

# How to Use the Chemical Aquatic Fate and Effects Database: CAFE, Version 1.2

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**U.S. DEPARTMENT OF COMMERCE**  
National Oceanic and Atmospheric Administration  
National Ocean Service  
Office of Response and Restoration  
Emergency Response Division

# How to Use the Chemical Aquatic Fate and Effects Database: CAFE, Version 1.2

May 2016



U.S. DEPARTMENT OF COMMERCE  
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## How to Use the Chemical Aquatic Fate and Effects Database: CAFE, Version 1.2

The Chemical Aquatic Fate and Effects (CAFE) database is a software program you can use to estimate the fate and effects of thousands of chemicals, oils, and dispersants. It serves as a tool to help responders in their assessment of environmental impacts from chemical or oil spills into aquatic environments.

Using CAFE, you can choose between four different spill scenarios: chemical, oil only, dispersant only, and dispersants mixed with oil. You can also add your own toxicity data, and view short-exposure hazard concentration estimates (Short Exposure Risk Reports) that were derived for selected chemicals using empirical toxicity data.

Data in CAFE are presented in two modules, which can provide complementary information to responders:

- Aquatic Fate module
- Aquatic Toxicity (Effects) module

This document provides a brief overview of how to navigate and perform queries in CAFE. You are encouraged to review the CAFE User's Manual for additional details, as well as the Quality Assurance/Quality Control (QA/QC) Plan contained in the manual (Appendix A).

Development of CAFE and its application for use in spill response is described in the following paper: Bejarano, A. C., Farr, J. K., Jenne, P., Chu, V. and Hielscher, A. (2016), The Chemical Aquatic Fate and Effects database (CAFE), a tool that supports assessments of chemical spills in aquatic environments. *Environmental Toxicology and Chemistry*, 35: 1576–1586.

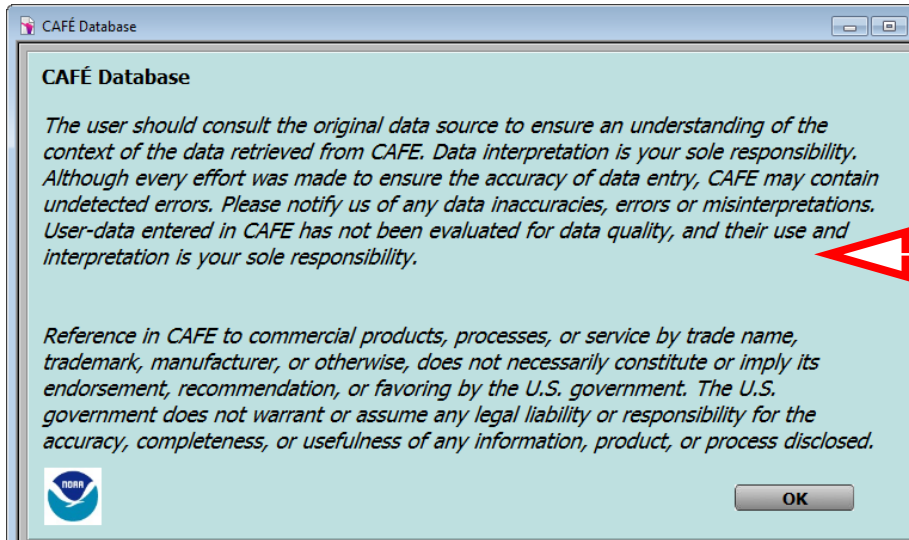
### Performing Queries in CAFE

Shown below are instructions and screenshots that will guide you through some sample queries in CAFE.

Before performing queries in CAFE, note that:

- CAFE is a repository of data that will continue to be updated as additional sources of data are identified.
- Data queries and interpretation are the sole responsibility of you, the user.
- The CAFE development team assumes no responsibility for the use or misuse of the data and information contained within the tool.

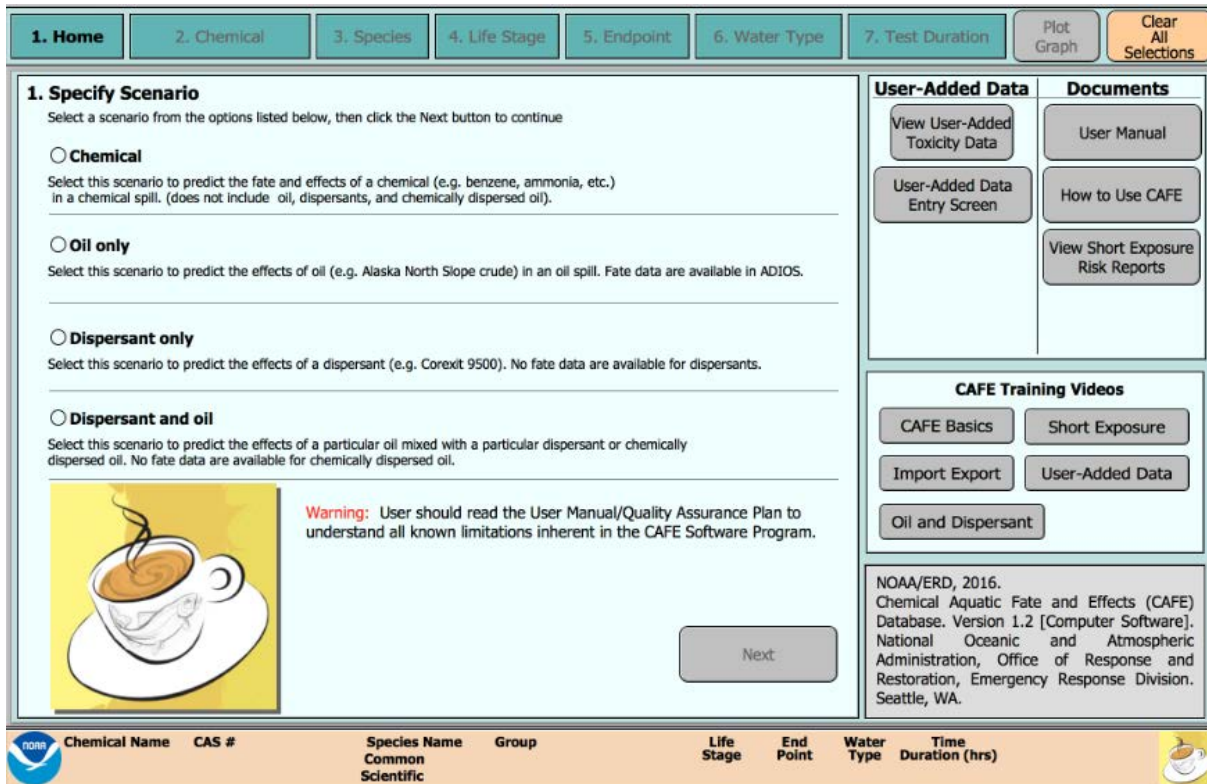
# Disclaimer



By reading this disclaimer and clicking OK, you show that you understand the potential pitfalls of this database, and more importantly, that data interpretation is at your own risk.

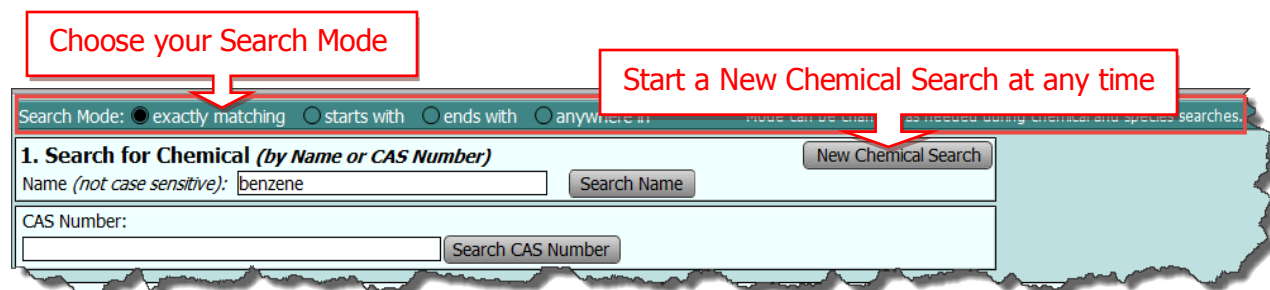
## Getting Started

**Home.** To begin, choose between four different spill scenarios: Chemical, Oil only, Dispersant only, or Dispersant and oil. The Chemical scenario allows you to view both fate and toxicity effects; whereas the Oil and Dispersant scenarios only allows you to view effects.



## Chemical Scenario

For a Chemical scenario, choose to search by name or by Chemical Abstracts Service (CAS) number, without dashes. If you search by name, you can search for chemicals that exactly match, start with, end with, or contain your chemical of interest.



Choose your Search Mode

Start a New Chemical Search at any time

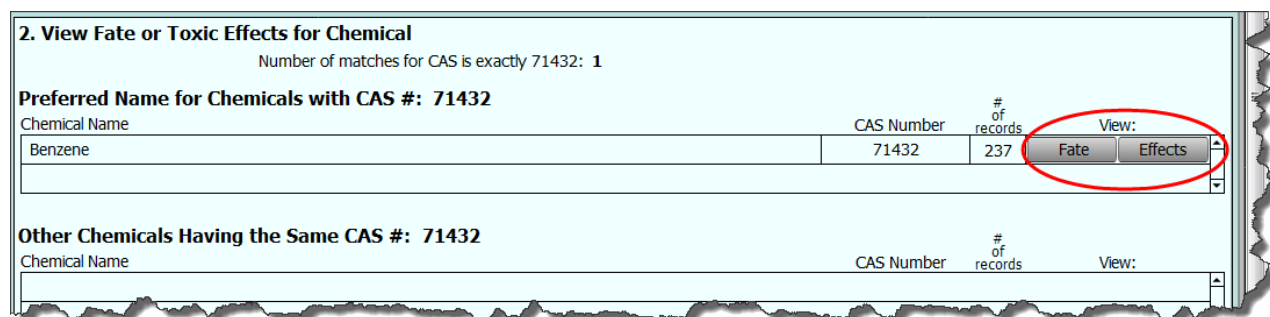
Search Mode:  exactly matching  starts with  ends with  anywhere in  mode can be changed as needed during chemical and species searches.

**1. Search for Chemical (by Name or CAS Number)**

Name (not case sensitive):

CAS Number:

Next, choose to view the **Fate** (Aquatic Fate module) or **Effects** (Aquatic Toxicity module) of the search result(s).



**2. View Fate or Toxic Effects for Chemical**

Number of matches for CAS is exactly 71432: 1

**Preferred Name for Chemicals with CAS #: 71432**

Chemical Name	CAS Number	# of records	View:
Benzene	71432	237	<input type="button" value="Fate"/> <input type="button" value="Effects"/>

**Other Chemicals Having the Same CAS #: 71432**

Chemical Name	CAS Number	# of records	View:
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## Aquatic Fate Module

There are three sub-modules within the Aquatic Fate module, shown by three buttons at the top of the screen:

1. Structure and Physical Properties
2. Environmental Fate
3. Analytical Methods and Uses

Printing is available on all three sub-modules.

**Structure and Physical Properties sub-module.** Help buttons, , are located at the side of the data to help guide you.

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

Fate Data - Physical Properties Chemical Name **Benzene** CAS 71432

Odor: Aromatic odor  
Gasoline-like odor; rather pleasant aromatic odor

Color/Form: Rhombic prisms  
Colorless to light-yellow liquid (a solid below 42°F)

Skin, Eye, and Respiratory Irritation: Skin irritant.  
Severe eye and moderate skin irritant.  
Skin irritant upon occupational exposures of >60 ppm for three weeks.


Structure:

Hazards of searched chemical

Physical Properties Data

Boiling Point (°C)	80° C (Experimental)	Flash Point	12°F (-11°C) (Closed Cup) (Experimental)
Melting Point (°C)	5.5° C (Experimental)	Ionization Potential (eV)	9.24 eV
Density		Hvap (cal/g)	
Autoignition Temp.	928°F (497°C)	HLC (atm-m3/mol)	.00555 at 25°C (Experimental)
Vapor Density	2.8 (Air= 1)	Log Kow	2.13 (Experimental)
Viscosity	0.604 cP at 25°C	Vapor Pressure (mmHg)	94.8 mm Hg at 25°C (Experimental)
Explosive/Flammable Limits	Lower 1.4%; Upper 8.0%	Water Solubility (mg/L)	1790 at 25°C (Experimental)

## Environmental Fate sub-module

Help buttons, , are located at the side of the data to help guide you. There are also some Environmental Explanations that summarize the data in paragraph form.

Home Return Physical Properties **Environmental Fate** Print

Fate Data - Environmental Properties Chemical Name **Benzene** CAS 71432

Soil Adsorption: Estimated Koc 165.5

Primary Biodegradation: Estimated Biodegradation Timeframe days-weeks

Estimated Volatilization from Water: Estimated Half-life from Model River (hours) .9951; Model Lake (hours) 84.96

Estimated Hydrolysis at pH=7: Half-life (days)

Estimated Atmospheric: Half-life (days) 5.486

Estimated Environmental Partitioning: Percent to air 37.6; Percent to water 48.1; Percent to soil 14.1; Percent to sediment .219

Estimated Wastewater Removal (%): Total Removed 76.22; Due to Biodegradation 21.66; Due to Sludge Adsorption .97; Due to Volatilization 53.59

Environmental Explanations

If released to the environment, Benzene is expected to be found predominantly in water (48.1%). It is also expected to be found in soil (14.1%), air (37.6%) and sediment (.22%).

SOIL

- In soil, Benzene is expected to have moderate mobility based upon a KOC of 165.5 (Estimated).
- Benzene may volatilize from dry soil surfaces based upon a vapor pressure of 94.8 mm Hg (Experimental).
- Benzene may volatilize from moist soil surfaces based upon a Henry's Law constant of .00555 atm-cu m/mole (Experimental).

WATER

- Benzene may volatilize slowly from water surfaces is expected to be an important fate process based on a Henry's Law constant of .00555 atm-cu m/mole (Experimental).
- Estimated volatilization half-lives for a model river and model lake are 1 hours and 84.96 hours, respectively.
- In water, Benzene is not expected to adsorb to suspended solids and sediment based upon a KOC of 165.5 (Estimated).

The Aqueous Hydrolysis Rate Program (HYDROWIN) estimates aqueous hydrolysis rate constants for only certain chemical classes: esters, carbamates, epoxides, halomethanes 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 Benzene. 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 Benzene is hydrolytically stable, it may contain functional group(s) for which HYDROWIN cannot estimate a hydrolysis rate constant.

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.

- Benzene will exist solely as a vapor in the atmosphere based upon a vapor pressure of 94.8 mm Hg (Experimental).
- The half-life for the reaction of Benzene with photochemically generated hydroxyl radicals is 5.486 days, assuming a hydroxyl radical concentration of 1.5E+6 OH/cm3 and a 12-hour day.

Environmental Fate Data

Detailed Environmental Explanations in paragraph form

## Analytic Methods sub-module

The upper section of the screen shows the methods used to measure the chemical. Click on a Method Number with an associated media type. A description of the method will be shown in the Method Type text box. The lower section of the screen shows the uses for the chemical. Click on a Use in the lower left and an expanded description will be shown in the Use text box.

**Media Type**

**List of Media Numbers**

Method #	Media
1	1624.0
2	602.2 (by PID)
3	22
4	602
5	6200B
6	6200C
7	624
8	8021B (by GC-ELCD)
9	8021B (by GC-PID)
10	8260B
11	D5790
12	O-3115
13	O-4024-03
14	O-4127-96
15	1501
16	3700
17	3800
18	1005

**Method 1501**

This method updates NMAM 1501 issued on August 15, 1994 [1] which was based upon P&CAM 127 (benzene, styrene, toluene, and xylene) [2]; S22 (p-tert-butyltoluene) [3]; S23 (cumene) [3]; S29 (ethylbenzene) [3]; S26 ("methylstyrene) [3]; S40 (styrene); S311 (benzene) [4]; S343 (toluene) [4]; and S318 (xylenes) [4]. HYDROCARBONS, AROMATIC

Issue 3: 15 March 2003

**National Institute for Occupational Health and Safety**

**Scope Application:**  
This method is for peak, ceiling, and TWA determinations of aromatic hydrocarbons. Interactions between analytes may reduce breakthrough volumes and affect desorption efficiencies. Naphthalene, originally validated in S292 [4], failed to meet acceptable desorption efficiency recovery and storage stability criteria at the levels evaluated in this study. However, the application of this method to naphthalene levels at or near the REL/PEL continues to meet acceptable recovery criteria. Styrene failed to meet acceptable recovery criteria at the two lowest levels evaluated in this study (highest level to meet the criteria was 181 µg/sample).

**Application Concentration Range**  
benzene: 0.004-0.35 mg; p-tert-butyltoluene: 0.013-1.09 mg; cumene: 0.039-3.46 mg; ethylbenzene: 0.045-8.67 mg; alpha-methylstyrene: 0.036-3.57 mg; beta-methylstyrene: 0.036-0.728 mg; toluene: 0.024-4.51 mg; o-xylene: 0.044-10.4 mg; m-xylene: 0.043-0.864 mg; p-xylene: 0.043-0.861 mg; styrene: 0.181-8.49 mg

**List of Uses**

**Use Text Box**

**Use**  
Chemical intermediate for ethylbenzene, cumene, cyclohexane, nitrobenzene, maleic anhydride, chlorobenzenes, detergent alkylate, anthraquinone, benzene hexachloride, benzene sulfonic acid, biphenyl, hydroquinone, and resorcinol

**Citation**  
HSDB

**Source**  
HSDB

## Aquatic Toxicity Module: Data Selection Screens

There are several sequential steps to complete before proceeding to test duration.

**Species** – Select species by taxonomic group and/or select individual species before proceeding to Life Stage(s) Selection.

**Life Stage(s)** – Select from available life stages for the selected species before proceeding to the Endpoint(s) Selection.

**Endpoint(s)** – Select Endpoint(s) before proceeding to the Water Type Selection. Notice how there are no LOEC or NOEC data, so those options are grayed out.

**Water Type(s)** – Select Water Type(s) before proceeding to the Test Duration.

**Notes:**

- A minimum of 5 species is required for curve fitting.
- The number of toxicity records decreases as more parameters are selected.
- All or individual parameter selections can be cleared at any time.
- When specific data selections are not available, those options are grayed out (see example on End Point(s) screen below).
- Green dots denote species-parameter selections for which data are available.

Also note that going back steps will clear all settings you have made, based on your previous selections.

On the Species step, there are *three steps* to complete before you proceed to the next step (Life Stage). On all other steps, there are *two steps*.

1. Select Species Groups to view which species in the selected groups are available.
2. Select all or individual species.
3. Click the button, Life Stage Selection, in the upper right to proceed to the next step.

**1. Select Species Group(s)**

Number of toxicity records: Life Stage Selection

Coral  Crustacean  Fish  Mollusk  Other

*Hover over option to show toxicity record count*

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**2. Select Species** A minimum of 5 species is required for curve fitting. Number of toxicity records:

*Click once in the box for each desired species, or click Select All Clear Current Selection*

indicates toxicity data available; place pointer over icon to show record count **available** for the given parameter and species

Common Name	Scientific Name	Species Group	Life Stage					Endpoint				Water Type			Test Duration (hrs)				Data Appl.		
			Embryo	Larva	Juvenile	Adult	Unk.	LC50	EC50	LOEC	NOEC	Salt	Fresh	24	48	72	96	H	M	L	
African Clawed Frog	Xenopus laevis	Other																			
Aquatic S...	aquaticus	Crustacean																			
Arctic Gray	ilus arcticus	Fish																			
Bluegill	is macrochirus	Fish																			
Brine Shrim	a salina	Crustacean																			
Brine Shrim	a sp.	Crustacean																			
Calanoid Copepod	Diaptomus forbesi	Crustacean																			
California Bay Shrimp	Crangon franciscorum	Crustacean																			
Carp	Leuciscus idus ssp. melanotus	Fish																			
Channel Catfish	Ictalurus punctatus	Fish																			
Chinook	Oncorhynchus tshawytscha	Fish																			
Crab	Scylla serrata	Crustacean																			
Crab	Palaemonetes pugio	Crustacean																			
Damselfly	Ischnura elegans	Other																			
Diatom	Thalassiosira pseudonana	Other																			
Dolly Varden	Salvelinus malma	Fish																			
Dover Sole	Solea solea	Fish																			
Dungeness Or Edible Crab	Cancer magister	Crustacean																			
Fathead Minnow	Pimephales promelas	Fish																			



The Life Stage(s), Endpoints, and Water Type selection steps are listed below.

**At any point selections can be cleared**

**Select Life Stage(s)**

**Select Endpoint(s)**

**At any point page selections can be cleared**

**Select Water Type(s)**

**Summary of all the parameters selected**

The interface consists of three sequential selection screens:

- Screen 1: Select Life Stage(s)**
  - Navigation: 1. Home, 2. Chemical, 3. Species, **4. Life Stage**, 5. End Point, 6. Water Type, 7. Test Duration
  - Selections:  Adult,  Embryo,  Juvenile,  Larva,  Unknown
  - Table: Lists species with columns for Life Stage (Embryo, Larva, Juvenile, Adult, Unk), End Point (LC50, EC50, LOEC, NOEC), Water Type (Sat, Fresh), and Duration (24, 48, 72, 96, H, M, L).
- Screen 2: Select End Point(s)**
  - Navigation: 1. Home, 2. Chemical, 3. Species, **4. Life Stage**, **5. End Point**, 6. Water Type, 7. Test Duration
  - Selections:  EC50,  LC50,  LOEC,  NOEC
  - Table: Same as Screen 1, but with End Point columns highlighted.
- Screen 3: Select Water Type(s)**
  - Navigation: 1. Home, 2. Chemical, 3. Species, 4. Life Stage, 5. End Point, **6. Water Type**, 7. Test Duration
  - Selections:  Fresh Water,  Salt Water
  - Table: Same as previous screens, but with Water Type columns highlighted.

**Summary of all the parameters selected**

Chemical Name	CAS #71432	Species Name	Group	Multiple Species Selected	Life Stage	Multiple	End Point	Multiple	Water Type	Multiple	Time	Duration (hrs)	Multiple									
Benzene		Common Name	Latin Name	Species Group	Embryo	Larva	Juvenile	Adult	Unk	LC50	EC50	LOEC	NOEC	Sat	Fresh	24	48	72	96	H	M	L

## Test Duration and Applicability Selection

There are two steps to complete before data are plotted.

**Test Duration** – Select **one** Test Duration before proceeding to plot the graph. Note that the numbers of records displayed are the records that correspond to the selected test duration.

**Data Applicability** – Each data source was given an applicability score (High, Moderate, or Low) to spill response. Select the Data Applicability (optional) prior to plotting the data.

### High applicability

- 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

### Moderate applicability

- 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 75- $<90\%$  active ingredient purity

### Low applicability

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

### Notes

An additional screen summarizes all the selected parameters in text form. Printing is available.

Number of toxicity records for all durations and applicabilities

1. Home 2. Chemical 3. Species 4. Life Stage 5. End Point 6. Water Type 7. Test Duration 8. All Selections

1. Select One Test Duration (hours) 2. Select Data Applicability *Number of toxicity records: 235* 2. Proceed to: Plot Graph

24  48  72  96  High  Moderate  Low

*Hover over option to show toxicity record count* Clear All On Page

*Number of toxicity records for selected test duration: 13*

indicates toxicity data available

Common Name	Latin Name	Species Group	Emb	Life Stage	End Point	Water Type	Test Duration (hrs)			Data Applic.				
							24	48	72	96	H	M	L	
Aquatic Sowbug	Asellus aquaticus	Crustacean												
Crab	Scylla serrata	Crustacean												
Great Pond Snail	Lymnaea stagnalis	Mollusk												
Green Algae	Pseudokirchneriella subcapitata	Other												
Marine Bivalve	Katelysia opima	Mollusk												
Scud	Gammarus fossarum	Crustacean												
Snail	Amphimelania holandri	Mollusk												
Striped Bass	Morone saxatilis	Fish												
Tigerfish	Terapon jarbua	Fish												

Number of toxicity records shown on the graph

Chemical Name: Benzene CAS #71432 Species Name: Multiple Species Selected Group Multiple Life Stage: Multiple End Point: Multiple Water Type: Multiple Time Duration (hrs): 72

Show Selection Summary

## Graph Output – The Result

The selection screens generate Species Sensitivity Distributions (SSD). SSDs describe the sensitivity of aquatic species to the exposure media, by ranking the relative sensitivity of the species tested from the least to most sensitive.

- The name of the chemical, oil or dispersant and the exposure duration (in parenthesis) are labeled as the title of the SSD
- The x-axis represents the concentration in  $\mu\text{g/L}$  (plotted on a log scale) required to adversely affect a unique species and the y-axis represents the percentage of species.
- Each point on the curve represents data available for a unique species, and each open circle represents the geometric mean of all the toxicity data available for a unique species.
- SSDs can be used to derive a protection threshold or a hazard concentration (HC) as a measure of risk. Here the 1st and 5th percentiles of the SSD<sup>1</sup> (HC1 and HC5, respectively; in  $\mu\text{g/L}$ ) are used as benchmark concentrations under the assumption that these would be protective of 99% and 95%, respectively, of the species on the SSD.
- HC1 and HC5 values are displayed and automatically updated with every query.

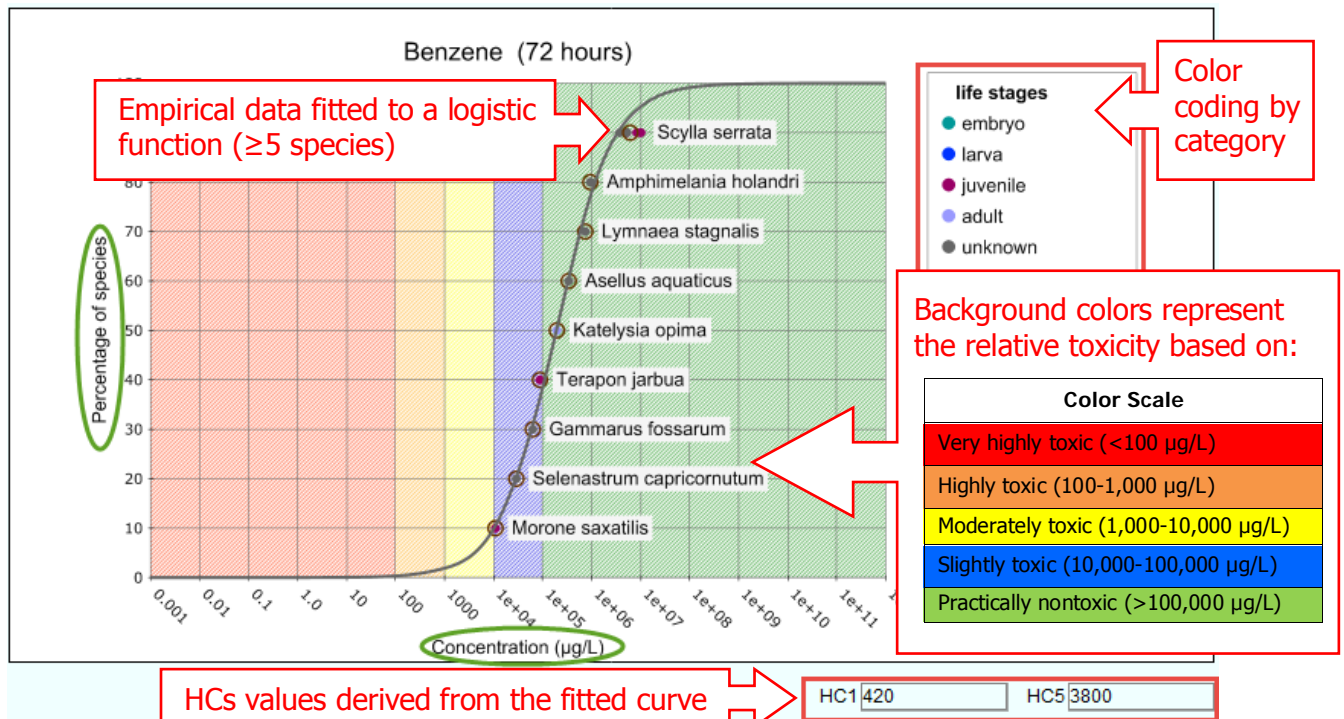
<sup>1</sup> While there is debate in the scientific literature regarding the appropriateness of one versus another HC percentile, the HC5 selected here was chosen because this is the most commonly used percentile, while a lower percentile (HC1) would offer an additional safety factor preferable when dealing with very highly toxic chemicals.

- The colors in the Toxicity key represent the relative toxicity of the exposure media<sup>2</sup>.
- All final query plots can be printed.



## Data Limitations

- This version of CAFE only provides data for acute 24, 48, 72, and 96 hour exposures. No other time durations are available in this version.
- Some chemicals have limited acute toxicity data available; not enough to generate SSDs.
- Most of the toxicity tests were done in a laboratory setting. These conditions do not accurately simulate real testing conditions.
- 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. 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. The user is encouraged to be critical of the fitted curve.
- SSDs are not intended to address 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.



<sup>2</sup> Source: [http://www.epa.gov/oppefed1/ecorisk\\_ders/toera\\_analysis\\_eco.htm#Ecotox](http://www.epa.gov/oppefed1/ecorisk_ders/toera_analysis_eco.htm#Ecotox)

There are a number of options that facilitate data visualization, including: shading by attributes, display of all values or just geometric means, viewing species by common or scientific names. You can also view a selection summary of your data by clicking the Show Selection Summary button on the bottom right of the SSD.

**Adjust data by going back to any of the navigation tabs**

**Graph display adjustments**

**Graph can be printed**

**Change the shade by feature to improve data visualization**

**View the original studies by clicking on the next to each unique species**

**HC1 and HC5 (µg/L) values**

**Show Selection Summary**

**View by Scientific Names**  
 View by Scientific Names  
 View by Common Names

To view original study click on **i**

**life stages**

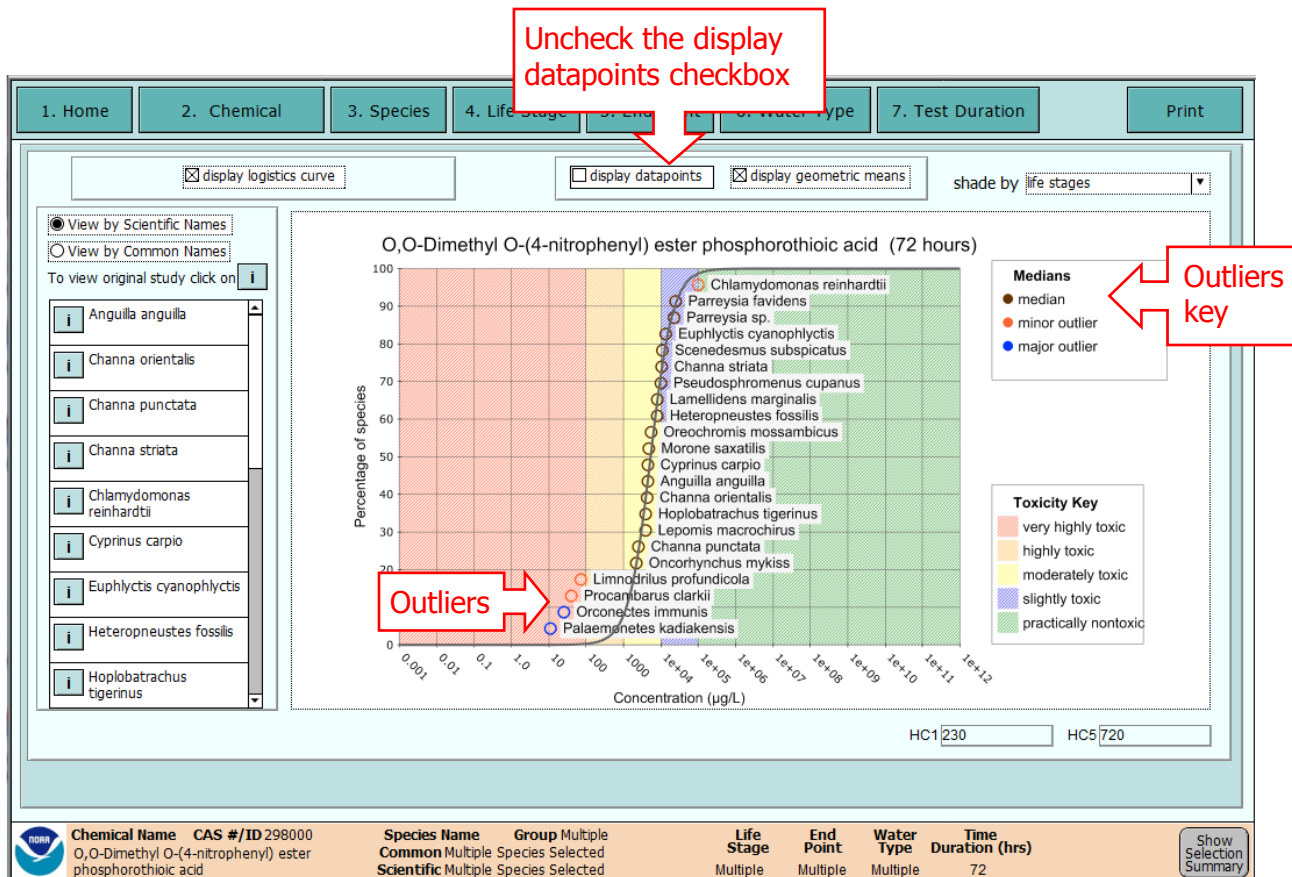
- embryo
- larva
- juvenile
- adult
- unknown

**Toxicity Key**

- very highly toxic
- highly toxic
- moderately toxic
- slightly toxic
- practically nontoxic

Species Name	Group	Multiple	Life Stage	End Point	Water Type	Time Duration (hrs)
Common Multiple Species Selected			Multiple	Multiple	Multiple	72
Latin Multiple Species Selected						

You can also shade by outliers. The logistics curves are computed using the geometric means. In certain cases, the curves were being skewed by outlier geometric means. The curves do not include these points in the computations, but the points are still displayed on the graph. When the user displays the geometric means only, the outlier points are shaded. Most chemicals don't have outliers, but some do. See the example, below.



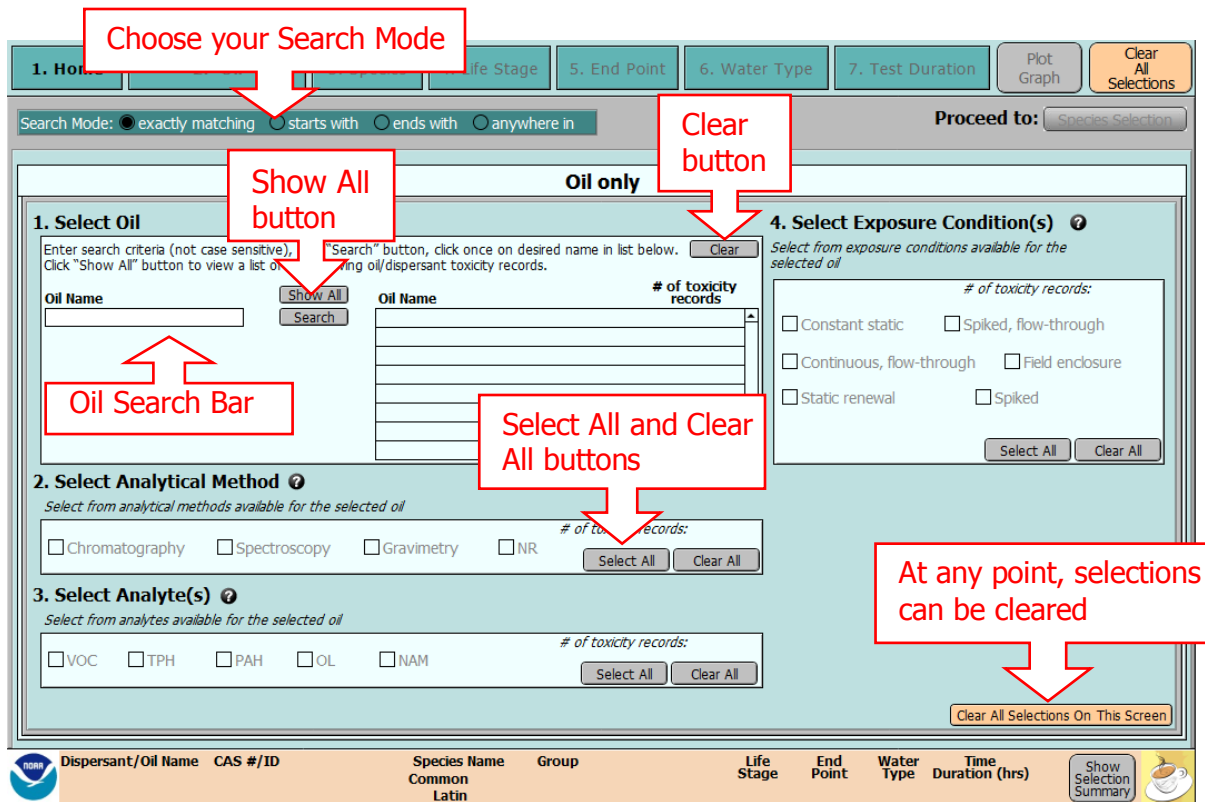
Each individual species plotted on the SSD has an associated report displaying important details from the original data source. Useful information includes chemical characteristics (e.g., grade, purity), test conditions (e.g., water type, exposure duration), species (e.g., scientific name, life stage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

Click on the **i** button next to each species to view the associated report (original studies). Then click on any of the numbered reports by data point. The source of the data point is listed next to each report button.

The screenshot displays the 'ECOTOX: Aquatic Reports' interface. At the top, there is a plot for 'Katelysia opima' with a concentration axis from 10<sup>-12</sup> to 10<sup>+12</sup> µg/L. A data point is plotted at approximately 10<sup>+05</sup> µg/L. Below the plot is a detailed report form for 'ECOTOX: Aquatic Report' with 'AQUATIC TEST #' 127989 and 'CHEMICAL Benzene'. The form includes sections for 'TEST CONDITIONS', 'TEST CONCENTRATION', and 'EFFECT RESULTS'. A red callout box points to the 'i' button next to the species name, with the text 'Click on the numbered report to view'. Another red callout box points to the numbered report button '(1) 127989\_a' in the left sidebar, with the text 'The reports are numbered by data point'.

## Oil only Scenario

After selecting an oil, the toxicity data selection screens are shown. There are three steps to complete before proceeding to the Species Selection. The number of Toxicity records adjusts, based on your selections.



**Oil** – Search for the desired oil using the search bar. Click once on the desired name in the Search Results.

**Analytical Method(s)** – Select Analytical Method(s) used to quantify the oil. NR stands for Not Recorded.

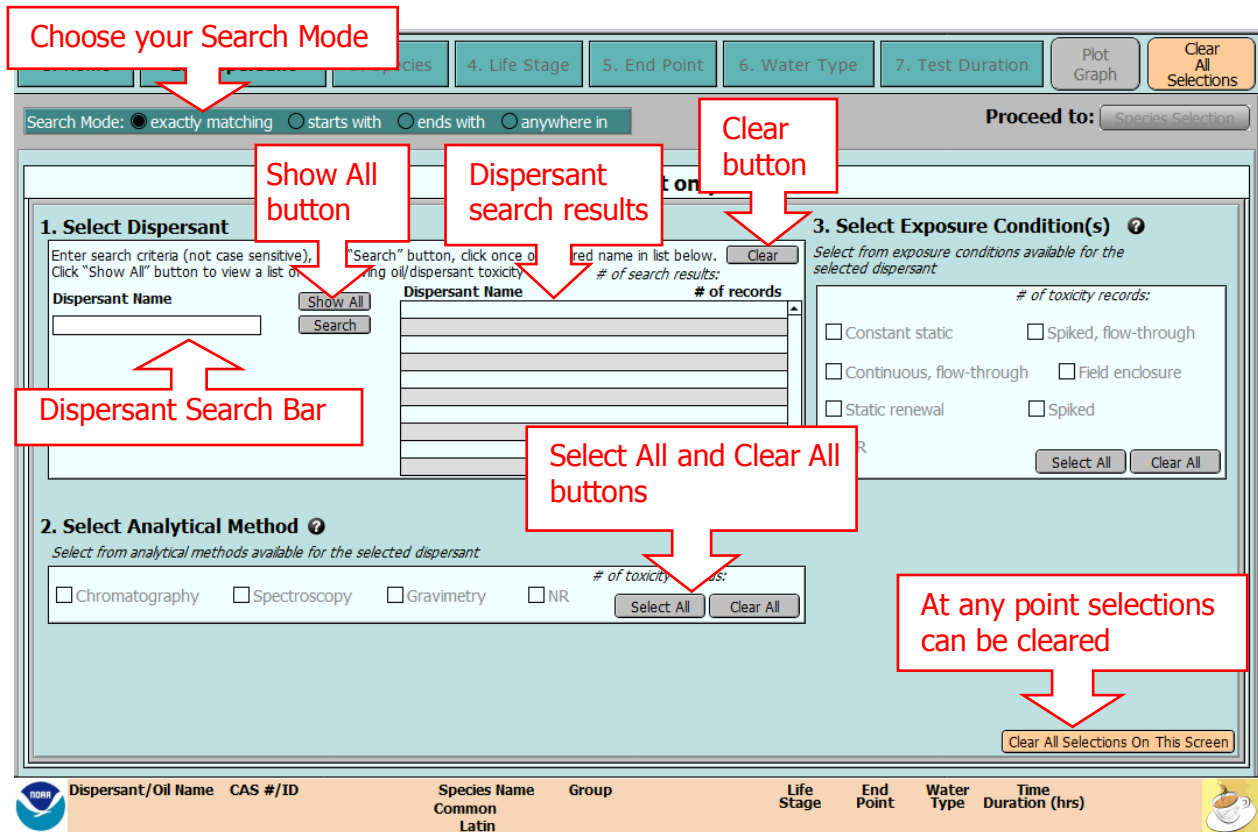
**Analyte(s)** – Select Analyte(s) measured in the chemical analysis. OL stands for Oil Loading and NAM stands for No Analyte Measured.

**Exposure Condition(s)** – Select Exposure Condition(s) used in the toxicity experiment(s).

## Dispersant only Scenario

After selecting a dispersant, the toxicity data selection screens are shown. There are two steps to complete before proceeding to the Species Selection. The number of Toxicity records adjusts, based on your selections.





**Dispersant** – Search for the desired dispersant using the search bar. Click once on the desired name in the Search Results.

**Analytical Method(s)** – Select analytical method(s) used to quantify the dispersant.

**Exposure Condition(s)** – Select exposure condition(s) used in the toxicity experiment(s).

## Dispersant and Oil Scenario

After making a dispersant and oil selection, the toxicity data selection screens are shown. There are six steps to complete before proceeding to the Species Selection. The number of Toxicity records adjusts, based on your selections.

**Oil** – Search for the desired oil using the search bar. Click once on the desired name in the Search Results.

**Dispersant** – Select a dispersant from the dropdown menu. Only dispersants that have data with the selected oil appear in the dropdown menu.

**Dispersant/Oil Ratio** – Select a Dispersant/Oil Ratio from the dropdown menu. Only ratios that have data with the selected oil and dispersant appear in the dropdown menu.

**Analytical Method(s)** – Select Analytical Method(s) used to quantify the oil and dispersant mixture. NR stands for Not Recorded.

**Analyte(s)** – Select Analyte(s) measured in the chemical analysis. OL stands for Oil Loading and NAM stands for No Analyte Measured.

**Exposure Condition(s)** – Select Exposure Condition(s) used in the toxicity experiment(s).

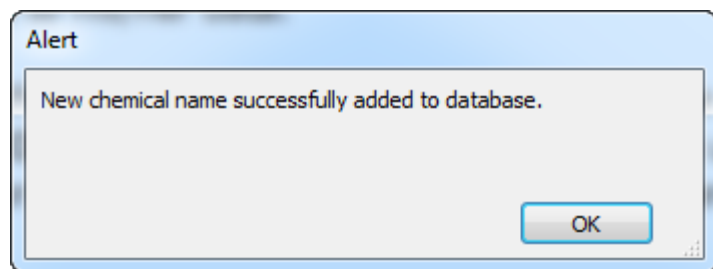
## User-Added Data

CAFE gives you the option to add your own data. There are eight to fourteen steps to complete before your data are submitted. To graph accurately, all steps must be complete and submitted (indicated by the green section labels) before clicking the final green "Submit" button. As you add your data, the orange summary bar will populate with your selections. You also have the ability to add some notes to your data.

**Scenario** – First, specify the scenario. The screen will adjust to the specified scenario.

**Chemical/Dispersant/Oil** – Select Chemical, Dispersant, or Oil. You can search for the chemical/dispersant/oil, or add a new one if the chemical/dispersant/oil of interest to you doesn't appear in the search.

If you choose to add a new chemical/dispersant or oil, you must submit the new chemical/dispersant/oil by clicking on the "Submit New Chemical/Dispersant/Oil" button. This is confirmed by a message such as:



Your new chemical/dispersant/oil should also appear in the search results.



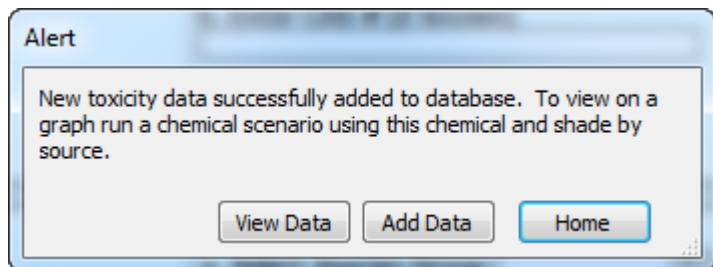
**Note:** If a chemical is added without an associated CAS number, CAFE will enter CAS numbers as defaults (e.g, User/1)

**Species** – Select the species for which data are available. You can search a species' common or scientific name, or add a new one if the species of interest to you doesn't appear in the search.

If you choose to add a new species, you must select a species group (fish, crustacean, mollusk, coral, or other). Then add a common and scientific name for your new species. Submit the new species by clicking on its "Submit" button. This is confirmed by a message and your species' name should appear in the search results.



After the user-added data records are submitted, an Alert message will prompt you to go back to your specified scenario (Home button) and include your user-added records in your query. You also have the option to view your added data or add more data.



The View Data screen is shown below.

**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.

Export User-Added Data Import User-Added Data Add Data Entry Screen

**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	Delete
Value Crab	Valus Crabby	Crustacean	1	Delete
Value Fish	Valus fishes	Fish	1	Delete

**Toxicity Data** 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 Test Type	Dur.	Analyte	Analytical Method	Disp/Oil Ratio	Conc. (µg/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	

Data Code Key: 1 = Chemical 2 = Dispersant Only 3 = Oil Only 4 = Dispersant and Oil

The **Chemicals/Oils/Dispersants** and **Species Names** sections displays new user-added chemicals/oils/dispersants and species names.

- These chemicals/oils/dispersants and species names can only be deleted when they do not have a complete record associated with them (e.g., a concentration, life stage, etc.). Otherwise, you would have to delete your individual record associated with the new chemical/oil/dispersant. The number of records of the chemical/oil/dispersants and/or species names column(s) should reduce with your deletion. Then you can delete the chemicals/oils/dispersants and species names.

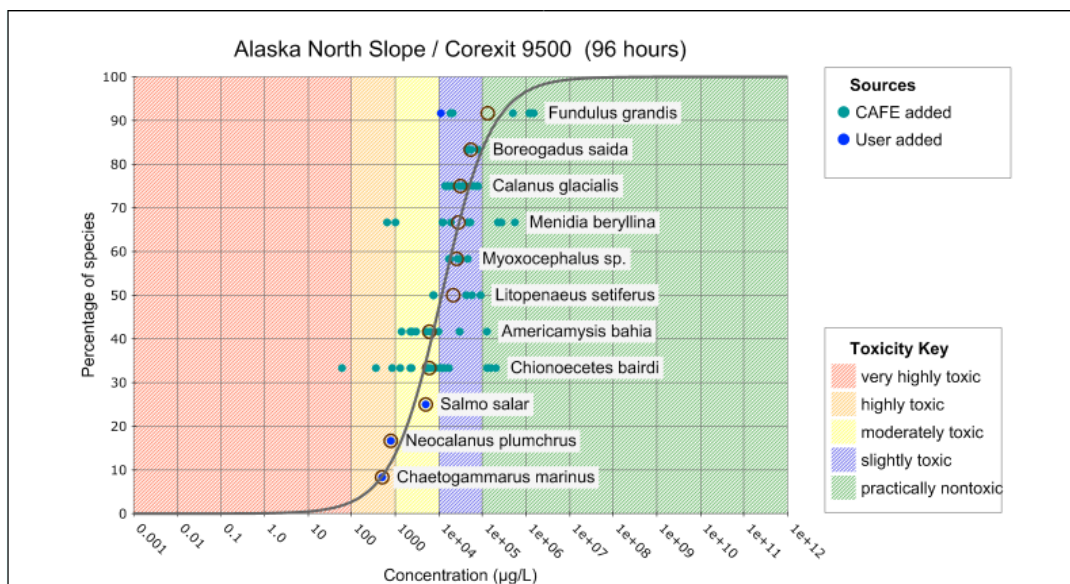
Under **Toxicity Data**, individual records display by toxicity parameter.

- Click on the pencil icon to edit a record.
- Click on the red X button to delete a record.
- Some toxicity parameters don't apply to a given scenario. For example, a chemical record would not have the following toxicity parameters: Analyte, Analytical Method, Dispersant, Oil Name, or Exposure Conditions.

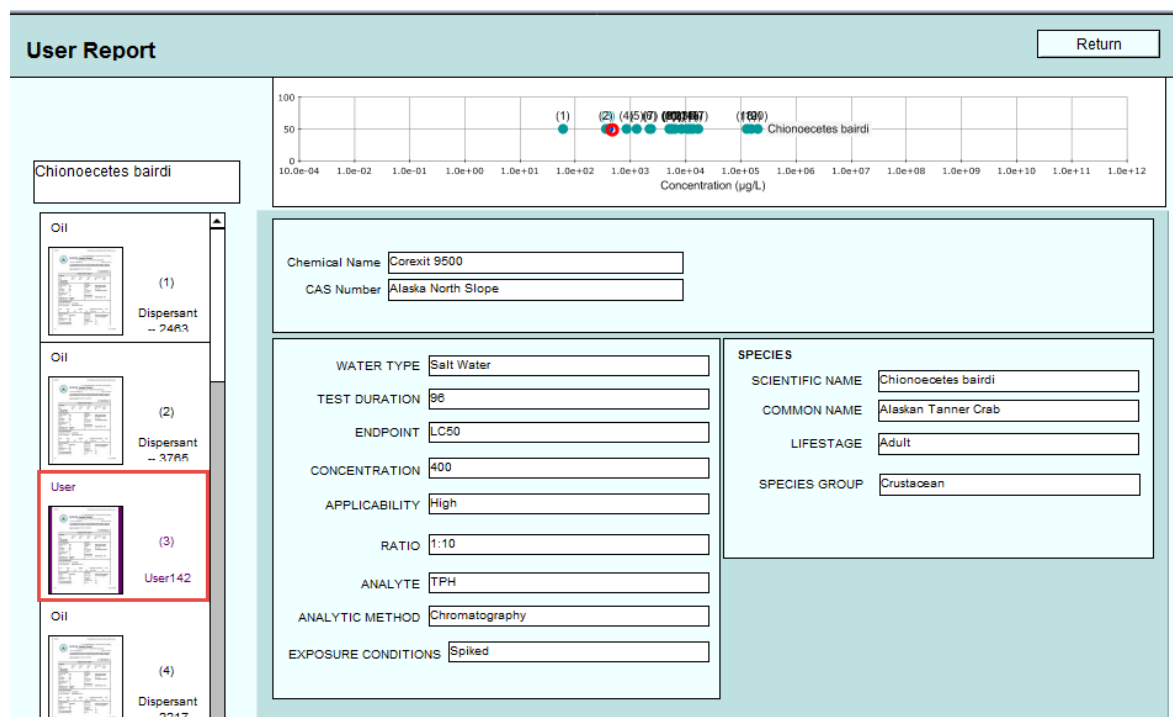


Oils and dispersants display as CAS numbers under the CAS#/ID field.

Once you have plotted your graph, you can choose to shade by "Sources," which helps you distinguish between the data you added and the CAFE data. In the example below, the user-added data points are labeled with blue dots.



Similar to the CAFE data, the user-added data points have an associated report providing greater detail about the data.




## User-Added Data Limitations

- For the Dispersant and Oil scenario, you can only input five dispersant and oil ratios per test duration.
- 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, you can search for and locate the oil/dispersant combination, Alaska North Slope and Corexit 9527; however, you 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 you want to add an oil/dispersant record for Agha Jari Iran and Actusol, you 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

## User-Added Data Import and Export

CAFE now has an import and export feature. When you click to view your user-added data, you can see the new feature.

 **NOTE:** You will not be able to import or export your user-added data from CAFE version 1.1. You will only be able to import and export your user-added data with version 1.2. or later.

### Export User-Added Data

To export user-added data, first make a backup copy of CAFE. Then click the button below.

**Instructions for moving your user-added data from your old into your new version of CAFE.** Return

**Export User-Added Data**

The following instructions will walk you through the process of exporting your user-added data from your old version of CAFE.

You should be in your old copy of CAFE.

Be sure to make a backup copy in case you need try this more than once.

Three files, main\_data.mer, chemical names.mer and species\_data.mer containing exported data will be put into a UserData folder in your CAFE runtime folder.

Export user-added data

Keep track of where this UserData folder is. You will need to move it into your new copy of CAFE.

The export is confirmed with summary text

4 user records successfully exported.  
3 chemical names successfully exported.  
3 species names successfully exported.

Three files are created with your export: main\_data.mer, chemical\_names.mer and species\_data.mer containing the exported data. These files are placed in a folder called UserData in your CAFE folder. Make sure you make copy of your UserData folder. It contains the three files you need. Keep track of where your UserData folder is.



Name	Date modified	Type	Size
de	3/16/2016 12:40 PM	File folder	
en	3/16/2016 12:40 PM	File folder	
es	3/16/2016 12:40 PM	File folder	
Extensions	3/16/2016 12:40 PM	File folder	
fr	3/16/2016 12:40 PM	File folder	
it	3/16/2016 12:40 PM	File folder	
ja	3/16/2016 12:40 PM	File folder	
ko	3/16/2016 12:40 PM	File folder	
nl	3/16/2016 12:40 PM	File folder	
pt	3/16/2016 12:40 PM	File folder	
SASL2	3/16/2016 12:40 PM	File folder	
sv	3/16/2016 12:40 PM	File folder	
Themes	3/16/2016 12:40 PM	File folder	
<b>UserData</b>	3/16/2016 12:40 PM	File folder	
XTPTrans	3/16/2016 12:40 PM	File folder	
zh-Hans	3/16/2016 12:40 PM	File folder	
CAFE.caf	3/16/2016 2:04 PM	CAFE	779,708 KB
CAFE.exe	4/22/2015 7:32 PM	Application	9,566 KB
ClientUI.dll	4/22/2015 7:32 PM	Application extens...	286 KB
DBEngine.dll	4/22/2015 7:32 PM	Application extens...	8,058 KB
Field_Names_as_Header.xsl	9/13/2012 5:37 PM	XSL Stylesheet	1 KB
FMEngine.dll	4/22/2015 7:32 PM	Application extens...	6,068 KB
FMP Acknowledgements.pdf	4/22/2015 7:26 PM	Adobe Acrobat D...	127 KB
FMRSRC.dll	4/22/2015 7:32 PM	Application extens...	10,882 KB
FMWrapper.dll	4/22/2015 7:32 PM	Application extens...	191 KB
Interop.dll	4/22/2015 7:32 PM	Application extens...	1,177 KB
libcurl.dll	4/22/2015 7:32 PM	Application extens...	454 KB
libeay32.dll	4/22/2015 7:32 PM	Application extens...	1,567 KB
Libetpan.dll	4/22/2015 7:32 PM	Application extens...	428 KB
libsasl.dll	4/22/2015 7:32 PM	Application extens...	356 KB
mfc120chs.dll	10/5/2013 1:58 AM	Application extens...	46 KB

## Import User-Added Data

After you complete a fresh install of CAFE, make sure you copy and replace the UserData folder with your exported UserData folder.

Once you have completed those steps, open your new copy of CAFE. Click the View User-Added Toxicity Data button then click the Import User-Added Data button.

**Instructions for moving your user-added data from your old into your new version of CAFE.** Return

**Import User-Added Data**

The following instructions will walk you through the process of importing your user-added data into your new version of CAFE.

During the export of your user-added data some files were created.

First move these files from the UserData folder where they currently reside into the UserData folder in your new copy of CAFE.

Alternately you can replace your whole UserData folder in your new version of CAFE with the UserData folder in your old version.

At the very least you will have a file maindata.mer which contains your user-added data records. If you also exported user-added chemical names and user-added species names then you will also have the files chemicalnames.mer and speciesdata.mer.

After you have moved your files click on Import user-added data to proceed with your import.

Import user-added data

On the Import User-Added Data screen, click the Import user-added data button. A summary confirming the import should appear.

Importing Data records  
Importing Chemical Names  
Importing Species Data  
Finished

Then you can view your imported user-added data to confirm.

**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.

Export User-Added Data Import User-Added Data Add Data Entry Screen

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Common Name	Latin Name	Species Group	# of records	
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Value Crab	Valus Crabby	Crustacean	1	Delete
Value Fish	Valus fishes	Fish	1	Delete

**Toxicity Data** 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. (µg/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	

## Short Exposure Risk Reports

Documents are available for a select number of chemicals (46 total), outlining the risks of these chemicals for short exposure durations. These reports were created by using existing toxicity data (LC<sub>50</sub> or EC<sub>50</sub>) from tests performed under longer exposure durations (e.g., 24, 48, 72, 96 h) to estimate short-term toxicity (1, 2, and 4 h). These reports were created using the methodology described in the following paper:

Bejarano, A.C. and J. K. Farr. 2013. [Development of Short Acute Exposure Hazard Estimates: A Tool for Assessing the Effects of Chemical Spills in Aquatic Environments](#). Environmental Toxicology and Chemistry. Environmental Toxicology and Chemistry. 32 (8): 1918-1927.




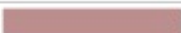


Users are highly encouraged to print the short exposure risk reports.

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

## Benzene -- CAS# 71432

Synonyms: Cyclohexatriene, Benzole

Color Schemes	Description	Color Scheme
Inherent acute toxicity	Moderately toxic	
	Slightly toxic	
	Practically nontoxic	
Risk Estimate Reliability	Moderate	

Color key

### Data availability

This table shows all toxicity data for aquatic species, by representative groups and exposure duration, available in CAFE as of 10/20/2015 for benzene.

Exposure duration (h)	Number of Species	Species Group*
24	34	C=8, F=13, M=3, O=10
48	37	C=12, F=10, M=3, O=12
72	9	C=3, F=2, M=3, O=1
96	35	C=10, F=19, M=4, O=2

Table of Data availability used in analysis

\*C=Crustaceans, F=Fish, M=Mollusks, O=Other

### General Observations

- Most of the currently available acute toxicity data (LC<sub>50</sub> and EC<sub>50</sub>) used fish and crustaceans as the test species
- Based on the available data, fish and crustaceans appear equally sensitive to this chemical, while mollusks, other (i.e., invertebrates/spiders) appear less sensitive than fish and crustaceans
- Analyses focused on fish and crustaceans since these appear to be the most sensitive groups to this chemical and are equally represented across all exposure durations

Observations about the data available

### Data summary

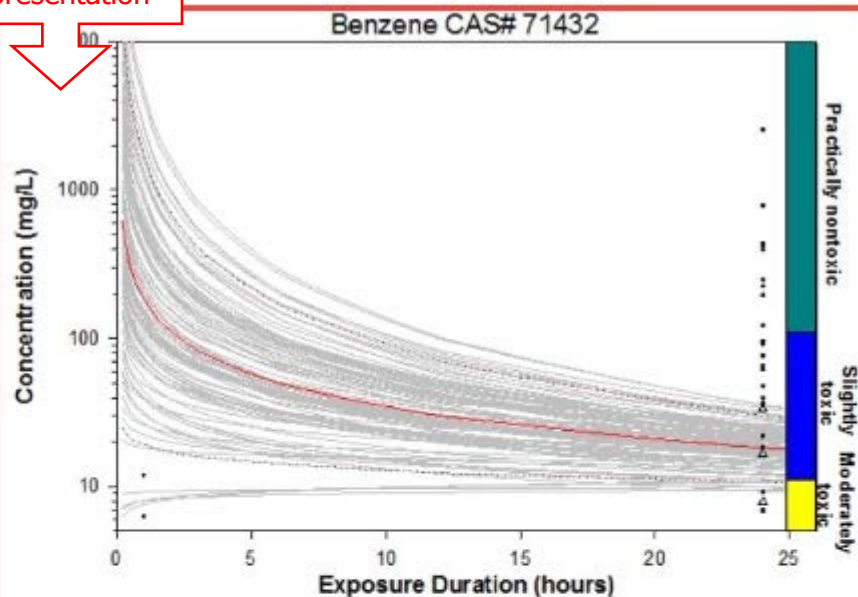
Evaluation of fish and crustacean aquatic toxicity data from CAFE (empirical) for benzene. Only curve with ≥5 species are shown. \* Kolmogorov-Smirnov test only.

Exposure duration (h)	Number of Species	Number of Outliers	Goodness of Fit	Estimated 5th percentile concentrations (95%CI) mg/L (ppm)**
24	21	1	Passed	17 (8-34)
48	22	1	Passed	14 (7-26)
96	29	1	Passed*	6 (3-12)

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

Evaluation of data included in analysis

Short Exposure Graphical representation



Graphic representation of the analysis used to estimate concentrations for short exposure durations using fish and crustaceans. Triangles: 5<sup>th</sup> percentiles and confidence interval concentrations from individual SSD curves; dots: available empirical data; light gray: bootstrapped lines; red: mean response (solid), 95% confidence interval (dashed); color scheme (right): inherent acute toxicity. These curves were derived from LC<sub>50</sub> and EC<sub>50</sub> data; therefore, these represent estimated LC<sub>50</sub>/EC<sub>50</sub> values.

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

Estimated short-exposure concentrations

Short exposure duration (h)	Estimated 5th percentile concentrations (95%CI) mg/L (ppm)*	Risk Estimate Reliability
1	184 (19-1,650)	Moderate
2	111 (17-679)	Moderate
4	67 (15-283)	Moderate
8	40 (14-117)	Moderate
24	18 (11-30)	Moderate

\*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
- Given initial data observations on relative sensitivity by group of species these estimates may be protective of most aquatic groups
- 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

Considerations

**Documentation:** CAFE uses two documents to provide guidance to users: this “How-To” Document and a User’s Manual. Also available are CAFE training videos.

**How-To Document** – This document helps users get started on how to use CAFE.

**User’s Manual** – This document provides a more in-depth analysis on the use of CAFE and the extensive QA/QC process that went into developing CAFE.

**Training Videos-** 5 different training videos contained in a .zip file on how to use CAFE.

**Recommended citation:** NOAA, 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.

Review the following scenarios to help you use outputs from CAFE:

## Scenario 1: Benzene (CAS No. 71432)

*Incident Occurrence: Benzene Release, Parachute Creek, Colorado*

A fracking boom for fracked natural gas processor, Williams Energy, spilled an estimated 241 barrels of benzene (CAS No. 71432) into the ground, some of which eventually washed into Parachute Creek. Those responding to this incident would be seeking estimates for fate and effects of benzene.

*Question 1: What are the hazards of the chemical?*

Fate Data - Physical Properties		Chemical Name	Benzene	CAS Number	71432
Odor	Aromatic odor Gasoline-like odor; rather pleasant aromatic odor		Structure		
Color/Form	Rhombic prisms Colorless to light-yellow liquid (a solid below 42°F)				
Skin, Eye, and Respiratory Irritation	Skin irritant. Severe eye and moderate skin irritant. Skin irritant upon occupational exposures of >60 ppm for three weeks.				
Boiling Point (°C)	80° C (Experimental)	Flash Point	12°F (-11°C) (Closed Cup) (Experimental)		
Melting Point (°C)	5.5° C (Experimental)	Ionization Potential (eV)	9.24 eV		
Density		Hvap (cal/g)			
Autoignition Temp.	928°F (497°C)	HLC (atm-m3/mol)	.00555 at 25°C (Experimental)		
Vapor Density	2.8 (Air= 1)	Log Kow	2.13 (Experimental)		
Viscosity	0.604 cP at 25°C	Vapor Pressure (mmHg)	94.8 mm Hg at 25°C (Experimental)		
Explosive/Flammable Limits	Lower 1.4%; Upper 8.0%	Water Solubility (mg/L)	1790 at 25°C (Experimental)		

**Answer:** With benzene, there are two hazards to consider: (1) Benzene is a fire hazard. Its flash point is very low at 12°F (-11°C), making it highly flammable. With an ignition source, benzene could catch on fire and burn quickly. (2) Benzene can harm humans as a skin and eye irritant, as well as a carcinogen (cancer-causing threat).



Question 2: How will this chemical behave in the environment?

Fate Data - Environmental Properties		Chemical Name	Benzene	CAS Number	71432
EPI Suite v4.11					
<b>Soil Adsorption</b>	Estimated Koc	145.8	<b>Environmental Explanations</b>		
<b>Primary Biodegradation</b>	Estimated Biodegradation Timeframe	days-weeks	If released to the environment, Benzene is expected to be found predominantly in water (41.1%). It is also expected to be found in soil (26.7%), air (31.8%) and sediment (0.37%).		
<b>Estimated Volatilization from Water</b>	Half-life from Model River (hours)	0.995	<b>SOIL</b>		
	Half-life from Model Lake (hours)	84.96	- In soil, Benzene is expected to have high mobility based upon a KOC of 145.8 (Estimated).		
<b>Estimated Hydrolysis at pH=7</b>	Half-life (days)		- Benzene may volatilize from dry soil surfaces based upon a vapor pressure of 94.8 mm Hg (Experimental).		
<b>Estimated Atmospheric</b>	Half-life (days)	5.486	- Benzene may volatilize from moist soil surfaces based upon a Henry's Law constant of 0.00555 atm-cu m/mole (Experimental).		
<b>Estimated Environmental Partitioning</b>	Percent to air	31.8	<b>WATER</b>		
	Percent to water	41.1	- Volatilization from water surfaces is expected to be an important fate process based on a Henry's Law constant of 0.00555 atm-cu m/mole (Experimental).		
	Percent to soil	26.7	- Estimated volatilization half-lives for a model river and model lake are 0.995 hours and 84.96 hours, respectively.		
	Percent to sediment	0.37	- In water, Benzene is not expected to adsorb to suspended solids and sediment based upon a KOC of 145.8 (Estimated).		
<b>Estimated Wastewater Removal (%)</b>	Total Removed	68.94	<b>AIR</b>		
	Due to Biodegradation	0.04	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.		
	Due to Sludge Adsorption	1.11	- Benzene will exist solely as a vapor in the atmosphere based upon a vapor pressure of 94.8 mm Hg (Experimental).		
	Due to Volatilization	67.78	- The half-life for the reaction of Benzene with photochemically generated hydroxyl radicals is 5.486 days, assuming a hydroxyl radical concentration of 1.5E+6 OH/cm3 and a 12-hour day.		
			<b>OTHER</b>		
			- The Sewage Treatment Model provides an estimate of the fate of a chemical present in the influent to a conventional activated sludge plant as it becomes subject to evaporation, biodegradation, sorption to sludges and loss in the final effluent. The Total Estimated Wastewater Removal is an estimate of the percentage of the chemical removed from the effluent stream by evaporation, biodegradation, and sorption to sludges. Benzene, is predicted to be removed from the effluent by these three processes. The percent lost to biodegradation, sludge adsorption, and air are 0.04, 1.11, and 67.78%, respectively.		

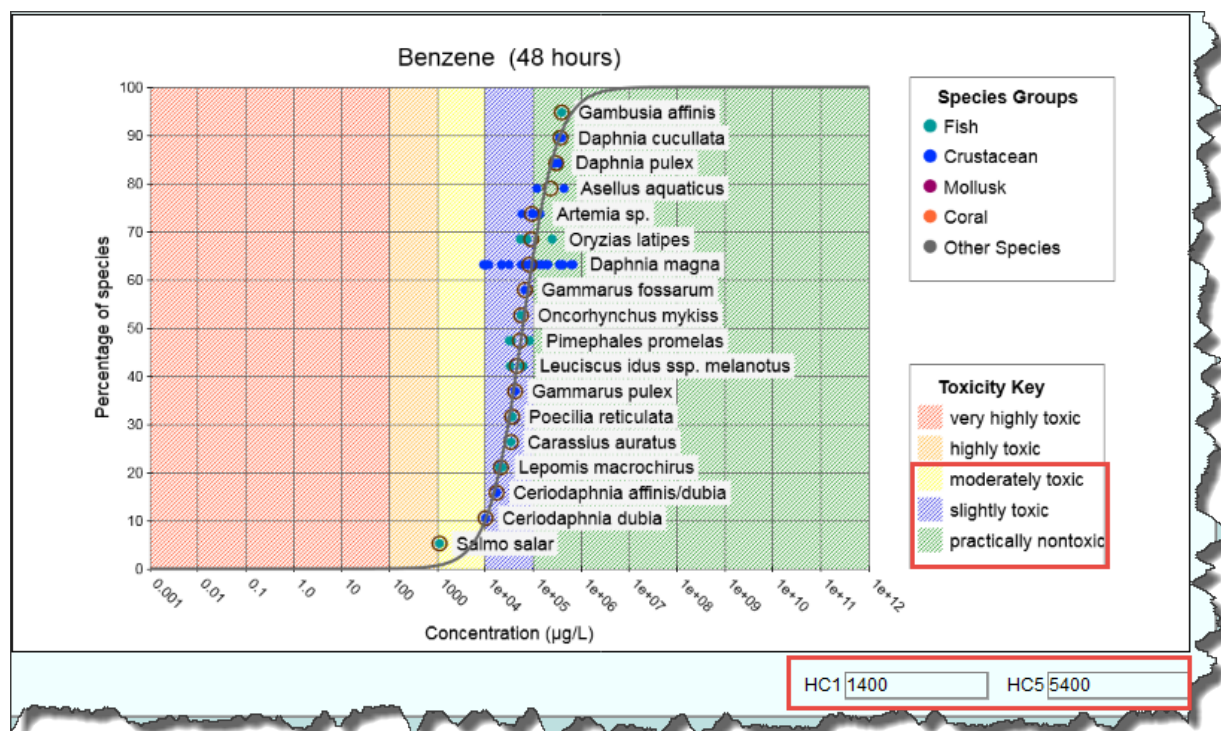
**Answer:** With a relatively high Henry's Law Constant (0.00555 atm·m<sup>3</sup>/mol) and vapor pressure (94.8 mm Hg), benzene is moderately soluble in water and will volatilize easily. Estimated Environmental Partitioning by the fugacity model predicts that if released into the environment, benzene is expected to be found predominately in water (41.1%), followed by air (31.8%), soil (26.7%), and sediment (0.37%). Estimated Volatilization from Water predicts that from a model river and lake, benzene will volatilize at 0.995 and 84.96 hours, respectively.

Question 3: How might you monitor and use this chemical?

Fate Data - Analytic Methods		Chemical Name	Benzene	CAS Number	71432															
<b>Method #</b>	<b>Media</b>																			
1	1624.0	Water																		
2	502.2 (by PID)	Water																		
3	524.2	Water																		
4	602	Water																		
5	6200B	Water																		
6	6200C	Water																		
7	624	Water																		
8	8021B (by GC-ELCD)	Various																		
9	8021B (by GC-PID)	Various																		
10	8260B	Various																		
11	D5790	Water																		
12	O-3115	Water																		
13	O-4024-03	Water																		
14	O-4127-96	Water																		
15	1501	Air																		
16	3700	Air																		
17	3800	Air																		
18	1005	Air																		
<b>Contamination and Interferences</b>		(A) Analytical system: Impurities in the purge gas, organic compounds out-gassing from the plumbing upstream of the trap, and solvent vapors can interfere. (B) Sample contamination: Samples can be contaminated by diffusion of volatile organic compounds through the bottle seal during shipment and storage. (C) Carry-over: Rinse the purging device and sample syringe with reagent water between samples.																		
<b>Maximum Holding Time</b>		14 days (after collection)																		
<b>Sample Handling</b>		Collect grab samples in glass containers having a total volume greater than 20 mL. Make sure no air bubbles are entrapped and maintain the hermetic seal until analysis. Store at 0-4 degrees C from time of collection until analysis. If residual chlorine is present, add 10mg/40mL of sodium thiosulfate prior to collection. Adjust pH to about 2 by adding HCl (1+1) while stirring.																		
<b>Quality Control Requirements</b>		The minimum requirements consist of an initial demonstration of laboratory capability, analysis of samples spiked with labeled compounds to evaluate and document data quality, and analysis of standards and blanks as tests of continued performance.																		
<b>References</b>		EPA Method Guidance CD-ROM (includes MC4WW Methods, and most current EPA Methods)																		
<b>Uses</b>		<table border="1"> <thead> <tr> <th>Use</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>Manuf of industrial chemicals such as</td> </tr> <tr> <td>2</td> <td>Chemical intermediate for ethylbenzene,</td> </tr> <tr> <td>3</td> <td>Benzol (benzene) discontinued by crowly tar</td> </tr> <tr> <td>4</td> <td>Was used extensively in the tire industry</td> </tr> <tr> <td>5</td> <td>Has been used as a veterinary disinfectant</td> </tr> <tr> <td>6</td> <td>Manufacture of explosives, pcb gasoline,</td> </tr> <tr> <td>7</td> <td>In the past, benzene has been used in the</td> </tr> </tbody> </table>				Use	1	Manuf of industrial chemicals such as	2	Chemical intermediate for ethylbenzene,	3	Benzol (benzene) discontinued by crowly tar	4	Was used extensively in the tire industry	5	Has been used as a veterinary disinfectant	6	Manufacture of explosives, pcb gasoline,	7	In the past, benzene has been used in the
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<b>Citation</b>		Budavari, S. (ed). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996. pp. 179																		
<b>Source</b>																				

**Answer:** According to Method Number 1624.0, you need to exercise caution when handling benzene. In an analytical system, other organic compounds and solvent vapors can interfere. While handling this chemical, you should select samples in glass containers having a total volume greater than 20 mL. Store the chemical at 0-4 °C and make sure no air bubbles are entrapped until analysis. Benzene has many uses, including the manufacture of industrial chemicals such as polymers, detergents, pesticides, pharmaceuticals, dyes, plastics, and resins, and as a solvent for waxes, resins, oils, natural rubber, etc.

Question 4: What is the toxicity of this chemical?



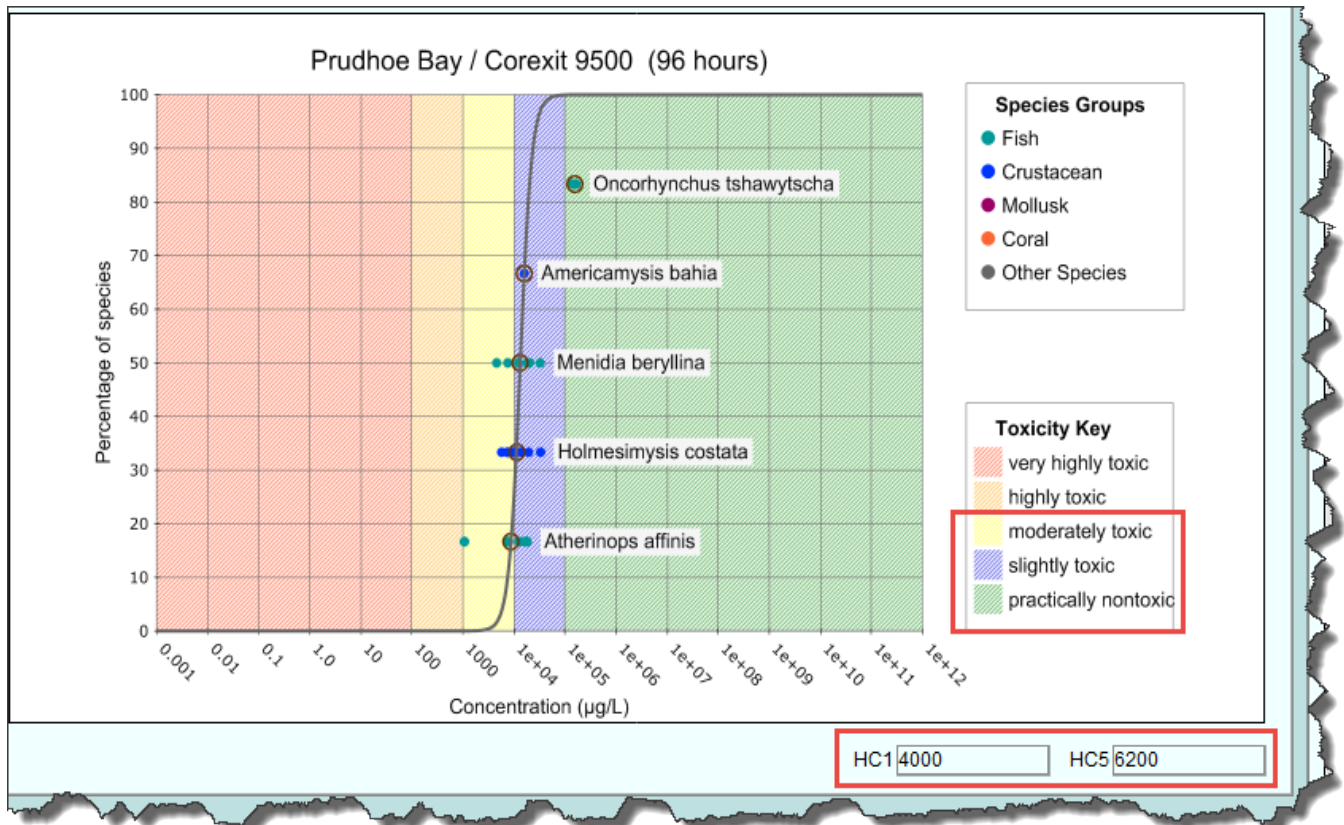
**Answer:** In an acute 48-hour exposure, benzene is moderately toxic to practically nontoxic to freshwater fish and crustaceans. The hazard concentrations indicate a HC5 protective value of 7,700 µg/L or 7.7 mg/L (7.7 ppm).

## Scenario 2: Alaska North Slope Crude and Corexit 9500

*Incident Occurrence: Oil Spill, Prince William Sound, Alaska*

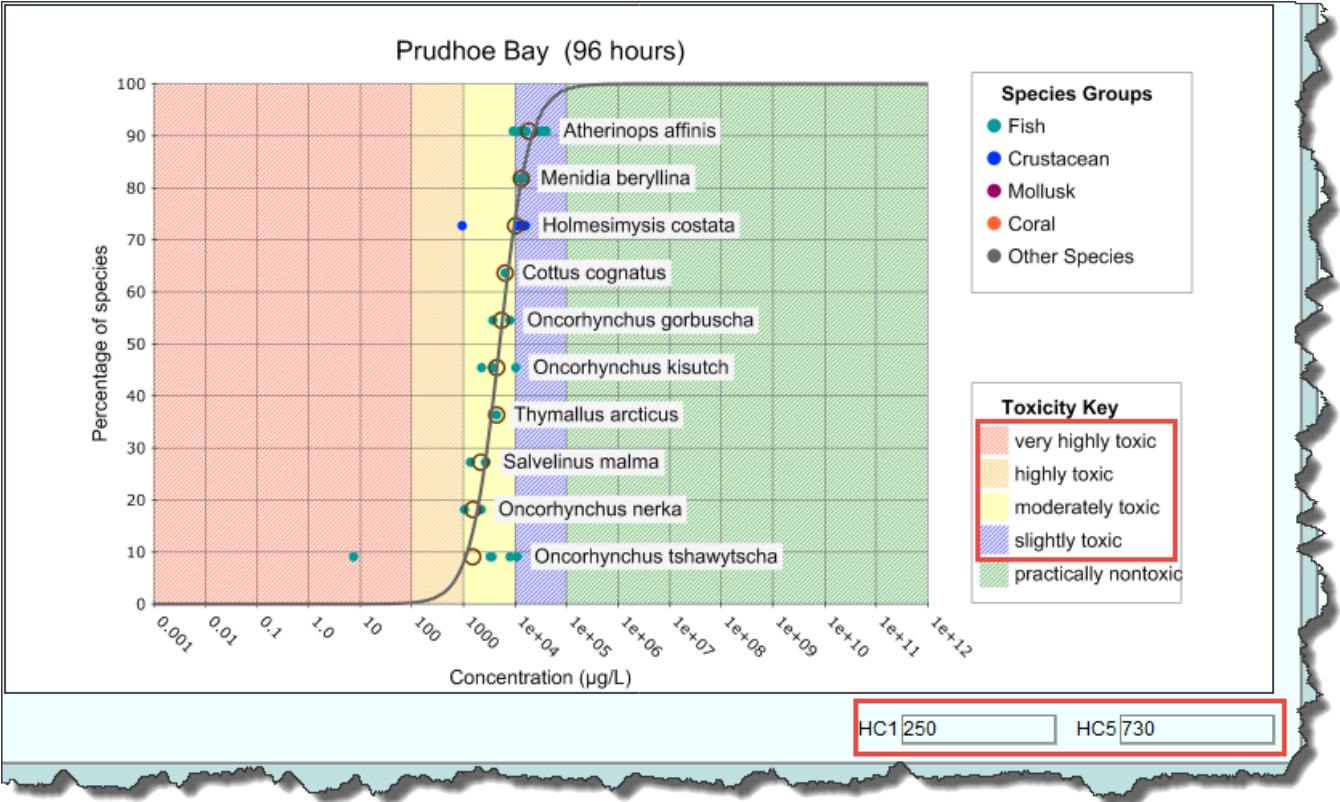
A barge collided near shore, spilling about 1,000 gallons of Prudhoe Bay crude in Prudhoe Bay, Alaska. Corexit 9500 was applied at the spill site at a 1:10 dispersant and oil ratio. The analytical methods used were chromatography. The analytes measured were TPHs and PAHs. Prudhoe Bay is a major fishing ground in the commercial fishing industry. You are concerned about how toxic the mixture is to fish and crustaceans.

*Question 1: How toxic is this mixture to fish and crustaceans?*



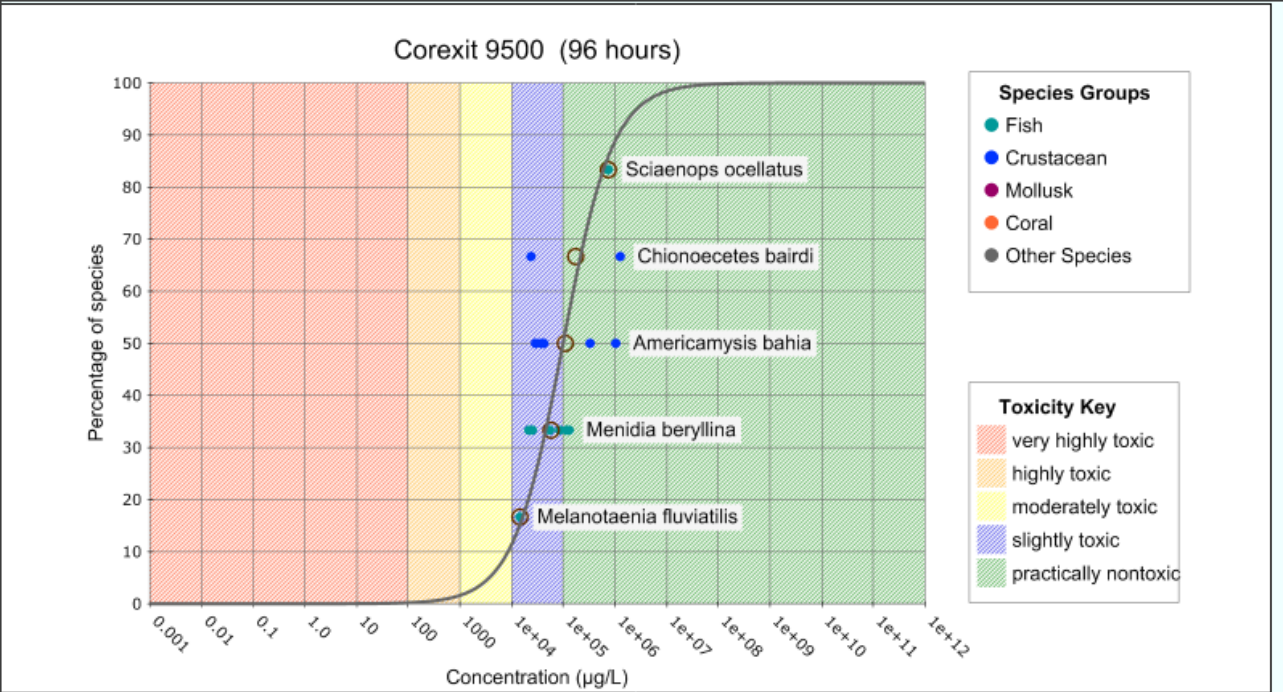
**Answer:** In an acute 96-hour exposure, Prudhoe Bay crude and Corexit 9500 together are moderately toxic to practically nontoxic to fish and crustaceans. The hazard concentrations indicate a HC5 protective value of 6,200  $\mu\text{g/L}$  or 6.2 mg/L (6.2ppm).

Question 2: How toxic is Prudhoe Bay crude (alone) to fish and crustaceans?



**Answer:** In an acute 96-hour exposure, Prudhoe Bay crude is very highly toxic to slightly toxic to fish and crustaceans. The hazard concentrations indicate a HC5 protective value of 730 µg/L or 0.73 mg/L (0.73 ppm).

Question 3: How toxic is Corexit 9500 (alone) to the fish and crustaceans?



HC1 580      HC5 3700

**Answer:** In an acute 96-hour exposure, Corexit 9500 is moderately toxic to practically nontoxic to fish and crustaceans. The hazard concentrations indicate a HC5 protective value of 3,700 µg/L or 3.7 mg/l (3.7 ppm).



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