

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- Renn Hanson, Genwest Systems, Inc.
- Rick Cardwell, Toxicological, Ecological & Water Quality Assessments
- Catherine Evans, Alberta Energy Regulator, Canada
- Marie DeLorenzo, Center for Coastal Environmental Health and Biomolecular Research, NOAA
- Pete Key, Center for Coastal Environmental Health and Biomolecular Research, NOAA
- Morgan Willming, US EPA⁸

⁸ *Disclaimer: US EPA scientists provided their personal technical review of CAFE. Their views and opinions do not necessarily reflect the views or policies of the US EPA. Reviews by US EPA scientists do not constitute endorsement of any commercial product by the US EPA.*



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8.0 Glossary

Aquatic Fate Module

Structure and Physical Properties

Boiling Point: The temperature at which a given liquid changes from a liquid to vapor. At the boiling point, the liquid and vapor phases exist in equilibrium. At the standard atmospheric pressure of 1 bar (760 mm Hg), the boiling point of water is 100 °C (212 °F).

Melting Point: The temperature at which a given solid changes from a solid to liquid. At the melting point, the solid and the liquid phase exist in equilibrium. At standard atmospheric pressure (1 bar), the melting point of ice is 32 °F (0 °C).

Density (kg/m³): Density (kg/m³): The mass per unit volume of any substance. Density is directly related to the buoyancy of a material. For example, borane has a low density of 0.18 g/mL at 17°C and silver azide has a high density of 5.1 g/mL. If these chemicals were placed in water (density 0.9970 g/mL at 25°C), borane would float, while silver azide would not. Density can also be used as an indication of purity.

Autoignition Temperature: The lowest temperature at which a material will catch on fire without the aid of a flame or spark. A substance with a low autoignition temperature poses a higher risk than one with a high autoignition temperature because it will be more likely to spontaneously combust under the same conditions. For instance, white phosphorus has a low autoignition temperature of 30°C (86 °F) while carbon has a high autoignition temperature of over 452 °C (846 °F). Thus, white phosphorus would be more likely to spontaneously combust than carbon.

Vapor Density: The ratio of the density of a gas to the density of air at the same temperature. A gas with a vapor density greater than 1.0 is heavier than air and will sink in the atmosphere. For example, tetrachloroethylene (5.7) has a high vapor density while anhydrous ammonia has a low vapor density (0.6). This indicates that tetrachloroethylene is heavier than air and will sink to ground level, while ammonia is lighter than air and will rise.

Viscosity (centipoise, cP): The property of a liquid that causes it to resist flow or movement in response to an external force applied to it. The less viscous a fluid is, the more easily it can move. For example, water is thin and has a low viscosity (0.894 cP) while honey is thick and has a high viscosity (2,000-10,000 cP).

Explosive/Flammable Limits: The lowest and highest concentrations of a combustible gas in air that will catch on fire when exposed to an ignition source, expressed as a percent volume in air. The lower limit (LFL or LEL) describes the leanest mixture that can sustain a flame, while the upper limit (UFL or UEL) describes the richest flammable mixture. The fire hazard posed by a combustible gas can be described in part by the size of this range. A smaller range means that the gas is less susceptible to catching on fire. For example, benzene has a small flammability range (1.4% LFL to 8% UFL) while ethylene oxide has a large flammability range (3% LFL to 100% UFL). Ethylene oxide poses a greater fire hazard than benzene because it is much more likely that a mixture of ethylene oxide and air will be flammable than a mixture of benzene and air.



Flash Point: The lowest temperature at which a volatile material gives off enough vapor to form an ignitable mixture in air. The lower the flash point, the more susceptible the material is to catching on fire. For example, ethanol has a relatively low flash point of 12.78°C (55 °F) and tall oil has a relatively high flash point of 182 °C (360 °F). There are two basic types of flash point measurement: open cup and closed cup. In open cup measurements, the sample is contained in an open cup which is heated and, at intervals, a flame is brought over the surface. In closed cup measurements, the cups are sealed with a lid through which the ignition source can be introduced. These different measurement methods can give different values for the flash point, with the closed cup method typically giving lower temperatures.

Ionization Potential (electron volts, eV): The energy required to remove electrons from chemicals in the gas phase. Larger chemicals have lower ionization energy, while small chemicals tend to have higher ionization energies. For example, helium (small) has a high ionization energy of 24.59 eV and cesium (large) has a low ionization energy of 3.89 eV.

Heat of Vaporization: The energy required to transform a given quantity of a substance from a liquid into a gas at a given pressure or temperature. The more polar the substance, the more energy is required for this phase change. For example, the value for water is relatively high (540 cal/g at its normal (1 atm pressure) boiling point of 100 °C), while the value for diazinon is low at 10.4 cal/g. Water requires more energy because it has a higher polarity than diazinon, making water molecules “stick together” more tightly.

Henry's Law Constant: The ratio of a dissolved chemical's concentration in the gas phase to its concentration in water at equilibrium. For example, tetrachloroethylene has a relatively high Henry's Law constant ($1.8 * 10^{-2}$ atm-m³/mol), and acetone has a low Henry's Law constant ($3.97 * 10^{-5}$ atm-m³/mol), indicating that acetone is more likely to partition preferentially from air into water than tetrachloroethylene is.

Log Octanol-Water Partitioning Coefficient (log K_{OW}): The logarithm of the K_{OW}. The K_{OW} is the ratio of the solubility of a chemical in octanol (a non-polar solvent) to its solubility in water (a polar solvent). The higher the log K_{OW}, the less polar the compound. For example, the polar amino acid lysine has a low log K_{OW} at -3.05, while the non-polar lipid cholesterol has a high log K_{OW} at 8.74. Because octanol is much less polar than water, a chemical's log K_{OW} indicates the likelihood of that chemical to partition into non-polar organic matter in soils. A low log K_{OW} means that the substance is likely to partition preferentially into water, while a high log K_{OW} means that the substance is instead more likely to adsorb onto carbon-rich matter such as soot. Log K_{OW} is also used in models to estimate soil-to-plant and soil-to-invertebrate bioaccumulation factors, with high log K_{OW} values indicating a high likelihood that the chemical will accumulate in tissue.

Vapor Pressure (mmHg): The pressure exerted by the gas form of a substance when it is in thermodynamic equilibrium with its solid or liquid phases within a closed system. This pressure is a measure of the volatility of a substance, since a highly volatile solid or liquid will release more vapor into the surrounding air at a given temperature than less volatile solids or liquids, and will thus have a higher vapor pressure. For example, non-volatile xenon difluoride has a low vapor pressure of $4.65 * 10^{-9}$ mmHg at 25 °C, while volatile carbon disulfide has a high vapor pressure of 359 mmHg at 25 °C.



Water Solubility (mg/L): The maximum amount of a chemical that will dissolve in pure water at a specified temperature. Water solubility depends on the polarity of the compound, and more polar molecules typically have higher water solubilities than less polar molecules. For example, highly polar ammonia has a high water solubility (482,000 mg/L at 25 °C), while highly non-polar methane has a low water solubility (22 mg/L at 25 °C).

Environmental Fate (courtesy of the US EPA EPI Suite™ program)

Soil Adsorption: (Soil Organic Carbon-Water Partitioning Coefficient) (K_{OC}) The equilibrium ratio of the solubility of a chemical in a soil's organic carbon to its solubility in water. The solubility of the chemical in the soil's organic carbon is expressed as the mass of the adsorbed chemical per unit mass of organic carbon in the soil, while the solubility of the chemical in water is expressed as the concentration of the chemical in a unit volume of water. K_{OC} is useful for predicting the mobility of organic soil contaminants: higher K_{OC} values correlate to less mobile organic chemicals while lower K_{OC} values correlate to more mobile organic chemicals. PCB 1254 has a high K_{OC} value (around 130,500) and therefore rapidly and tightly adsorb to soil particles and organic matter and have a low mobility in soil. Dipropylene glycol, a common ingredient in cosmetics, has a low K_{OC} value (around 1) and therefore has a high mobility in soil and leaches readily into groundwater.

Primary Biodegradation Timeframe: The approximate amount of time needed for a substance in an aquatic environment to be broken down into other substances with different behavior in the environment than the original material. Substances that contain carbon, nitrogen, oxygen, or other elements commonly found in biological molecules typically degrade more quickly in aquatic environments than substances that do not contain those elements. For example, furfuryl alcohol contains carbon and oxygen and takes days to biodegrade, whereas lead does not contain carbon, nitrogen, or oxygen and takes weeks-months to biodegrade. In CAFE, these timeframes are estimated using the EPA's BIOWIN™ model.

Estimated Volatilization from Water (half-life): The estimated time needed for a sample dissolved in water to vaporize. In CAFE, these values are calculated using EPA's Water Volatilization model, which assumes a Model Lake and Model River, and they are expressed as half-lives ($t_{1/2}$). The Model River is defined to be 1 m deep, flowing at a velocity of 1 m/sec, and with a wind velocity of 5 m/sec. The Model Lake is defined to be 1 m deep, with a current velocity of 0.05 m/sec and a wind velocity of 0.5 m/sec.

The rate of volatilization depends largely on the polarity of the chemical. The more polar the chemical, the more the chemical is attracted to water and the longer it takes to volatilize. For example, methyl chloride, which is relatively non-polar, takes just 0.772 hours to volatilize from the Model River and 68.01 hours to volatilize from the Model Lake, while ethanol, which is relatively polar, takes 80.17 hours to volatilize from the Model River and 931.5 hours to volatilize from the Model Lake.

Estimated Hydrolysis at pH=7 (half-life): The estimated half-life (in days) of the acid- or base-catalyzed breakdown of a chemical by water, based on the rate constants for acid- or base-catalyzed hydrolysis calculated by the EPA's HYDROWIN™ model. For example, 1,2-dibromo-1,1-difluoroethane is predicted to be rapidly hydrolyzed, with a short half-life of 0.0001246 days, while pipazethate is not predicted to be broken down by water, with an extremely long



hydrolysis half-life of $8.28E+26$ days. This calculation does not account for neutral hydrolysis (that is, any type of hydrolysis not catalyzed by acid or base).

Estimated Atmospheric Photooxidation (half-life): The estimated half-life (in days) of a chemical compound upon reaction with photochemically-generated hydroxyl radicals, as calculated using the EPA's AOPWIN™ model. For example, isoprene, which is predicted to react quickly with hydroxyl radicals, has a relatively short estimated half-life of 0.102 days. In contrast, acetyl chloride, which is predicted to react slowly with hydroxyl radicals, has a much longer estimated half-life of 1,170 days.

Estimated Environmental Partitioning: The estimated distribution of a chemical among environmental media (air, water, soil, and sediment) as predicted by the EPA's Fugacity model. This model mathematically compares the rates at which a chemical diffuses or is transported between environmental media, then predicts the amount of the chemical that will end up in the air, water, soil, and underwater sediment. A chemical's molecular weight greatly affects its partitioning among media. For example, acetylene, a small organic molecule, is expected to be found predominately in the air (50.4%) and water (47.2%), with very little in the soil (2.26%) or underwater sediment (0.113%). In contrast, polychlorinated biphenyls (PCBs), which are large non-polar organic molecules, are expected to be found predominately in the soil (70.7%) and sediment (26.3%), with very little in the water (2.57%) or air (0.412%).

Estimated Wastewater Removal: A means of quantifying the predicted fate of a chemical as it passes through a conventional activated sludge wastewater treatment plant, where it is subjected to volatilization, biodegradation, sorption onto sludges, and loss in the final effluent (as predicted by EPA's Sewage Treatment Model). First, Total Percent Removed, representing the total percentage of the chemical removed from the effluent stream during treatment, is shown. The Total Percent Removed is then subdivided to indicate the percentage of the chemical predicted to be removed by biodegradation, sorption to sludges, and/or volatilization. For example, a total of 93.8% of DDT present in wastewater is predicted to be removed during treatment, with nearly all of it removed by sludge absorption (93.02%) and only a small amount removed by biodegradation (0.78%). In contrast, a total of 91.57% of carbon tetrachloride is predicted to be removed during treatment, with the largest percentage removed by volatilization (89.51%) and much smaller percentages lost due to sludge adsorption (2.02%) and biodegradation (0.03%).

Aquatic Effects Module

Water Type

Fresh water (F) – Water type characterized by salinities below 1 psu.

Salt water (SW) – Water type characterized by salinities above 1 psu; encompasses waters that resemble salinities from brackish, estuarine, or marine environments.

Reported Analytes

Measured concentrations (M) – Concentration or amount of chemical present in the exposure media and quantified via analytical methods.

Nominal/unmeasured concentrations (N) – Concentration or amount of chemical expected to be present in the exposure media, but not quantified by any analytical methods.

**Exposure Conditions** (chemical scenario)

Flow-through Exposures (F) – Laboratory toxicity tests performed with continuous or frequent passage of aqueous exposure media through a test chamber with no recycling.

Static Exposures (S) – Laboratory toxicity tests performed with aqueous exposure media that typically remains unchanged throughout the duration of the test.

Static Renewal Exposures (R) – Laboratory toxicity tests performed without continuous flow of solution, but with renewal of aqueous exposure media.

Exposure Conditions (oil, dispersant, and oil and dispersant scenarios)

Constant static (with or without open vessels) – Refers to toxicity tests performed in the absence of flow. Aqueous exposure media typically remains unchanged throughout the duration of the test.

Static or semi-static renewal – Refers to a test without continuous flow of solution, but with renewal of aqueous exposure media.

Flow-through test – Refers to the continuous or very frequent passage of aqueous exposure media through a test chamber with no recycling.

Spiked, pulsed, and spiked, flow-through (with or without open vessels) – Refers to initial spike in concentrations in the exposure media, which is allowed to decline over the duration of the exposure period.

Endpoints

Endpoint – Refers to the biological metric used to characterize toxicity.

EC₅₀ – Median effects concentration that causes a sublethal response in 50% of the exposed organisms at a specific time interval.

LC₅₀ – Median lethal concentration that kills 50% of the exposed organisms at a specific time interval.

LOEC (Lowest Observed Effect Concentration) – The lowest concentration that causes a response statistically different from controls.

NOEC (No Observed Effect Concentration) – The highest concentration that causes a response statistically different from controls.

Endpoints (oil, dispersant, and oil and dispersant scenarios)

Endpoint – For the purpose of these databases, endpoints are grouped by Mortality (primarily LC₅₀ data); Growth and Development (e.g., blue sac disease, embryo abnormalities) (primarily EC₅₀ data); Reproduction (e.g., fecundity, fertilization inhibition, percent hatch) (primarily EC₅₀ data); Biochemical (e.g., CYP1A induction, EROD activity) (primarily EC₅₀ data); Physiology (e.g., heart rate, impaired byssal activity, impaired shell-closure) (primarily EC₅₀ data); and Behavior (e.g., feeding rate, impaired swimming) (primarily EC₅₀ data).



Analytes and Analytical Methods (oil, and oil and dispersant scenarios)

Volatile Organic Compounds – Group of volatile organic compounds (VOCs) found in petroleum derivatives. VOCs include benzene, toluene, ethylbenzene, and xylenes (BTEX).

Total Petroleum Hydrocarbons – Group of hydrocarbons of varying carbon chains (e.g., C6 to C44) contained in crude oil.

Polycyclic Aromatic Hydrocarbons – Group of hydrocarbons characterized by having multiple aromatic rings

Oil Loading – Amount of oil (by weight or volume) used in the preparation of aqueous exposures of oil

Chromatography – Analytical method for quantifying and separating compounds based on their differential partitioning between a mobile and a stationary phase.

Spectroscopy – Semi-quantitative analytical method used for characterizing compounds based on their wavelength at which light is absorbed and emitted.

Gravimetry – Semi-quantitative analytical method used for characterizing compounds based on their relative mass.



9.0 Appendices

Appendix A: Quality Assurance/Quality Control (QA/QC) Plan for CAFE

A.1.0 Introduction

The Chemical Aquatic Fate and Effects (CAFE) Database, developed and maintained by the Emergency Response Division (ERD) of the National Oceanic and Atmospheric Administration's Office of Response and Restoration, is a tool that aids responders in their assessment of the environmental impacts associated with chemical spills. CAFE is comprised of two modules, the **Aquatic Fate** and **Aquatic Effects Modules**. The **Aquatic Fate Module** contains data (e.g., chemical properties, partitioning, and degradation) useful in understanding and predicting chemical behavior in aquatic environments; while the **Aquatic Effects Module** contains acute toxicity data for a wide variety of aquatic organisms, which can be used to characterize the potential risks of the spilled material to aquatic communities. Because CAFE is a compilation of several data types from a variety of sources and providers, this document is intended to provide a detailed description of the data compilation, review, and standardization process. As a result, the purpose of this Quality Assurance/Quality Control (QA/QC) Plan is to provide a detailed description of the steps undertaken to ensure data quality during the development of CAFE.

A.2.0 Data Sources

This section describes each of the data sources used in the development of CAFE. The two modules in CAFE contain data collected by agencies and organizations outside NOAA. All data sources obtained by ERD were received in electronic formats (e.g., database files, ASCII files, Excel files), which were carefully reviewed to ensure that only data of the highest quality are used in the development of the CAFE user interface.

A.2.1 *Aquatic Fate Module*

The Aquatic Fate Module contains chemical-specific information helpful in assessing the fate of chemicals in aquatic environments. Data within this module include:

- Molecular structure.
- General description of individual chemicals and information on human exposure (e.g., skin, eye, respiratory irritation).
- Physical properties (e.g., boiling point, water solubility, molecular weight) of over 30,000 chemicals.
- Information on the estimated environmental fate of individual chemicals (e.g., partitioning, biodegradation times, photooxidation, hydrolysis).
- Detailed descriptions of environmental fate in different media.
- Analytical methods used in the quantification of chemicals in different media.



- Information on the intended use of individual chemicals.
- Citations of the original data sources.

This module was compiled from the following sources:

- SRC, Inc., formerly Syracuse Research Corporation, PHYSPROP database, <http://www.srcinc.com/what-we-do/product.aspx?id=133>.
- National Library of Medicine, Hazardous Substances Data Bank (HSDB), <http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB>.
- US Department of Commerce, National Institute of Standards and Technology (NIST), <http://www.nist.gov/srd/>.
- US EPA Office of Pollution Prevention and Toxics, Estimation Program Interface (EPI) Suite (EPI Suite™, formerly EPIWIN), <http://www.epa.gov/opptintr/exposure/pubs/episuite.htm>.

In all cases, data reporting in CAFE's Aquatic Fate Module is identical to the information provided by each data source. Information compiled from these sources (**Table A.2.1**) includes:

- Structure and physical properties:
 - Display of molecular structure.
 - Physical description of individual chemicals: odor, color and form, and human exposure (e.g., skin, eye, respiratory irritation).
 - Physical properties important in modeling the environmental fate of individual chemicals: boiling, melting and flash points, density, vapor pressure, water solubility, octanol-water partitioning coefficient (log K_{OW}).
- Environmental fate:
 - Soil adsorption, biodegradation half-life, estimates of volatilization from water, hydrolysis, photooxidation and media partitioning.
 - Detailed environmental explanations on the fate and behavior of individual chemicals in different media (air, water, soil, other).
- Analytical methods and uses:
 - Complete description of the different methods used to quantify individual chemicals, including the complete citation of the original source.
 - Description of the current and intended uses of individual chemicals, including the complete citation of the original source.

Table A.2.1. Summary of the type of information in CAFE's Aquatic Fate Module from each data source.

Data Fields in CAFE	SRC ¹	HSDB ²	NIST ³	EPI ⁴
<i>Structure and Physical properties</i>				
Odor		X		
Color/Form		X		



Data Fields in CAFE	SRC ¹	HSDB ²	NIST ³	EPI ⁴
Skin, Eye and Respiratory Irritation		X		
Boiling Point (°C)	X			
Melting Point (°C)	X			
Density	X			
Autoignition Temperature		X		
Vapor density		X		
Viscosity		X		
Explosive/Flammable limits		X		
Flash Point		X		
Ionization potential (ev)		X	X	
Hvap (cal/g) [Heat of Vaporization]	X			
HLC (atm·m ³ /mol) [Henry's Law Constant]	X			X
Log Kow [Octanol Water partitioning coefficient]	X			
Vapor Pressure (mm Hg)	X			
Water solubility (mg/L)	X			
<i>Environmental Fate</i>				
Soil Adsorption - Estimated Koc				X
Primary Biodegradation - Estimated Biodegradation Time				X
Estimated Volatilization - Half-life from Model River (hours)				X
Estimated Volatilization - Half-life from Model Lake (hours)				X
Estimated Hydrolysis at pH=7 - Half-life (days)				X
Estimated Environmental Partitioning - Percent to air				X
Estimated Environmental Partitioning - Percent to water				X
Estimated Environmental Partitioning - Percent to soil				X
Estimated Environmental Partitioning - Percent to sediment				X
Estimated Wastewater removal (percent) - Total Removed				X
Estimated Wastewater removal (percent) - Biodegradation				X
Estimated Wastewater removal (percent) - Sludge Adsorption				X
Estimated Wastewater removal (percent) - Volatilization				X
<i>Analytical Methods and Uses</i>				
Analytical Methods	X	X	X	X
Uses		X		

¹ SRC, Inc., formerly Syracuse Research Corporation; ² Hazardous Substances Data Bank; ³ National Institute of Standards and Technology; ⁴ US EPA Office of Pollution Prevention and Toxics, Estimation Program Interface (EPI) Suite.

A.2.2 Aquatic Effects Module

The **Aquatic Effects Module** contains chemical-specific information helpful in assessing the effects on aquatic receptors. Data within this module include:



- Aquatic toxicity data for individual chemicals.
- Acute toxicity data for a variety of aquatic receptors.
- Toxicity data for different exposure durations (e.g., 24, 48, 72, and 96 h).
- Toxicity data for two water types: salt water, fresh water.
- Toxicity data by life stage of the tested species.
- Toxicity data by taxonomic group (e.g., fish, crustaceans, other).
- Toxicity data in the form of median lethal concentrations (LC₅₀), median effects concentrations (EC₅₀), Lowest Observed Effect Concentration (LOEC), No Observed Effect Concentration (NOEC).
- Toxicity data by database source.
- Citations of the original data sources.

The toxicity data in this module was compiled from the following sources:

- ECOTOX database (<http://cfpub.epa.gov/ecotox/>).
- ECETOC database (<http://www.ecetoc.org>).
- DTox database (<http://www.researchplanning.com/projects/dtox-worldwide-quantitative-database-toxicity-dispersants-chemically-dispersed-oil/>).
- Expert consultations, peer-reviewed publications, open literature.
- User-provided data.

A description of the data inclusions criteria of each database is provided in the sections below.

A.2.2.1 Aquatic Effects Data Sources

A.2.2.1.1 ECOTOX

The ECOTOX database (<http://cfpub.epa.gov/ecotox/>) was developed, maintained, and is continuously updated by the US Environmental Protection Agency, Office of Research and Development (ORD), and the National Health and Environmental Effects Research Laboratory's (NHEERL's) Mid-Continent Ecology Division (MED). This database contains toxicity information of single chemicals for a number of taxonomic groups extracted primarily from peer-reviewed literature and internal government reports. Data from ECOTOX included in CAFE are queried periodically (four times a year), as this database is continuously updated. The large majority of toxicity data in CAFE (95%) comes from ECOTOX.

Basic criteria for data inclusion in ECOTOX are:

- Toxicity data associated with single chemical exposure.
- Toxicity data using aquatic plant or animal species.
- Toxicological endpoints on live, whole organisms.
- Data sources reporting environmental chemical concentration/dose or application rate.
- Toxicity data associated with an explicitly reported exposure duration.



- Full articles published in English.
- Documents and articles that are publicly available.

A.2.2.1.2 ECETOC

The ECETOC Aquatic Toxicity (EAT) database (<http://www.ecetoc.org>) was developed and maintained by the European Centre for Ecotoxicology and Toxicology of Chemicals, based in Brussels, Belgium. This database contains toxicity information of single chemicals for aquatic species in fresh and marine waters from peer-reviewed literature and internal government reports. Data from ECETOC was provided as a single file, with potential data additions pending future updates.

Basic criteria for data inclusion in ECETOC are:

- Data should be from original, scientific publications rather than from reviews or unpublished reports.
- Test methods employed should be described, or reference made to an appropriate published method.
- Only measured exposure concentrations are included in the database, except when the stability and physico-chemical properties of the tested material can be demonstrated.
- Chemical analysis used to define the exposure concentrations should be described or referenced.

A.2.2.1.3 Dispersant, Oil, and Dispersed Oil Toxicity Data

The oil and dispersant database (DTox) (<http://www.researchplanning.com/projects/dtox-worldwide-quantitative-database-toxicity-dispersants-chemically-dispersed-oil/>) was originally developed by Adriana C. Bejarano, Research Planning, Inc. through funds provided by NOAA and the University of New Hampshire's Coastal Response Research Center, but with future maintenance and updates to be supported by ERD. DTox contains toxicity data on dispersants and chemically dispersed oil for aquatic species from peer-reviewed literature, internal government reports, independent consultant and industry reports, and gray literature. Data from DTox was provided as a single file.

Basic criteria for data inclusion in DTox are:

- Toxicity data using aquatic species.
- Toxicological endpoints on live, whole organisms.
- Data should be from original, scientific publications rather than from reviews or unpublished reports.
- Test methods employed should be described, or reference made to an appropriate published method.
- Toxicity data associated with an explicitly reported exposure duration.
- Full articles published in English, except when information in another language could be accurately translated.



- Chemical analysis used to define the exposure concentrations should be described or referenced.
- Effect-concentrations that were easily converted to mg/L.
- Careful evaluation of the entire database for duplicate data.

A.2.2.1.4 Expert Consultations, Peer-Reviewed Publications, Open Literature

These types of data are rare in CAFE, but data additions from independent literature searches or through consultation with experts have also been undertaken by ERD.

Basic criteria for data inclusion by ERD are the same as those used in the development of ECOTOX.

A.2.2.1.5 User-Provided Data

These types of data are rare in CAFE, but data additions by users are also allowed. There are no basic criteria for data inclusion by users.

A.2.2.2 Additional Criteria for Data Inclusion in CAFE

Data reporting in CAFE's **Aquatic Effects Module** contains elements from each of the data sources above; however, additional exclusions were applied in addition to those implemented during the development of the original databases.

Additional criteria for data inclusion in CAFE are as follows:

- Those criteria used for data inclusion in ECOTOX and ECETOC.
- Studies including only one chemical per test (mixture data are not included).
- Studies with reported chemical name or CAS registry numbers.
- Laboratory testing only (monitoring studies are not included).
- Only aquatic toxicity data (toxicity data for terrestrial species are not included).
- Toxicity data reported as LC₅₀, EC₅₀, LOEC, NOEC (toxicity data reported as any other endpoint type are not included).
- Toxicity data based only on aqueous exposures.

A more complete discussion of data inclusions and manipulations is described in later sections of this document. Because of the amount of information handled particularly in the development of CAFE's **Aquatic Effects Module**. Sections below are dedicated to describing data manipulation, verification, and quality control implemented during the compilation of toxicity data.

A.3.0 Quality Assurance

The Quality Assurance/Quality Control (QA/QC) Plan of CAFE's **Aquatic Effects Module** is intended to meet the following goals:

- Summarize data management procedures and manipulations used during the development of CAFE.
- Provide a means by which the quality of information can be maintained in future updates.



- Provide a sound basis for documenting, evaluating, and verifying the accuracy of the data compilation process.
- Provide guidelines for the preparation and review of reports emerging from CAFE.
- Provide the means that would allow the user to assess the quality of data compilation efforts.

As part of the QA/QC components of CAFE's **Aquatic Effects Module**, data compiled from different sources are periodically reviewed to ensure accurate data entry. The ultimate goal is to review for accuracy and completeness a minimum of 5% of all data used in CAFE.

A.3.1 Data Inclusions

A.3.1.1 Active Ingredient and Mixtures

Inclusion of chemicals in CAFE required toxicity testing with a reported active ingredient purity, and not with chemical mixtures. Mixtures are excluded, except for chemicals that do not commonly occur as single chemicals (e.g., oils, dispersants, PCBs, salts, metals).

A.3.1.2 Chemical Names and Chemical Abstracts Service Registry Number

Each toxicity record in the database is required to have the chemical name of the tested compound and its associated Chemical Abstracts Service (CAS) Registry number. A CAS number is required because all queried data and data display are based on CAS numbers and not on chemical name. Records without CAS numbers are not included in the database. While chemical names and CAS numbers are entered in CAFE as reported in the original database, both are checked for consistency. Missing information (e.g., original database providing chemical names or CAS numbers) is filled in based on other existing records within the database, but records with inconsistent or uncertain chemical names and CAS numbers are either corrected or removed from the database. Any changes to chemical names or CAS numbers are documented within new columns in the master database, keeping the originally reported information unchanged.

A.3.1.3 Aquatic Organisms

This database only includes toxicity data for aquatic organisms. Toxicity data for terrestrial species are not included. Each toxicity record in the database is required to have a common name and/or scientific name, or at a minimum, information on genus. Records providing only family or kingdom are not included in the database. All records reporting or missing information on the specific life stage used in toxicity testing (if applicable) are included in the database, but missing records are given a specific code (NA). Additional information on data standardization of life stages is provided in Section A.4. Each species within the database should have an associated water type (if applicable) of either fresh water (salinities <1 practical salinity units [psu]) or salt water (estuarine or marine). This information is often reported as part of the experimental regime. However, records missing this information are assigned a water type based on the knowledge of the species and life stage habitat requirements, or based on information for that particular species/life stage from other records already in the database. In cases where water type



cannot be determined, records are given a specific code (NR). Each aquatic species within the database is assigned to the appropriate taxonomic group (currently, coral, crustacean, fish, mollusk, and other). Records missing taxonomic group information are assigned to the appropriate group based on the knowledge of the species, or based on information for that particular species from other records already in the database. Any changes to life stages, water type, or taxonomic group are documented within new columns in the master database, keeping the originally reported information unchanged.

A.3.1.4 Exposure Conditions and Toxicity Endpoints

Most toxicity records included in the database are from controlled laboratory exposures. Lotic, lentic, and osmotic exposures were also included, as long as measured concentrations were reported. Toxicity data from monitoring, mesocosm, or studies on community assemblages are not included. Similarly, only toxicity records from aqueous exposures are included in the database. Toxicity data from sediment exposures, from dietary and oral exposures, or from intraperitoneal/abdominal, intravenous, or other type of injections are not included.

CAFE includes toxicity data from various experimental regimes including static, flow-through, static renewal, pulse exposures, etc. and from studies reporting toxicity values on the basis of measured, nominal, unmeasured, or unreported. However, studies based on flow-through (and related laboratory settings) and measured concentrations are given a different treatment within the database (see Section A.4.3 on Applicability). All exposure durations are included in CAFE; however, data display within the tool is only based on the standard exposure durations: 24, 48, 72, and 96 h (see Section A.5). In all cases, toxicity endpoints must be reported as LC₅₀, EC₅₀, NOEC, LOEC. Toxicity data reported as any other LC or EC value (e.g., LC₁₀) are not included.

A.3.2 Database Fields

All the aquatic toxicity data compiled from different sources is reduced to a specific list of data fields, which are later used to develop CAFE's user interface. A summary of these data fields is shown in **Table A.3.2**.

Table A.3.2. Representative list of data fields currently in the master file of CAFE. This information is later integrated into the user interface (Section A.5).

Data Field	Description
ReferenceNumber	Unique reference number identification for individual records (rows) ¹ .
TestCAS	CAS number identification for individual records (rows) ¹ . [<i>Data field used in queries. See Section A.5.</i>]
Test ID	Unique Test ID identification for individual records (rows) ¹ .
ChemicalName	Chemical name associated with TestCAS.
SpeciesNumber	Numeric code assigned to unique species in the database, and associated with individual records (rows) ¹ .
SpeciesScientificName	Scientific name associated with SpeciesNumber. [<i>Data field used in queries. See Section A.5.</i>]



Data Field	Description
SpeciesGroup	Taxonomic group of the species tested.
LifestageCode	Life stage used in toxicity testing ¹ . Includes 91 code types. Examples: embryo (E), larva (L), juvenile (J), adult (A), subadult (SA), sac fry (SF), and unknown (U). [Data field used in queries. See Section A.5.]
Endpoint	Toxicity endpoint associated with individual records (rows) ¹ . Includes LC ₅₀ , EC ₅₀ , LOEC, and NOEC. [Data field used in queries. See Section A.5.]
TestDurationOP	Qualifiers (e.g., <, >) associated with test exposure duration.
TestDuration	Exposure duration (h) associated with toxicity record (rows). [Data field used in queries. See Section A.5.]
DurationUnits	Exposure duration units. All units converted to hours (h).
Concentration1MeanOP	Qualifiers (e.g., <, >) associated with the mean toxicity response value.
Concentration1Mean	Mean toxicity response value (rows). [Data field used in queries. See Section A.5.]
Concentration1MinOP	Qualifiers (e.g., <, >) associated with the minimum toxicity response value.
Concentration1Min	Minimum toxicity response value (rows).
Concentration1MaxOP	Qualifiers (e.g., <, >) associated with the maximum toxicity response value.
Concentration1Max	Maximum toxicity response value (rows).
ConcentrationUnits	Toxicity response value. All units converted to micrograms/liter (µg/L).
WaterType	Water type used in the derivation of toxicity endpoints for individual records (rows). Includes fresh water (FW), salt water (SW), or not reported (NR). [Data field used in queries. See Section A.5.]
ExposureType	Laboratory setting used to perform toxicity tests ¹ . Includes flow-through (F), static (S), static renewal (R), pulse (P), and not reported (NR), as well as from lotic, lentic and osmotic exposures.
TestMethod	Indicates whether a test method was used to characterize aquatic exposures to chemicals. Includes measured (M), nominal/unmeasured (N), and not reported (NR).

¹ Primarily from ECOTOX; exposures other than aqueous exposure (e.g., diet, injection, oral, or other) were not included.

A.4.0 Data Standardization and Missing Information

Because the **Aquatic Effects Module** of CAFE combines large amounts of information, data standardization was undertaken to facilitate further data integration (Section A.5). In all cases, any changes made to the original data source are clearly documented. Similarly, many records for key field attributes may contain missing information limiting the use of these records. However, in some cases, this missing information can be filled in. Procedures on the handling of missing information are provided below.



A.4.1 Aquatic Organisms

A.4.1.1 Scientific Name Verification

Each toxicity record in the database is required to have a common name and/or scientific name, or at a minimum, information on genus. Scientific names were verified and checked for changes of official names, as well for spelling errors (examples **Table A.4.3**). This verification was made through online sources including Integrated Taxonomic Information System (ITIS; www.itis.gov) and World Registry of Marine Species (WoRMS; www.marinespecies.org), or related sources (www.fishbase.com). Additionally, other global changes made include standardization of common names. For example, species with different common names, but with the same reported scientific name, are standardized to a single common name. Any changes to common or scientific names are documented within new columns in the master database, keeping the originally reported information unchanged.

Table A.4.3. Examples of species with reported scientific names modified to the currently accepted names. At least 480 species names were modified.

Reported name	Currently accepted name
<i>Acanthomysis costata</i>	<i>Holmesimysis costata</i>
<i>Arius felis</i>	<i>Ariopsis felis</i>
<i>Balanus albicostatus</i>	<i>Fistulobalanus albicostatus</i>
<i>Barbus conchoniis</i>	<i>Puntius conchoniis</i>
<i>Calanus plumchrus</i>	<i>Neocalanus plumchrus</i>
<i>Chrysophrys major</i>	<i>Pagrus major</i>
<i>Clupea harengus pallasii</i>	<i>Clupea pallasii</i>
<i>Brachydanio rerio</i>	<i>Danio rerio</i>
<i>Bufo cognatus</i>	<i>Anaxyrus cognatus</i>
<i>Gambusia holbrooki</i>	<i>Gambusia affinis</i>
<i>Homarus vulgaris</i>	<i>Homarus gammarus</i>
<i>Mysidopsis almyra</i>	<i>Americamysis almyra</i>
<i>Mysidopsis bahia</i>	<i>Americamysis bahia</i>
<i>Nereis glandicincta</i>	<i>Neanthes glandicincta</i>
<i>Oncocottus hexacornis</i>	<i>Myoxocephalus quadricornis</i>
<i>Pecten opercularis</i>	<i>Aequipecten opercularis</i>
<i>Penaeus setiferus</i>	<i>Litopenaeus setiferus</i>
<i>Penaeus vannamei</i>	<i>Litopenaeus vannamei</i>
<i>Pleuronectes flesus</i>	<i>Platichthys flesus</i>
<i>Rasbora heteromorpha</i>	<i>Trigonostigma heteromorpha</i>
<i>Salmo clarkia</i>	<i>Oncorhynchus clarkii</i>
<i>Salmo gairdneri</i>	<i>Oncorhynchus mykiss</i>
<i>Salvelinus malma</i>	<i>Salvelinus malma malma</i>



Reported name	Currently accepted name
<i>Stenonema ithaca</i>	<i>Maccaffertium ithaca</i>
<i>Tympanotonus fuscatus</i>	<i>Tympanotonos fuscatus</i>

A.4.1.2 Life Stage

The life stages of the species tested are classified into embryo, larva, juvenile, adult, or unknown, and reported as entered in the original data source. Life stage standardization of 91 unique ECOTOX codes are shown in **Table A.4.4**. If records are missing from the original data source, life stage information is filled in if the original data provides identifying information (e.g., length, size, weight, age in days, days of post hatch, etc.). This information is then used to enter life stage missing information based on the knowledge of the life cycle of the species, or based on information for that particular species from other records already in the database (examples, **Table A.4.5**). If life stage cannot be determined, records are given a specific code (U=unknown). Any changes to life stages are documented within a new column in the master database, keeping the originally reported information unchanged.

Table A.4.4. Standardization of life stage information.

Original ECOTOX Entries	CAFE Standardized Entries
Adult(s); imago; mature organism(s); mature organism(s); post-smolt; pre-spawning; sexually mature organism(s); young adult	Adult
Elver; fingerling; immature organism(s); juvenile(s); naiad; neonate; parr; post-hatch; post-larvae; pre-, sub-, semi-, or near adult; smolt; spat; subadult(s); swim-up; underyearling; yearling; young of year	Juvenile
Alevin; copepodid; copepodite; instar; larvae(e); larvae-pupa; mysis; prolarvae; protolarvae; rotzoaea; pupa(e); sac fry, yolk sac fry; tadpole; veliger; yolk sac larvae, sac larvae; zoea	Larva
Blastula; cleavage stage; cyst; egg(s); embryo(s); eyed egg or stage, eyed embryo; oocyte, ova; pre-larvae	Embryo
Exponential Growth Phase (Log); F0 generation; F1 generation; F11 generation; F2 generation; F6 generation; gestation; intermolt; lag growth phase; male gametophyte(s); mature (side-green stage) organism(s); megalopa; molt; morula; neurala; new, newly or recent hatch; newborn; not coded; not reported, unknown; organisms at different lifestages; post-emergence; post-molt; post-spawning; pre-molt; rooted cuttings; scape elongation; seed(s); seedling(s); sexually immature organism(s); shoot; sperm; spore; stationary growth phase; tissue culture callus; trophozoite; unspecified; young organism(s); zygote nauplii; nymph(s)	Unknown



Table A.4.5. Examples of the information used to assign life stage information to missing records.

Scientific Name	Identifying Information	Entered Missing Life Stage	New Life Stage Source
<i>Acipenser gueldenstaedtii</i>	2 yr old	Juvenile	Records within database
<i>Ambassis sp.</i>	840 mg	Adult	Records within database
<i>Ameiurus melas</i>	125 mm, 15 g	Adult	Records within database
<i>Ameiurus melas</i>	Fingerlings	Juvenile	Species specific life history
<i>Americamysis bahia</i>	8 day old	Juvenile	Species specific life history
<i>Amia calva</i>	1-1.5 g	Juvenile	Records within database
<i>Anabas scandens</i>	35 g, 14-16 cm	Juvenile	Records within database
<i>Balanus balanoides</i>	Cyprid, 10 D	Larva	Species specific life history
<i>Balanus improvisus</i>	Stage II nauplii, 3 h old	Larva	Records within database
<i>Cambarus robustus</i>	3.98 cm, 19.63 g	Adult	Records within database
<i>Carassius auratus</i>	7.62 cm	Adult	Records within database
<i>Daphnia magna</i>	<24 h old	Juvenile	Records within database
<i>Gammarus duebeni</i>	1.8 CM, 0.08 g	Adult	Records within database
<i>Gammarus pulex</i>	8-12 mm	Adult	Species specific life history
<i>Gasterosteus aculeatus</i>	4-5 wk old	Juvenile	Species specific life history
<i>Homarus americanus</i>	450 g	Adult	Records within database
<i>Ictalurus punctatus</i>	2 wk old	Larva	Records within database
<i>Litopenaeus vannamei</i>	Nauplius I	Larva	Records within database
<i>Oncorhynchus kisutch</i>	1.10 g, 5.0 cm, Fingerlings	Juvenile	Records within database
<i>Pimephales promelas</i>	30-35 d old	Juvenile	Records within database
<i>Puntius sophore</i>	1.8 g, 50 mm	Juvenile	Records within database

Life stages vary across species. In CAFE, “fry” (a life stage of salmon and other fishes) is classified as juvenile, while “glochidia” (a life stage of mussels) is classified as larva. As some identifying information is difficult to classify as embryo, larva, juvenile, or adult, a master list of species-specific life stages was created in a separate file (e.g., **Table A.4.6**). Identifying life stage information provided in the original data is compared against the compiled species-specific life stage information, and decisions made on the appropriate life stage. If identifying information is provided as a range value, the mean value is used to assign the appropriate life stage to records with missing information. For instance, *Palaemonetes pugio* reported range “1.5-4 CM,” with a mean value 2.75 cm, was classified as an adult.

**Table A.4.6.** Representative examples of life stage classification by species.

Scientific Name	Life Stage Conditions
<i>Americamysis bahia</i>	Adult >10 Days, 10 MM Juvenile 0-10 Days Embryo <0 Day
<i>Cyprinodon variegatus</i>	Adult > 3 CM Juvenile 12 D, <0.7 g Larva <11 D, <10 mg Embryo < 0 D
<i>Danio rerio</i>	Adult 3 CM, 6 MO, 0.4 G Juvenile < 6 MO, < 3 CM <0.4 G Larva <0.1 G, 10 D- Embryo < 0 D
<i>Daphnia magna</i>	Adult after 7 days, > 2MM Juvenile <7 days, <2 M Embryo <0 days
<i>Farfantepenaeus duorarum</i>	Adult >140 MM, max male 169 MM, max female 280 MM Juvenile 10-140 MM Larva <1.5 g, 10 MM, 24 hours
<i>Gambusia affinis</i>	Adult >2.3 CM, > 0.25 G Juvenile 1-3 CM, 0.1 - 0.25 G, >1 Wk Larva <10 MM, <0.1 G
<i>Ictalurus punctatus</i>	Larva <0.3 G, 2 weeks Juvenile >0.3 G to 14 MO Adult 2 years
<i>Labeo rohita</i>	Adult >20 CM Juvenile >0.1 G, > 2.5 CM Larva < 0.1 G, < 2.5 CM
<i>Menidia beryllina</i>	Embryo <2 D old Larva < 33 D old - < 0.1 G Juvenile 0.1 G- 1 G
<i>Oncorhynchus mykiss</i>	Larva < 15 Days old, <0.3 G, < 2.5 CM sac fry, alevin Juvenile 2.5 - 24 CM, < 1 year, 0.3 G - 300 G, swim up fry Adult >20 CM, >250 g, 1-3 years
<i>Oreochromis mossambicus</i>	Adult 8G, >6.5 CM Juvenile >40 D, >0.1 G, >15 MM Larva <40 D, <0.1 G, <15MM
<i>Palaemonetes pugio</i>	Adult >2.2 CM Juvenile <2.2 CM, >0.2 G, >6MM Larva <6MM, <20 D
<i>Pimephales promelas</i>	Adult >16 WK, 35 MM, 0.8 G Juvenile 14 D to 8 Wk, 0.05 G - 0.8G, >10 MM Larva <14 D, 0.05 G, <10 MM



Scientific Name	Life Stage Conditions
<i>Salmo salar</i>	Adult ~3 YR Juvenile 0.2G - 200 G Larva <0.2 G
<i>Semibalanus balanoides</i>	Adult 1 yr Larva cyprid, nauplii

A.4.1.3 Taxonomic Group

Each aquatic species within the database is assigned to one of the following taxonomic groups: corals, fish, crustaceans, mollusks, and other (e.g., algae, echinoderms). This is particularly important for data from ECETOC, as this database assigned records to taxonomic groups more specific than crustaceans. Records missing taxonomic group information are assigned based on the knowledge of the species, or based on information for that particular species from other records already in the database. Any changes to taxonomic group are documented within a new column in the master database, keeping the originally reported information unchanged.

A.4.2 Exposure Conditions and Toxicity Endpoints

A.4.2.1 Effects Concentrations and Units

Each toxicity record in the database is required to have a value associated with the reported endpoint (e.g., LC₅₀, EC₅₀, NOEC, LOEC), which is later used in data visualization plots (Section A.5). Open-ended toxicity values preceded by qualifiers (e.g., >, <) are excluded. For those values, a range of observed toxicity values is given (e.g., minimum and maximum), the arithmetic mean of which is calculated and used as the value associated with the reported endpoint.

All toxicity records are converted to µg/L (**Table A.4.7**). If units could not be determined, the toxicity records are not included. In all cases when conversions are used, an identifier is added to the database to keep track of conversions (0=as reported; 1=conversion to µg/L used during standardization). When information on molecular weight is needed for conversions, this information is obtained from CAFE's **Aquatic Fate Module**. Any calculated values or changes to reported units are documented within new columns in the master database, keeping the originally reported information unchanged.

Table A.4.7. Toxicity units and conversion factors. MW= molecular weight.

Reported Unit	Conversion to µg/L
pmol/L	unit / 10 ⁶
pg/L	unit / 10 ⁵
0/00, AI ng/L, ng, ng/L, ppt	unit / 1000
pg/g, pg/ml	unit /100
ae ppb, ae ug/L, AI ng/mL, AI ppb, AI ug/kg, AI ug/L, ng eq/ml, ng/g, ng/ml, ppb, ug/dm ³ , ug/kg, ug/L	Unit



Reported Unit	Conversion to µg/L
ng/0.5 ml	unit * 2
pg/ul, ug/10 L, ug/100 ml	unit * 10
ae mg/L, AI mg/kg AI mg/L, ai ppm, AI ug/ml, AI ul/L, mg, mg/dm ³ , mg/kg, mg/L, ppm, ppmv, ug/g, ug/ml, ul, ul/L	unit * 1000
mg/100g	unit * 10 ⁴
AI ml/L, g, g/dm ³ , g/kg, g/L, mg/g, mg/ml, ML, ml/kg, ml/L, ug/mm ³ , ul/ml % vol	unit * 10 ⁶
%, ml/10 L, % v/v, % w/v	unit * 10 ⁷
AI g/m ²	unit * 10 ⁸
g/m ³ , g/ml, mm ³ /L	unit * 10 ⁹
1e-9 M	unit / 10 ⁹ * MW
nM, nM/L, nmol, nmol/L	unit / 1000 * MW
nmol/g, nmol/ml, uM, uM/L, umol, umol/dm ³ , umol/kg, umol/L	unit * MW
mM, mM/L, mmol, mmol/kg, mmol/L, umol/g	unit * 1000 * MW
M, mmol/m ³ , mol, mol/dm ³ , mol/L	unit * 10 ⁶ * MW
mol/g, mol/m ³	unit * 10 ⁹ * MW

A.4.2.2 Exposure Duration

No standardization of exposure duration is performed, and only standard exposure durations equivalent to 24, 48, 72, and 96 h are displayed within CAFE's user interface (see Section A.5). Only conversions from days to hours (e.g., 1 day=24 h) are made, and any conversions of exposure duration are documented within new columns in the master database, keeping the originally reported information unchanged. Exposure durations such as days post hatch (dph) are not included.

A.4.2.3 Water Type

The water type used in toxicity testing is classified as fresh water, salt water, or not reported, and entered in CAFE as entered in the original data source. If records are missing from the original data source, water type is filled in based on scientific name and life stage information. This information is then used to fill in missing information based on the knowledge of the life cycle of the species, or based on information for that particular species from other records already in the database (examples **Table A.4.8**). If water type cannot be determined, records are given a specific code (U=unknown). Any changes to water type are documented within new columns in the master database, keeping the originally reported information unchanged.

Table A.4.8. Examples of the information used to assign water type to missing records.

Scientific Name	Life Stage	Entered Missing Water Type	New Water Type Source
<i>Acilius sulcatus</i>	Larva	FW	Records within database
<i>Aedes aegypti</i>	Larva	FW	Records within database



Scientific Name	Life Stage	Entered Missing Water Type	New Water Type Source
<i>Aeshna cyanea</i>	Larva	FW	Records within database
<i>Channa punctata</i>	Unknown	FW	Species specific life history
<i>Channa striata</i>	Juvenile	FW	Species specific life history
<i>Crassostrea virginica</i>	Unknown	FW	Species specific life history
<i>Danio rerio</i>	Unknown	FW	Records within database
<i>Daphnia magna</i>	Unknown	FW	Records within database
<i>Gambusia affinis</i>	Juvenile	FW	Records within database
<i>Ictalurus punctatus</i>	Juvenile	FW	Records within database
<i>Lepomis macrochirus</i>	Juvenile	FW	Records within database
<i>Oncorhynchus keta</i>	Juvenile	FW	Records within database
<i>Oryzias latipes</i>	Unknown	FW	Species specific life history
<i>Scylla serrata</i>	Adult	SW	Records within database

A.4.3 Check for Duplicates

As part of the QA/QC components of CAFE's **Aquatic Effects Module**, data compiled from different sources are reviewed in an effort to identify potential duplicate toxicity data (e.g., data published by authors in more than one published article or report). The identification of potential duplicate data was undertaken as follows: several species with the most records are selected, and duplicates identified by matching several fields (e.g., toxicity value, endpoint, CAS#, species scientific name, species life stage, exposure duration, and exposure type). If records sharing all the above information (i.e., identical information) are identified, these are flagged as potential duplicates, and original data sources checked for accuracy. Through these exercises, it is estimated that a small percent of data in CAFE (3%) are duplicate records.

A.5.0 DEVELOPMENT OF CAFE'S USER-INTERFACE

All data are currently stored in a database format that is migrated into a platform (FileMaker® Pro 12) with expanded capabilities. In FileMaker® Pro 12, data are filtered by specific attributes (e.g., life stage, taxonomic group, endpoints, data sources, water type, exposure duration), which are used as the selection criteria for data visualization of chemical-specific data.

A.5.1 Data Queries and Graphics

CAFE's user interface allows for selection of chemical-specific data, with graphics generated based on specific data selection. Data selection is based on the following fields:

- CAS number.
- Species Group (Coral, Crustacean, Fish, Mollusk, Other).
- Species common or scientific name.
- Life Stage (Embryo, Larva, Juvenile, Adult, Unknown).
- Endpoint (LC₅₀, EC₅₀, LOEC, NOEC).



- Water Type (salt water, fresh water).
- Exposure Duration (24 h, 48 h, 72 h, 96 h).
- Data Applicability (High, Moderate, Low).

Following data selection, the queried data are plotted and visualized on a separate window. Data are displayed in the form of Species Sensitivity Distributions (SSDs), which are constructed by calculating the geometric mean of toxicity data for each individual species (by scientific name). Data included in geometric mean calculations are:

- Toxicity data without qualifiers (toxicity data preceded by \geq , \leq , $>$, or $<$ are not included).
- Toxicity data calculated as the mean of minimum and maximum toxicity data values.
- Unique toxicity data (data identified as duplicates are not included).

During the development of SSDs, routines were implemented to identify and remove outlier effects on logistics curves. Outliers were identified as follows:

- In cases where logistic curves were skewed by one or two geometric means, values were removed from the final computation of the logistic curve.
- Predetermined boundaries were used to test each data point and to identify potential outliers. These boundaries were defined as follows:
 - Dividing all geometric mean calculations per curve into quarters, q1, q2, and q3, which are the numbers that mark the first, third, and middle quarters.
 - Concentrations falling outside of the $(q3 - q1) * 1.4$ range are considered to be minor outliers, while concentrations falling outside of the $(q3 - q1) * 3$ range are considered to be major outliers.
 - Both minor and major outliers were excluded prior to the calculation of the logistics curve.

Additional details on SSDs include:

- SSDs are generated by fitting the toxicity data to a logistic function defined by $F(x) = \frac{L}{(1+c*e^{(a*x)})}$, $x \in R$, where L is the curve's maximum value, and a and c the regression coefficients.
- Fitted SSDs do not include a goodness-of-fit test.
- SSDs are only generated for datasets with a minimum of 5 species.
- Two Hazard Concentrations (HC) (HC1 and HC5, equivalent to the concentrations at which 1% and 5%, respectively, of the species in the SSD may not be protected⁹) are included.

⁹ While there is debate in the scientific literature regarding the appropriateness of one versus another HC percentile, the HC5 selected here was chosen because this is the most commonly used percentile, while a lower percentile (HC1) would offer an additional safety factor preferable when dealing with very highly toxic chemicals.



- Data are displayed based on color coding selections (e.g., applicability, endpoints, life stage, data sources, species group, water type, analytes, analytical methods, exposure conditions, ratios).
- All SSDs are plotted over a colored background representing a common scale of relative toxicity for aquatic organisms. This color code scheme was adopted from the US EPA Office of Pesticide Programs¹⁰.

Scale
Very highly toxic (<100 µg/L)
Highly toxic (100-1,000 µg/L)
Moderately toxic (1,000-10,000 µg/L)
Slightly toxic (10,000-100,000 µg/L)
Practically nontoxic (>100,000 µg/L)

A.5.2 Data Applicability to Spill Response

Each toxicity data record (rows) within CAFE were scored (High, Moderate, Low) based on their applicability to chemical spill response. This score was judged based on source-specific considerations, and are as follows:

High

- Toxicity data with reported concentrations on the basis of measured concentrations (Test method: M).
- Toxicity data from laboratory setting performed under flow-through conditions (Exposure Type: F).
- Reported $\geq 90\%$ active ingredient purity (Chemical Scenario only).

Moderate

- Toxicity data with reported concentrations on the basis of measured concentrations (Test method: M).
- Toxicity data from laboratory setting performed under static or static renewal conditions (Exposure Type: S, R).
- Reported $\geq 75\%$ - $< 90\%$ active ingredient purity (Chemical Scenario only).

Low

- Toxicity data with reported concentrations on the basis of nominal or unmeasured concentrations (Test method: N).

¹⁰ Source: <https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/technical-overview-ecological-risk-assessment-0>



- Toxicity data not clearly stating if the reported concentration are nominal, unmeasured, or measured (Test method: NR).
- Toxicity data not clearly stating the laboratory conditions used during testing (Exposure Type: NR).
- Reported <75% active ingredient purity (Chemical Scenario only).

Note: Source applicability is assigned to individual records (rows) in the database. Source applicability is based on the relevance of these data to spill response, and not on the overall scientific merit of individual records.

A.6.0 Testing of CAFE

Prior to the release of the first version of CAFE, extensive testing was performed within the CAFE development team as well as by selected testers.

A.6.1 Internal Testing

The development team anticipated that users' test platforms would include Windows (Windows 7) and Macintosh (OS X Mountain Lion) operating systems.

Specific tests included:

- Testing every aspect of the program: buttons, checkboxes, fields, reports, tabs, windows.
- If a sequential process is required for the correct usage of the program, verify that the correct order of the steps must be followed and that processes are not active or indicated as active until the correct point in the process.
- Verify that searches return appropriate results for chemicals, dispersants, and oils as identified in search criteria, based on name or CAS Number.
- Verify that, if a checkbox is checked or unchecked, the correct filter has been applied to the data being displayed.
- If criteria are required for a process or function to occur, verify that the criteria are met (e.g., data for a minimum of 5 species are required for a curve to be drawn).
- Verify that hovering the cursor over an area in the window displays the correct number of records associated with that area (i.e., if a species has 6 records associated with it and only Low applicability, the screen should display the number 6 when the cursor is hovered over the Low applicability area for that record).

General issues that the CAFE development team focused on included:

- Checking for spelling errors, including error message boxes, headings, etc.
- Ensuring that CAFE performs searches, draws, etc. at a reasonable speed (less than 20 seconds).
- Ensuring that text does not run long or off the screen.
- Ensuring that incorrect searches and queries do not produce any results (e.g., searching for dispersant in the oil scenario).



- Ensuring that cursor-hovering over grid dots and individual toxicity parameters shows a record count.
- Ensuring that grayed-out radio buttons and checkboxes are not available for checking and selection.
- Ensuring that the number of records are reduced as selections are made within the tabs.

In addition to general checks, several queries were performed consistently (e.g., same queries, same chemicals, same selections, etc.) with the purpose of identifying and correcting programming and data display issues. A summary of these queries is included below.

Chemical Scenario

- Chemical Search:
 - Search Chemical Name “benzene” with all four search modes (Exactly matching, Starts with, Ends with, Anywhere in).
 - Search CAS Numbers (1327533, 12125029, 2691410, 2104645, 10108642).
 - View the Aquatic Fate and Effects Modules.
 - Ensure that all chemical names are spelled correctly.
 - Switch Search modes with the CAS number search.
 - Select a chemical with no Fate or Effects Data. The user should not be able to proceed to the next screen.
- Aquatic Fate Module:
 - Search Chemical Name “benzene” and click View Fate.
 - Check the Fate helps of each sub-module. The user should be able to clearly see the text and scroll up/down.
 - Click the Return button on each sub-module.
 - Click the Print button on each sub-module.
 - Repeat steps above with other chemicals (e.g., ethanol, acrylonitrile).
- Aquatic Effects Module – General Aquatic Toxicity Interface:
 - Click the “Clear All Selections on This Screen,” or “Clear All Selections” on any screen. The appropriate tables should be cleared.
 - Click buttons for the “go back” steps (e.g., from “4. Life Stage” to “2. Chemical”). A message should appear stating that the going-back steps will clear all selections.
 - Hovering over gridded data should display the total number of toxicity records.
 - Grayed-out radio buttons should not allow for selections.
 - The Plot Graph button should only be enabled at the end of the query selection.
 - All species should be correctly spelled (common names or scientific names).
 - All species should be assigned to the correct species group.



- SSDs:
 - Select each of the dropdown options of the Shade feature.
 - Only one type of shading by feature is allowed.
 - The “shade by” feature should be disabled for editing.
 - View the Aquatic Report fields. They should be disabled for editing.
 - Going back to the selection query should result in an updated SSD.
 - The Print button should prompt the user to their default printer screen.
 - The Show Selection summary screen should display the entire data query selected by the user.

Oil, Dispersant, and Dispersant and Oil Scenarios

- The “Proceed to” button should be disabled until all prior selections are made.
- All of the remaining steps should be identical to those for the Chemical Scenario.
- Dispersant and Oil Scenario:
 - Search “diesel” with all four search modes.
 - Select Diesel Fuel No. 2 and Corexit 9527 with a 1:1 ratio. Select All for the options on the rest of the page.
 - Select all defaults (all species, all life stages, etc.). Choose any test duration. Plot graph.
 - Refer back to the SSD Plots section.
 - The Shade by Ratios should be allowed under this scenario.
 - Go back and make different selections. The SSD should reflect the new query.
- Oil Only Scenario:
 - Search “diesel” with all four search modes.
 - Select Diesel Fuel No. 2 and Select all Analytical Methods and Analytes.
 - Select all defaults (all species, all life stages, etc.). Choose any test duration. Plot graph.
 - Refer back to the SSD Plots section.
 - Go back and make different selections. The SSD should reflect the new query.
- Dispersant Only Scenario:
 - Search “corexit” with all four search modes.
 - Select Corexit 9500 and Select all Analytical Methods and Analytes.
 - Select all defaults (all species, all life stages, etc.). Choose any test duration. Plot graph.
 - Refer back to the SSD Plots section.
 - Go back and make different selections. The SSD should reflect the new query.

Short Exposure Risk Reports

- Click on the Short Exposure Risk Report for ammonia.
- The user should be able to clearly see the text and scroll up/down.



- Press return. The User should be prompted to the list of reports.
- The reports should be disabled for editing.

User-Added Data Entry

- Search “benzene,” “diesel,” and “corexit” in their respective scenarios with all different search modes. Searches should not overlap between scenarios.
- Add a new “test” chemical, oil, or dispersant.
- Add a new species in any scenario. The user should not be able to submit a new species twice.
- Select various choices from each of the dropdown menus.
- Enter a random concentration.
- Add user notes.
- Check the green progress labels.
- Go back and search the “test” chemical, oil, or dispersant in their respective scenarios.
- Select the “test” chemical, oil, or dispersant and proceed to the Species selection.
- Go through the remaining parameters with the user-added data selections. The user-added data point should be displayed on the graph.

A.6.2 External Testing

Seven individuals extensively tested the pre-release version of CAFE and provided comments as well as feedback on opportunities for improvement of the interactive tool. The CAFE development team addressed the majority of these comments, while other comments/suggestions will be considered during future updates of CAFE. A summary of comments received during the testing phase of the pre-release version are included in **Table A.6.9**.



Table A.6.9. Strengths and limitations of CAFE (Version 1.1) based on feedback provided by users. Enhancements implemented in the most recent version are also indicated where applicable.

Comment	Response	Possible Solution (CAFE version)
General Comments		
The CAFE database is intuitive, comprehensive, and easy to use. It is very advantageous to have chemical fate and effects information compiled in one database.	None	None
The data compiled in CAFE includes thousands of chemicals, making it a very robust source of information. It is organized in a logical fashion.		
This is a product that has been needed for a while. It is comprehensive and user-friendly.		
The short term exposure files are a nice addition.		
The full name of the database should be included on the opening page.	Agree	The CAFE development team will make this update (Version 1.1).
The disclaimer should be expanded to clearly state the data selection process, and this should be included on the opening page, in addition to providing it in the user manual.	Agree with the overall comment. This information is captured in the manual, but more clear guidance will be provided to the user.	An additional note or disclaimer was added to the home page (Version 1.1).
The database is slow.	Data queries for data-rich chemicals can be slow. The CAFE development team is working on a solution to optimize performance.	Speed performance was substantially improved in Version 1.2. The CAFE development team will continue to explore programming solutions to speed performance (future versions).
The font size could be a bit larger.	Agree, but a larger font may cause screens to be even busier.	The CAFE development team will look into a larger font size (Version 1.1).



Comment	Response	Possible Solution (CAFE version)
The User-Added Data section has 2 buttons, and it is not immediately clear which to use or how to use them.	Agree. The “How to Use CAFE” document provides specific guidance on how to navigate through the User-Added Data section.	The User-Added Data screens were substantially improved in Version 1.2. The CAFE development team will continue to improve the User-Added Data screens (future versions).
Aquatic Fate Module		
Having all the fate data in one place is great, minimizing the need for looking in multiple references.	None	None
CAFE needs more fate and effect data for chemicals.	None	Fate and effects data were substantially improved in Version 1.2. The CAFE development team will continue to explore additional data sources (future versions).
Some of the fate parameters are off.		Fate parameters were substantially improved in Version 1.2.
Aquatic Effects Module		
I like the ability to access the original study data. This lends scientific value to the database.	None	None
The graphing feature is really nice, particularly the links to individual data points. I also like the color scheme and including the EPA toxicity categories.		
Under the Species Tab, “Latin Name” should be relabeled “Scientific Name.” Sorting by scientific name should be allowed.	Agree. Allowing sorting by common name or scientist name has been a programming challenge.	The CAFE development team will continue to explore programming solutions so that sorting by name can be implemented (future versions).
The black text on gray button (after “Proceed to:”) is not intuitive as a working button to click. Similar comment applies to “Plot Graph.” It should be made clear to the user that some features could not be used.	Agree. Making all buttons and features intuitive are programming challenges, as the user’s perceptions cannot be anticipated. This information is captured in the manual, but more clear guidance will be provided to the user.	The CAFE development team will continue to explore programming solutions to enhance the intuitive nature of the tool (future versions).



Comment	Response	Possible Solution (CAFE version)
Plot Graph should not appear or be faded until all the selections have been made.	Great suggestion.	The CAFE development team will make changes to this button (Version 1.2).
There should be a way to save the plot as a file, as well.	Agree. The user can right-click and copy/paste the plot into a document. This information is detailed in the manual and the "How To" document.	None
Explanations for the abbreviations (ECOTOX and ECETOC) are needed.	Agree. This information is detailed in the manual.	None
Selecting only one duration for effects will reduce the number of species/data points, and may be unnecessary.	Agree. However, the CAFE development team adopted these exposure durations as they are considered to be standard in most toxicity testing.	Keep the individual exposure durations, but allow for all durations to be combined (Version 2).
Selecting between fresh and salt water may be unnecessary.	This feature was added because it is known that water type can influence the toxicity of some chemicals.	Keep the individual water types, but allow for both water types to be combined (Version 2).
Consider the inclusion of toxicity data beyond the maximum duration (96 h).	Agree	Add and combine all toxicity data with exposure duration >96 h (future versions).
Statements on the user interpretation of SSDs should be cautioned.	Agree with the overall comment. This information is captured in the manual, but more clear guidance will be provided to the user.	An additional note or disclaimer will be added to the home page (Version 1.1).
The usefulness and applicability of the output could be improved by providing an output file of the data points and curve parameters.	Agree with the comment. These features would make CAFE more broadly useful to the scientific community, expanding its use in risk assessment.	Allow for export of output data (future versions).



Comment	Response	Possible Solution (CAFE version)
Place 95% confidence bands (CIs) around the SSDs.	We have long recognized the lack of CIs as a limitation on the data display. This has been a programming challenge and not an omission by the CAFE development team.	The CAFE development team will continue to explore programming solutions so that CIs can be implemented (future versions).
Eliminate HC1s.	While we agree that the HC1 is highly uncertain, this lower value provides an extremely conservative value of potential use for spill responders.	None
Some of the original references for the data points are missing.	Likely a coding issue.	This bug was fixed in CAFE version 1.2.



Appendix B: Technical Document: Short-Exposure Risk Estimate Concentrations for Selected Chemicals

Generally, in real spills of chemicals into rivers, estuaries, and the ocean, organisms are likely to be exposed to the spilled chemical in short pulses. However, the toxicological data from controlled laboratory testing takes the form of a more constant exposure of long duration (e.g., 96 h). Because of this mismatch between real exposure scenarios and those from standard laboratory testing, the CAFE development team developed a procedure by which more applicable exposure scenarios could be developed to derive more reasonable Hazard Concentrations. The following sections provide a general description of the methodology developed to estimate the potential risk to aquatic species following short exposures (a few hours) to the spilled chemical. In all cases, the estimated concentrations that may pose unacceptable risks to aquatic species represent the 5th percentile concentration on the Species Sensitivity Distribution (SSD) curve, or the concentration assumed to be protective of 95% of the species tested.

Chemicals selected for these analyses included those chemicals with sufficient acute toxicity data in CAFE that followed one or more of the following criteria:

- Involved in accidents by the Department of Transportation (DOT).
- Potentially toxic to humans and biological resources.
- Reasonably water soluble.
- Shipped in bulk and having a reasonable risk of being spilled in large quantities.

This document also includes a description of the color schemes included in the Short Exposure Risk Reports, as well as a summary of the level of the risk estimate reliability associated with each of the chemicals evaluated.

B.1.0 Data Sources

The large majority of data used in risk estimates were extracted from CAFE and a few additional data points were generated through online searches or peer-reviewed literature and reports, or were provided by colleagues. Because of data limitations, data were not separated by variables that have the potential to influence risk estimates. Some of these variables include life stages and water type (i.e., seawater, fresh water), or laboratory testing conditions (i.e., static, flow-through). In addition, acute toxicity data included nominal and measured concentrations, as well as median lethal (LC₅₀) and median effects (EC₅₀) concentrations. The lowest observed effects concentrations (LOEC) and the no observed effects concentrations (NOEC) were only used when limited data were available.



B.2.0 Data Analysis Process

Risk estimates were developed following the methodology reported in Bejarano and Farr, 2013¹¹. The following section summarizes this methodology:

- Visual observation of potential differences in sensitivity across groups of species for which acute toxicity are currently available:
 - If differences in sensitivity across groups¹² are suspected, analyses were performed separately for the most sensitive group(s), as well as for the combined remainder group(s).
 - If no obvious differences in sensitivity across groups are suspected, analyses were performed for the combined group(s).
 - To avoid potential group-bias, groups of species were excluded if they were not equally represented across the different exposure durations.
 - The analyses above were limited by availability of data.
- Species Sensitivity Distributions (SSDs) by exposure duration (typically 24, 48, 72, and 96 h) with a minimum of 5 species were constructed, assuming a log-normal family distribution:
 - For curves with limited empirical data that shared one common species across all exposure durations, data were augmented via the EPA's Web-based Interspecies Correlation Estimation (Web-ICE) application.
 - If several species are shared across all exposure durations, the most sensitive species was used as a Web-ICE surrogate.
 - To reduce uncertainty, only species with a cross-validation success rate $\geq 90\%$ and the closest taxonomic distance were included (see the Web-ICE User Manual for details; <http://epa.gov/ceampubl/fchain/webice/>). Only in the absence of the closest taxonomic distances (1=within the same genus, 2=within the same family) were other taxonomic distances considered (3=within the same order, 4=within the same class, 5=within the same phylum).
- Two goodness-of-fit tests (Kolmogorov-Smirnov and Anderson-Darling) were used to assess the fit of SSD curves under a log-normal family distribution:
 - Curves failing either of the goodness-of-fit tests at an $\alpha=0.05$ were evaluated for *gross* outliers via robust analysis (QQ plots and residual plots under the assumption of a log-normal form).
 - After removal of outliers, goodness-of-fit tests were performed again and curves failing the Kolmogorov-Smirnov test at an $\alpha=0.05$ were excluded from the analysis.

¹¹ Bejarano, A.C., Farr, J.K., 2013. Development of short acute exposure hazard estimates: A tool for assessing the effects of chemical spills in aquatic environments. *Environmental Toxicology and Chemistry* 32, 1918-1927.

¹² Groups refer to the following: fish, crustaceans, mollusks, amphibians, insects/spiders, invertebrates, worms.



- Curves passing the Kolmogorov-Smirnov test but failing the Anderson-Darling test were included only if less than 3 curves were available for short exposure extrapolations.
- Curves passing the Kolmogorov-Smirnov test but with insufficient data points to compute the Anderson-Darling test (small sample sizes, $n < 7$) were also included.
- Assuming a long-normal distribution, individual SSD curves for all available “longer exposure durations” (typically 24, 48, 72, and 96 h) were bootstrapped 2,000 times and the 5th percentile concentration¹³ with its associated 95% confidence interval estimated (**Figure B.2.1**, left plot).
- 5th percentiles and confidence interval concentrations for all SSD curves were plotted on a log-log scale versus the original exposure duration, and regressions linear bootstrap analysis (2,000 draws) was used to estimate concentrations at short exposure durations (1, 2, 4, 8, 24 hours) (**Figure B.2.1**, right plot). Note: bootstrap analysis would fit all possible curves among the given data points, and therefore, the resulting confidence intervals may differ from those of the “longer exposure durations.” (typically 24, 48, 72, and 96 h)
 - Bootstrap 95% confidence intervals of the slope, calculated via bias-corrected accelerated bootstrap (BCa), that included “0” were deemed to have failed the analysis and were excluded.
 - For chemicals with at least 4 exposure duration SSDs that did not pass the linear bootstrap, the mean 5th percentile concentration, but *not* its associated 95% confidence interval, was used to estimate concentrations at short exposure durations.
- Successful linear bootstraps were used to estimate concentrations for short exposure durations include the mean response as its associate 95% confidence interval.

¹³ Hazard concentration assumed to be protective of 95% of the species tested.

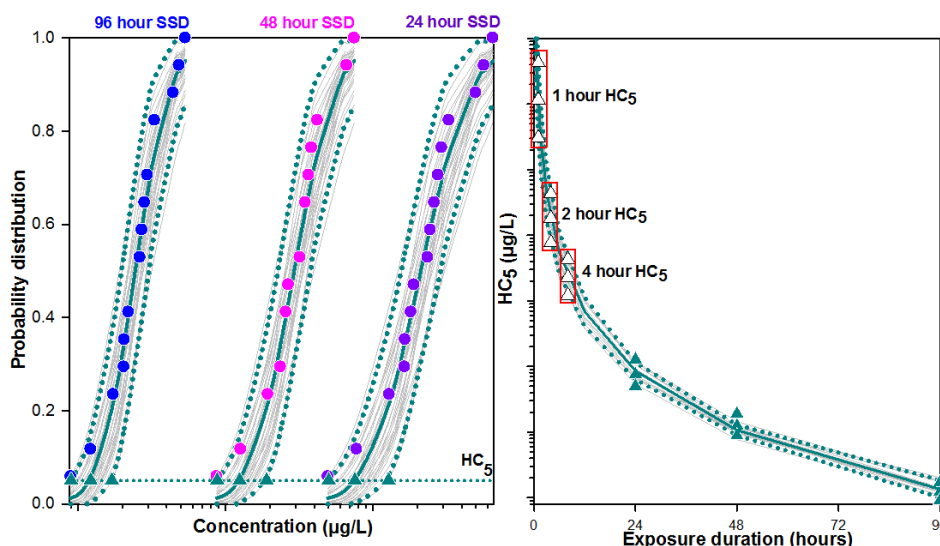


Figure B.2.1. Schematic representation of the method used to derive the 5th percentile hazard concentrations (HC5) for short exposure durations from Species Sensitivity Distributions (SSDs). Left plot: Empirical data (open circles) for several exposure durations (24, 48, 96 h) with their bootstrapped (grey lines), mean (solid green lines), and 95% confidence interval (95%CI) SSDs (dashed green lines), and the estimated HC5s (green triangles). Right plot: Estimated HC5s from longer exposures (green triangles), the bootstrapped mean (solid green line), and 95%CI concentrations (dashed green lines), and the estimated HC5s for short exposure durations (white triangles).

B.3.0 Color Schemes and Assessment of Reliability

B.3.1. Chemical Inherent Acute Toxicity

The following color scheme (**Table B.3.1**) was used to provide a visual representation of the inherent acute toxicity of chemicals with estimated exposure concentrations at short exposure durations (1, 2, 4, 8, 24 h). Tables and figures within Short Exposure Risk Reports include chemical-specific inherent toxicity color coding.

Table B.3.1. Color scheme used in all Short Exposure Risk Reports to denote the relative toxicity of individual chemicals. This color scheme is consistent with the toxicity category used in CAFE.

Toxicity Category	LC ₅₀ (µg/L)	Color Scheme
Very highly toxic	<100	Red
Highly toxic	100-1,000	Orange
Moderately toxic	1,000-10,000	Yellow
Slightly toxic	10,000-100,000	Blue
Practically nontoxic	>100,000	Teal

B.3.2. Decision Tree for Risk Estimate Analysis Reliability

The following criteria and color scheme (**Table B.3.2**) applies to chemicals that successfully passed the linear bootstrap analysis, and are associated with the level of risk estimate reliability. Tables showing risk estimates within Short Exposure Risk Reports include chemical-specific risk



estimate reliability color coding. Note that all estimates provided in Short Exposure Risk Reports are subject to change based on additional chemical-specific information.

Table B.3.2. Color scheme used in Short Exposure Risk Reports to denote the relative reliability of risk estimates.

Risk Estimate Reliability	Criteria
High	>7 data points for each of ≥ 3 exposure durations without additional data points from Web-ICE. No violations of goodness-of-fit tests. Limited data manipulation (fit, refit, outlier removal).
Moderate	≥ 5 data points for each of 3 exposure durations with or without additional data points from Web-ICE. Violations of the Anderson-Darling goodness-of-fit test. Curves with insufficient data points to compute the Anderson-Darling test (≤ 7). Limited data manipulation (fit, refit, outlier removal).
Low	< 5 data points for each of 3 exposure durations with or without additional data points from Web-ICE. Curves with insufficient data points to compute the Anderson-Darling test (≤ 7). Substantial data manipulation (fit, refit, outlier removal). Short exposure estimates based on mean 5th percentile concentration, but <i>not</i> its associated 95% confidence interval (i.e., analyses failing linear bootstrap).



B.4.0 Summary of Risk Estimates

The following table (Table B.4.3) summarizes the analytical steps used for each of the selected chemicals. Chemicals with two or more rows represent separate analysis for different taxonomic groups. Short Exposure Risk Reports are available for a subset of the chemicals below, for which sufficient acute toxicity data were available.

Table B.4.3. Summary of the analytical steps used for each of the chemicals of interest. Note that because of data constraints, Short Exposure Risk Reports were developed for a subset of these chemicals.

Chemical (CAS#)	Data Analysis						Risk Estimate Reliability	Report Available
	Insufficient Data	Data manipulation	Web-ICE data points	Violation of Anderson-Darling test*	Failed linear bootstrap	5 th mean		
Formalin (50000)		X					High	Yes
Tetrachloromethane (56235)	X			X			Low	Yes
Phosphorothioic acid, O,O-diethyl-O-(4-nitrophenyl)ester (56382)		X					High	Yes
		X					Moderate	
3-Isothiocyanato-1-propene (57067)	X							No
1,1-Dimethylhydrazine (57147)			X	X			Low	Yes
Monomethylhydrazine (60344)	X		X	X		X	Low	Yes
Ethanol (64175)					X	X	Low	Yes
Formic acid (64186)	X							No
Methanol (67561)							High	Yes
2-Propanol (67630)			X				Low	Yes
2-Propanone (67641)		X			X	X	Low	Yes
Trichloromethane (67663)	X		X	X	X	X	Low	Yes
Benzene (71432)		X		X			Moderate	Yes
Bromomethane (74839)	X	X	X	X			Low	Yes
Ethylene oxide (75218)	X		X	X	X	X	Low	Yes



Chemical (CAS#)	Data Analysis						Risk Estimate Reliability	Report Available
	Insufficient Data	Data manipulation	Web-ICE data points	Violation of Anderson-Darling test*	Failed linear bootstrap	5 th mean		
1,2,3,4,5,5-Hexachloro-1,3-cyclopentadiene (77474)			X				Low	Yes
Chloromethane (74873)	X							No
2-Butanone (78933)	X							No
Methanamine (74895)	X							No
Hydrocyanic acid (74908)	X							No
Acetaldehyde (75070)	X							No
Carbon disulfide (75150)	X							No
Propylene oxide (75569)	X							No
Tetramethyl lead (75741)	X							No
Acetone cyanohydrins (75865)	X							No
Dimethyl sulfate (77781)	X							No
Lactonitrile (78977)	X							No
1,1,2-Trichloroethane (79005)	X	X	X	X		X	Low	Yes
2-Propenoic acid (79107)	X							No
Butyl benzyl phthalate (85687)	X	X	X	X			Low	Yes
Hexachlorobutadiene (87683)		X		X			Moderate	Yes
1,2,3-Trichloropropane (96184)	X							No
Methyl acrylate (96333)	X							No
2-Furancarboxaldehyde (98011)				X			Moderate	Yes
Ethylbenzene (100414)		X		X	X		Low	Yes
Styrene (100425)	X	X		X	X	X	Low	Yes
Chloromethyl benzene (100447)	X		X	X	X	X	Low	Yes



Chemical (CAS#)	Data Analysis						Risk Estimate Reliability	Report Available
	Insufficient Data	Data manipulation	Web-ICE data points	Violation of Anderson-Darling test*	Failed linear bootstrap	5 th mean		
Chloromethyl oxirane (106898)	X		X	X	X	X	Low	Yes
1,2-Dibromoethane (106934)	X							No
2-Propenal (107028)		X	X		X	X	Low	Yes
1,2-Dichloroethane (107062)	X							No
2-Chloroethanol (107073)		X	X				Low	Yes
2-Propen-1-amine (107119)	X							No
*2-Propenenitrile (107131)		X		X			Moderate	Yes
1,2-Ethylenediamine (107153)	X							No
Chloroacetaldehyde (107200)	X							No
2-Propen-1-ol (107186)	X							No
1,2-Ethanediol (107211)	X	X		X	X			No
Vinyl acetate (108054)	X							No
Methylbenzene (108883)					X	X	Low	Yes
Chlorobenzene (108907)		X		X			Moderate	Yes
Phenol (108952)		X		X			Moderate	Yes
Tetrahydrofuran (109999)								No
Furan (110009)	X		X	X	X	X	Low	Yes
Hexane (110543)	X							No
Cyclohexane (110827)	X							No
Pyridine (110861)			X	X			Moderate	Yes
[(Dimethoxyphosphinothioyl)thio]butanedioic acid, Diethyl ester (121755)		X		X	X	X	Low	Yes
		X		X			Moderate	
Triethylamine (121448)	X							No



Chemical (CAS#)	Data Analysis						Risk Estimate Reliability	Report Available
	Insufficient Data	Data manipulation	Web-ICE data points	Violation of Anderson-Darling test*	Failed linear bootstrap	5 th mean		
Butyl ester, Acetic acid (123864)	X	X	X	X	X	X	Low	Yes
Acetic acid ethyl ester (141786)	X		X	X	X	X	Low	Yes
Methanesulfonyl chloride (124630)	X							No
N-Methylmethanamine (124403)		X	X		X	X	Low	Yes
Tetrachloroethene (127184)			X	X	X			No
Ethyl acrylate (140885)	X							No
2-Propenoic acid, Butyl ester (141322)	X							No
Acetic acid ethyl ester (141786)			X	X			Low	Yes
Aziridine (151564)	X							No
Hydrazine (302012)	X							No
Cyanogen chloride ((CN)Cl) (506774)	X							No
Isothiocyanatomethane (556616)	X							No
2,4-Diisocyanate-1-methylbenzene (584849)	X		X	X	X	X	Low	Yes
Tetraethylstannane (597648)	X							No
Xylene (1330207)		X	X	X	X		Low	Yes
2-Butenal (4170303)	X							No
Nitric acid ammonium salt (6484522)	X							No
Hydrochloric acid (7647010)	X							No
Cadmium (7440439)		X					High	Yes
		X		X			Moderate	
		X					High	



Chemical (CAS#)	Data Analysis						Risk Estimate Reliability	Report Available
	Insufficient Data	Data manipulation	Web-ICE data points	Violation of Anderson-Darling test*	Failed linear bootstrap	5 th mean		
Zinc (7440666)		X					Moderate	Yes
							High	
Ammonia (7664417)		X		X			Moderate	Yes
Sulfuric acid (7664939)	X							No
Nitric acid (7697372)	X							No
Potassium permanganate (7722647)		X					High	Yes
Hydrogen peroxide (H2O2) (7722841)			X	X			Low	Yes
Bromine (7726956)	X		X	X	X	X	Low	Yes
Chlorine (7782505)		X		X			Moderate	Yes
Hydrogen sulfide (7783064)							High	Yes
Nitrogen oxide (10102440)	X							No
Cadmium Chloride (10108642)							High	Yes
				X			Moderate	
Bromine chloride (13863417)				X	X	X	Low	Yes

* At least one of the ≥ 3 SSDs.



B.5.0 Representative Species used to Derive Short-Exposure Risk Reports

The following tables (**Table B.5.4** and **B.5.5**) summarize the species and data sources used to develop 2-pager reports for selected chemicals.

Table B.5.4. List of species from CAFE and by taxonomic group most frequently used in analyses for deriving short-exposure concentration estimates.

Common name	Scientific Name	Frequency of Use
Species Group: Fish		
Fathead Minnow	<i>Pimephales promelas</i>	113
Bluegill	<i>Lepomis macrochirus</i>	95
Rainbow Trout	<i>Oncorhynchus mykiss</i>	86
Guppy	<i>Poecilia reticulata</i>	52
Goldfish	<i>Carassius auratus</i>	48
Channel Catfish	<i>Ictalurus punctatus</i>	45
Common Carp	<i>Cyprinus carpio</i>	35
Western Mosquitofish	<i>Gambusia affinis</i>	35
Medaka, High-Eyes	<i>Oryzias latipes</i>	32
Striped Bass	<i>Morone saxatilis</i>	31
Zebra Danio	<i>Danio rerio</i>	30
Largemouth Bass	<i>Micropterus salmoides</i>	25
Tigerfish	<i>Terapon jarbua</i>	20
Mozambique Tilapia	<i>Oreochromis mossambicus</i>	18
Indian Catfish	<i>Heteropneustes fossilis</i>	15
Sheepshead Minnow	<i>Cyprinodon variegatus</i>	14
Green Sunfish	<i>Lepomis cyanellus</i>	14
Harlequinfish, Red Rasbora	<i>Rasbora heteromorpha</i>	14
Flagfish	<i>Jordanella floridae</i>	13
Brook Trout	<i>Salvelinus fontinalis</i>	13
Giant Gourami	<i>Colisa fasciata</i>	12
Golden Shiner	<i>Notemigonus crysoleucas</i>	11
Yellow Perch	<i>Perca flavescens</i>	11
White Sucker	<i>Catostomus commersoni</i>	10
Snake-Head Catfish	<i>Channa punctata</i>	10
Asiatic Knifefish	<i>Notopterus notopterus</i>	10
Carp, Hawk Fish	<i>Cirrhinus mrigala</i>	9
Threespine Stickleback	<i>Gasterosteus aculeatus</i>	9
Brown Trout	<i>Salmo trutta</i>	9
Lake Trout, Siscowet	<i>Salvelinus namaycush</i>	9
American Eel	<i>Anguilla rostrata</i>	8
Walking Catfish	<i>Clarias batrachus</i>	8
Cutthroat Trout	<i>Oncorhynchus clarki</i>	8
Chinook Salmon	<i>Oncorhynchus tshawytscha</i>	8
Nile Tilapia	<i>Oreochromis niloticus</i>	8
Starry, European Flounder	<i>Platichthys flesus</i>	8
Two Spot Barb, Dotted Barb	<i>Barbus siphore</i>	7
Spot	<i>Leiostomus xanthurus</i>	7
Atlantic Silverside	<i>Menidia menidia</i>	7



Common name	Scientific Name	Frequency of Use
Coho Salmon, Silver Salmon	<i>Oncorhynchus kisutch</i>	7
Sailfin Molly	<i>Poecilia latipinna</i>	7
Florida Pompano	<i>Trachinotus carolinus</i>	7
Black Bullhead	<i>Ameiurus melas</i>	6
Two-Spot, Tic Tac Toe Barb	<i>Barbus ticto</i>	6
Milkfish, Salmon-Herring	<i>Chanos chanos</i>	6
Northern Pike	<i>Esox lucius</i>	6
Banded Killifish	<i>Fundulus diaphanus</i>	6
Aholehole	<i>Kuhlia sandvicensis</i>	6
Loach	<i>Lepidocephalichthys thermalis</i>	6
Pumpkinseed	<i>Lepomis gibbosus</i>	6
White Perch	<i>Morone americana</i>	6
Leaping Grey Mullet	<i>Mugil saliens</i>	6
Pink Salmon	<i>Oncorhynchus gorbuscha</i>	6
Hirame, Flounder	<i>Paralichthys olivaceus</i>	6
Flounder	<i>Pseudopleuronectes yokohamae</i>	6
Species Group: Crustaceans		
Water Flea	<i>Daphnia magna</i>	62
Opossum Shrimp	<i>Americamysis bahia</i>	37
Daggerblade Grass Shrimp	<i>Palaemonetes pugio</i>	26
Brine Shrimp	<i>Artemia salina</i>	24
Aquatic Sowbug	<i>Asellus aquaticus</i>	23
Water Flea	<i>Daphnia pulex</i>	18
Water Flea	<i>Ceriodaphnia dubia</i>	17
Scud	<i>Gammarus pulex</i>	17
Common Shrimp, Sand Shrimp	<i>Crangon crangon</i>	14
Ostracod	<i>Cypris subglobosa</i>	12
Scud	<i>Gammarus minus</i>	11
Grass Shrimp, Freshwater Prawn	<i>Palaemonetes kadiakensis</i>	11
Scud	<i>Gammarus pseudolimnaeus</i>	10
Brine Shrimp	<i>Artemia sp.</i>	9
Scud	<i>Gammarus fasciatus</i>	9
Giant River Prawn	<i>Macrobrachium rosenbergii</i>	9
Scud	<i>Gammarus fossarum</i>	8
Fairy Shrimp	<i>Streptocephalus proboscideus</i>	8
Harpacticoid Copepod	<i>Nitocra spinipes</i>	7
Fleshy Prawn	<i>Penaeus chinensis</i>	7
Indian Prawn	<i>Penaeus indicus</i>	7
Kuruma Shrimp	<i>Penaeus japonicus</i>	7
Bay Shrimp, Sand Shrimp	<i>Crangon septemspinosa</i>	6
Water Flea	<i>Daphnia obtusa</i>	6
Redtail Prawn	<i>Fenneropenaeus penicillatus</i>	6
Greasyback Shrimp	<i>Metapenaeus ensis</i>	6
Crayfish	<i>Orconectes nais</i>	6
Northern Pink Shrimp	<i>Penaeus duorarum</i>	6
Jumbo Tiger Prawn	<i>Penaeus monodon</i>	6



Common name	Scientific Name	Frequency of Use
Species Group: Insects/Spiders		
Midge	<i>Chironomus riparius</i>	14
Midge	<i>Chironomus tentans</i>	8
Backswimmer	<i>Notonecta undulata</i>	8
Stonefly	<i>Pteronarcys californica</i>	8
Yellow Fever Mosquito	<i>Aedes aegypti</i>	7
Mayfly	<i>Baetis rhodani</i>	7
Stonefly	<i>Tallaperla maria</i>	7
Stonefly	<i>Claassenia sabulosa</i>	6
Golden Stonefly, Willow Fly	<i>Hesperoperla pacifica</i>	6
Beetle	<i>Peltodytes sp.</i>	6
Stonefly	<i>Pteronarcella badia</i>	6

Table B.5.5. List of species from Web-ICE and by taxonomic group most frequently used in analyses for deriving short-exposure concentration estimates.

Common name	Scientific Name	Frequency of Use
Species Group: Fish		
Goldfish	<i>Carassius auratus</i>	41
Common carp	<i>Cyprinus carpio</i>	37
Cape fear shiner	<i>Notropis mekistocholas</i>	36
Colorado squawfish	<i>Ptychocheilus lucius</i>	33
Cutthroat trout	<i>Oncorhynchus clarkii</i>	23
Coho salmon	<i>Oncorhynchus kisutch</i>	18
Green sunfish	<i>Lepomis cyanellus</i>	16
Largemouth bass	<i>Micropterus salmoides</i>	16
Razorback sucker	<i>Xyrauchen texanus</i>	16
Apache trout	<i>Oncorhynchus gilae</i>	15
Channel catfish	<i>Ictalurus punctatus</i>	15
Chinook salmon	<i>Oncorhynchus tshawytscha</i>	15
Fathead minnow	<i>Pimephales promelas</i>	15
Brown trout	<i>Salmo trutta</i>	14
Threespine stickleback	<i>Gasterosteus aculeatus</i>	14
Black bullhead	<i>Ameiurus melas</i>	12
Lake trout	<i>Salvelinus namaycush</i>	11
Mosquitofish	<i>Gambusia affinis</i>	11
Brook trout	<i>Salvelinus fontinalis</i>	10
Guppy	<i>Poecilia reticulata</i>	10
Leon springs pupfish	<i>Cyprinodon bovinus</i>	9
Bonytail chub	<i>Gila elegans</i>	8
Yellow perch	<i>Perca flavescens</i>	8
Species Group: Crustaceans		
Amphipod	<i>Hyaella azteca</i>	6
Species Group: Insects/Spiders		
Stonefly	<i>Claassenia sabulosa</i>	6



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