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

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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.

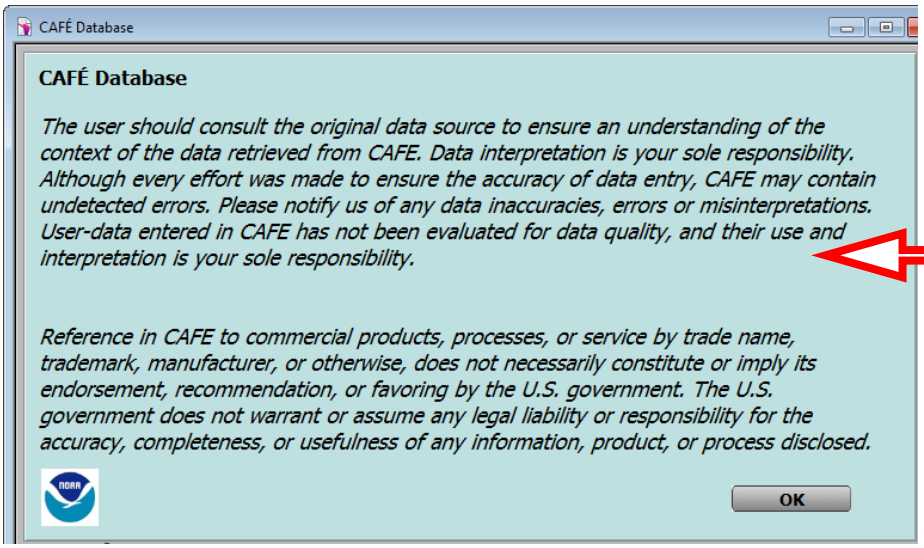
Performing Queries in CAFE

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.

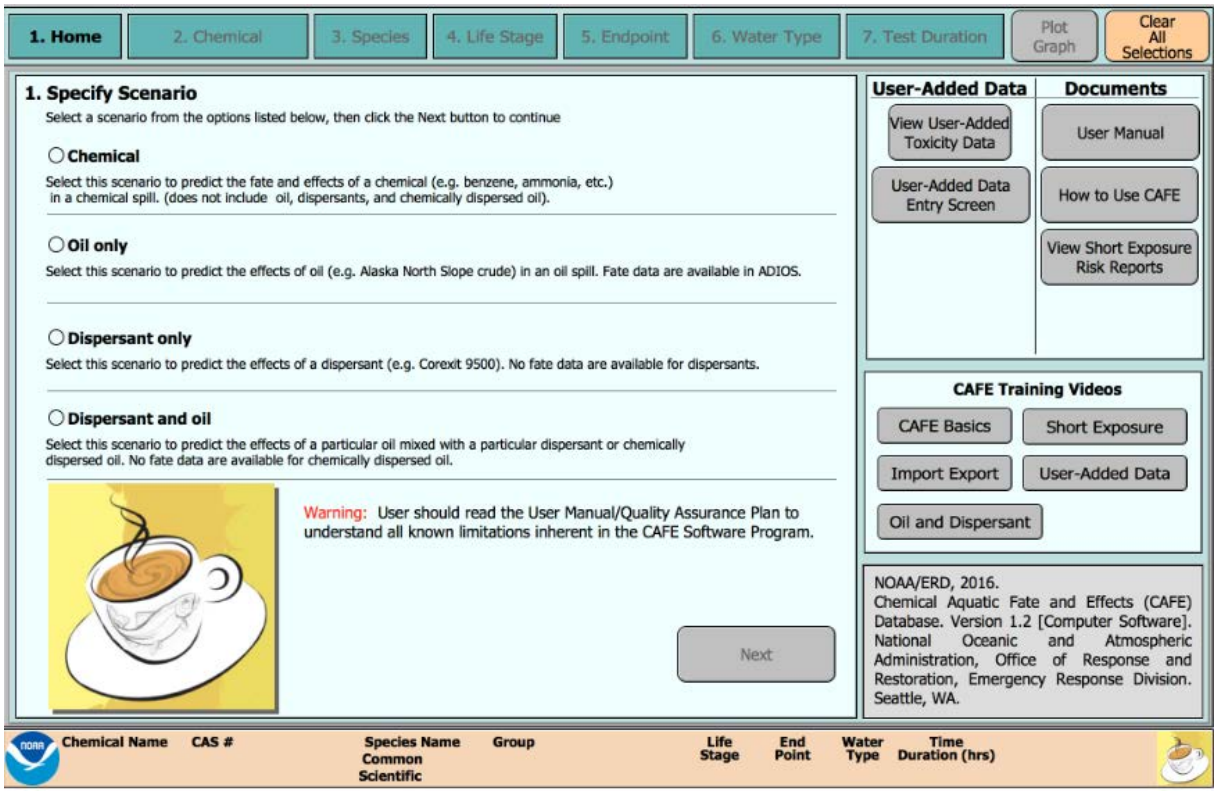
Disclaimer



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.

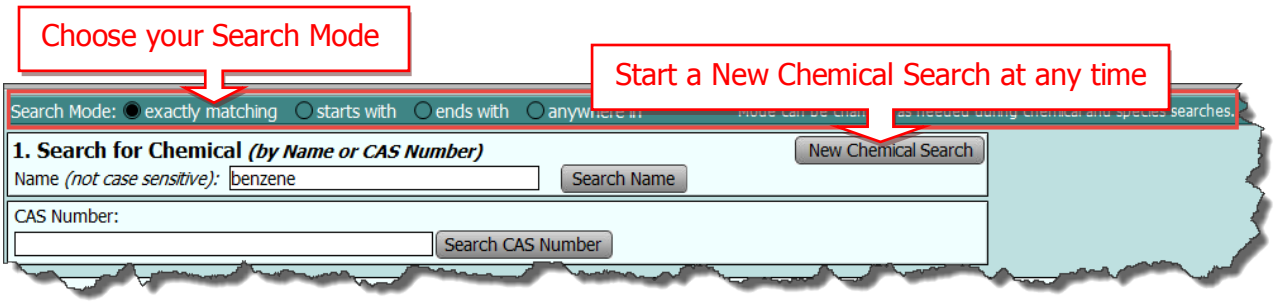
Getting Started

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.

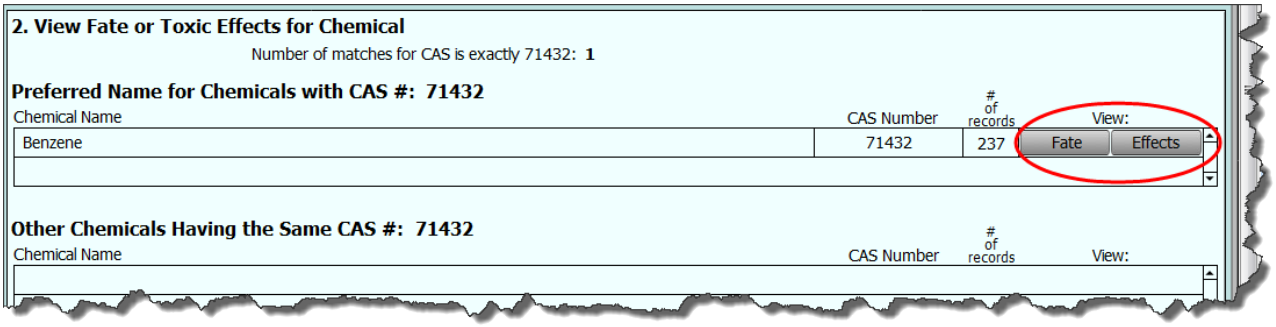


Chemical Scenario

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.



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



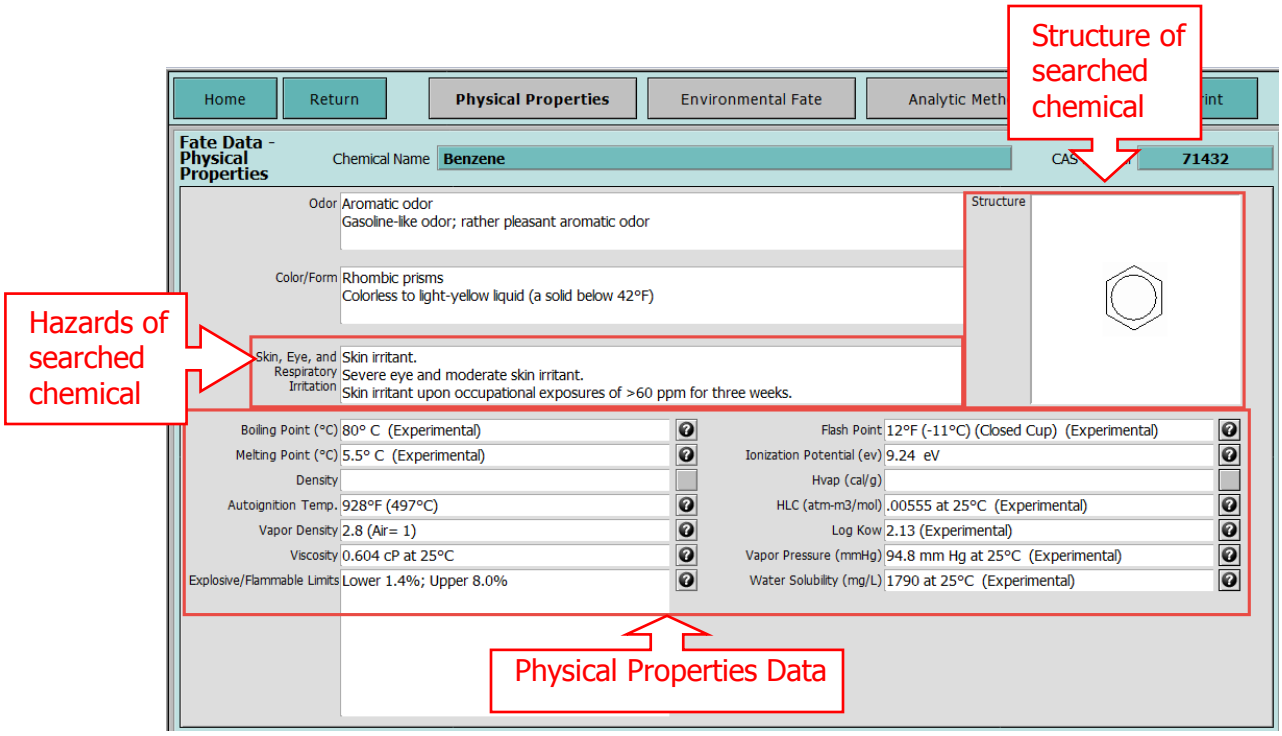
Aquatic Fate Module

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

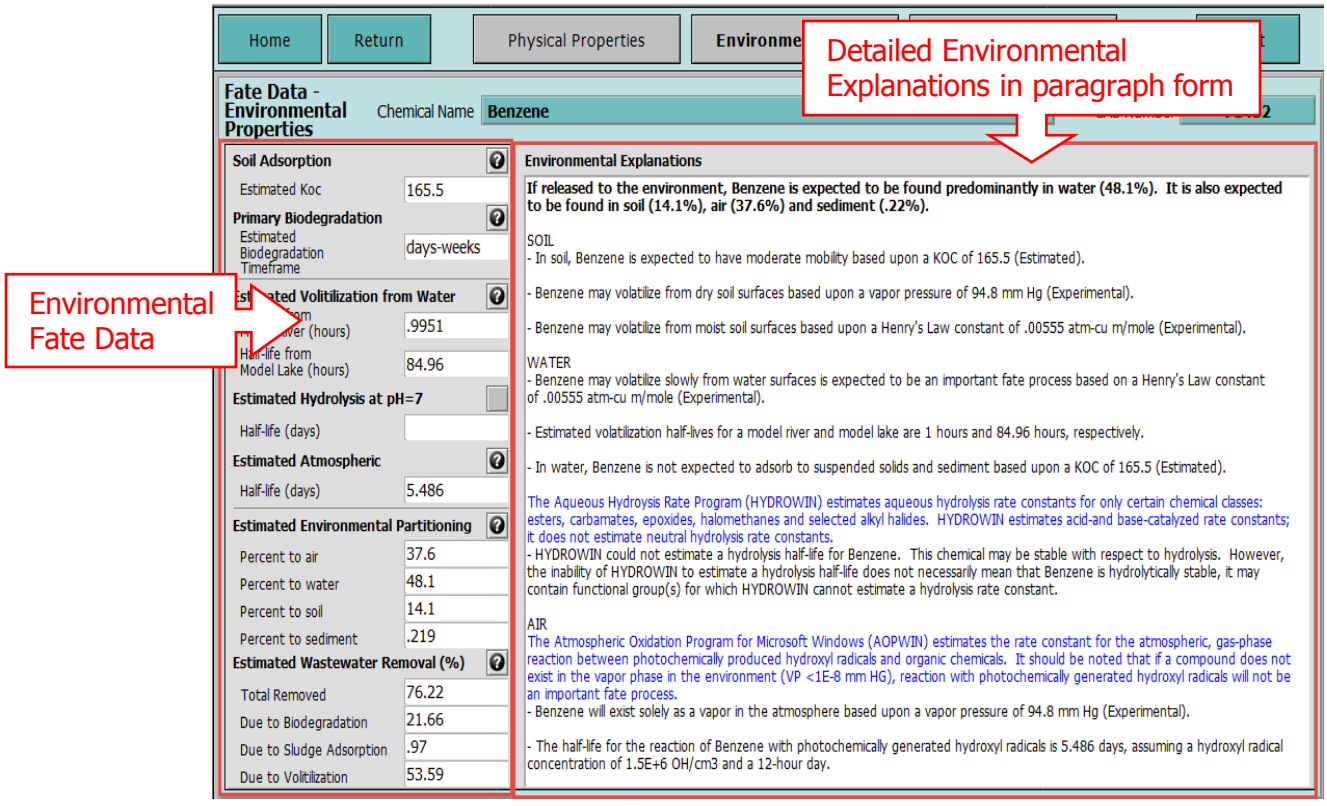
Printing is available on all three sub-modules.

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



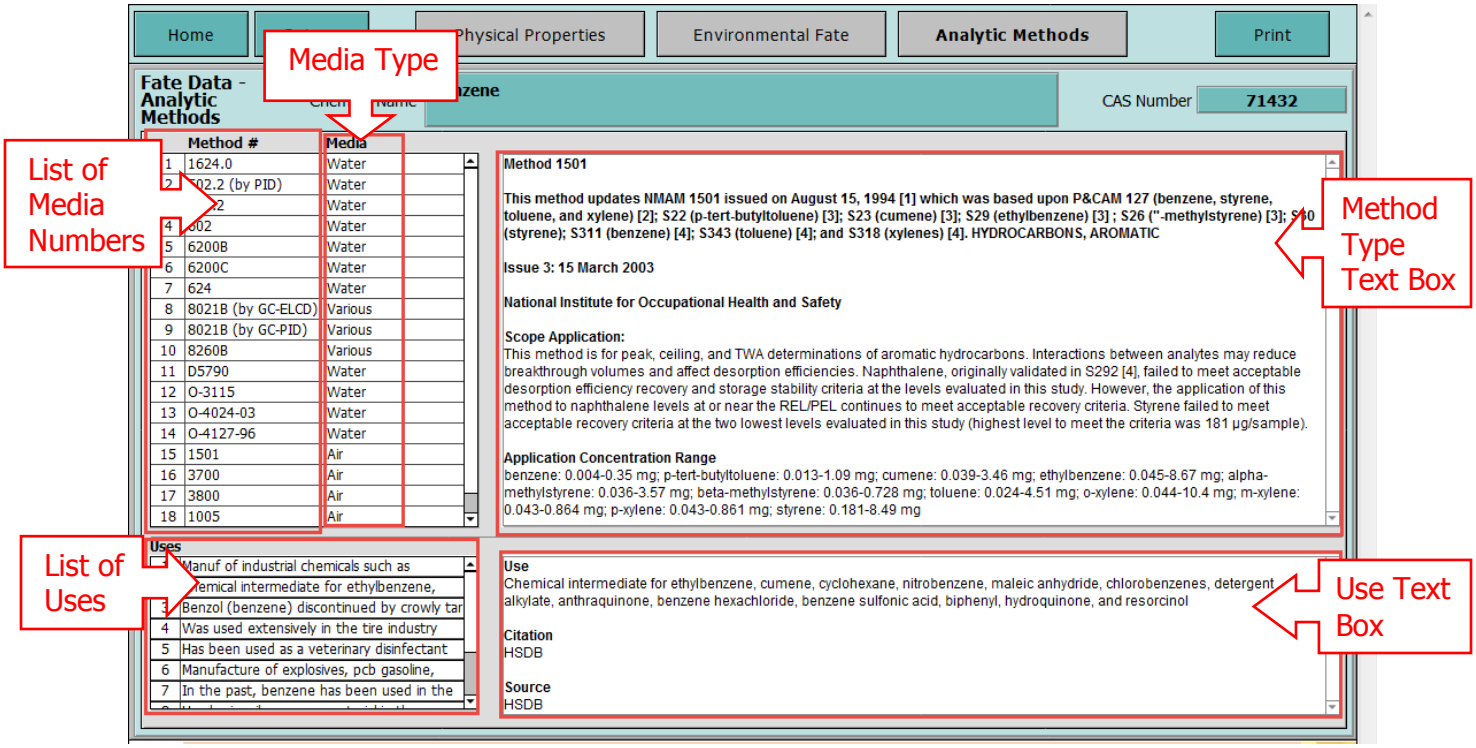
Environmental Fate sub-module

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.



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.



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.

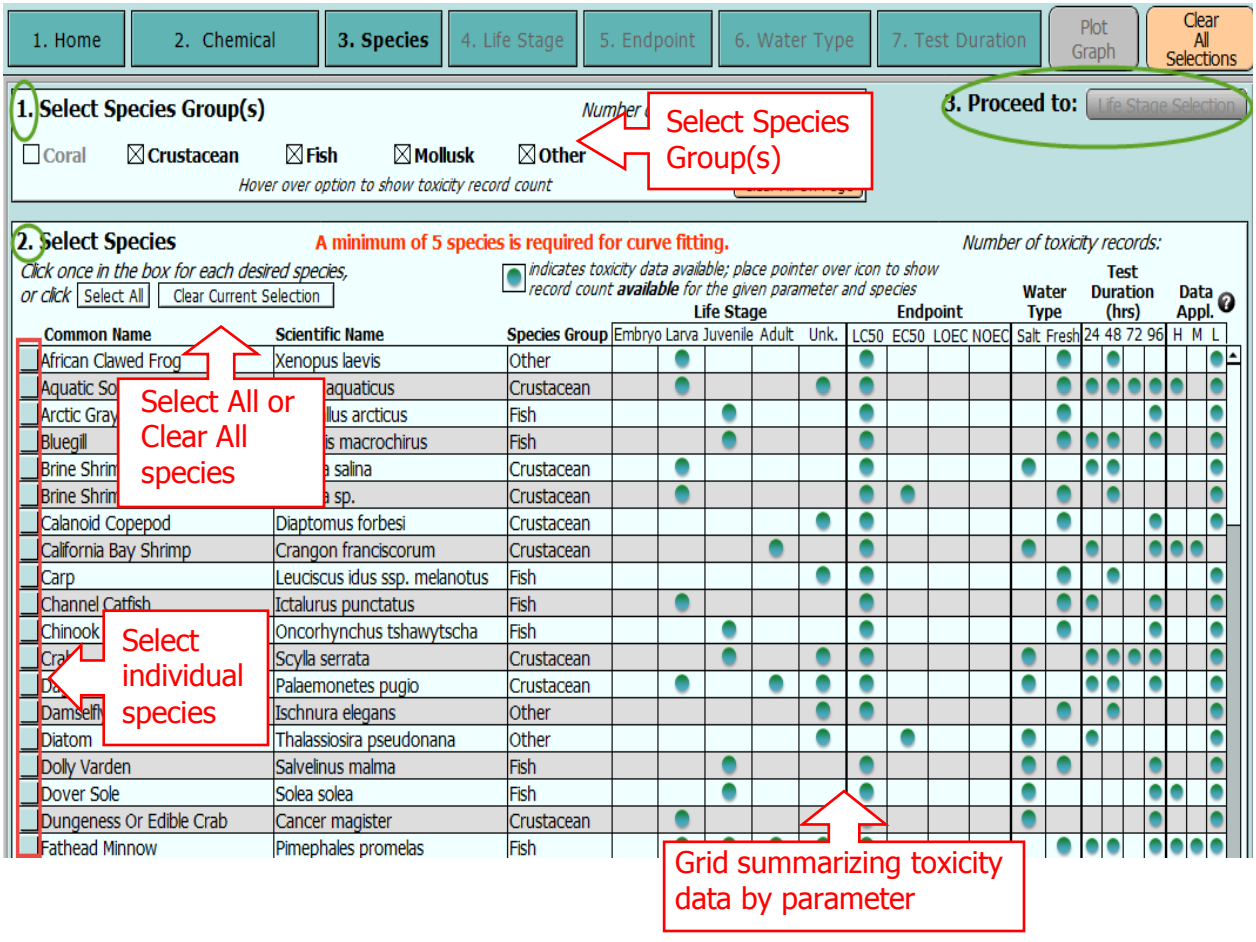
Also note that going back steps will clear all settings you have made, based on your previous selections.

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*.

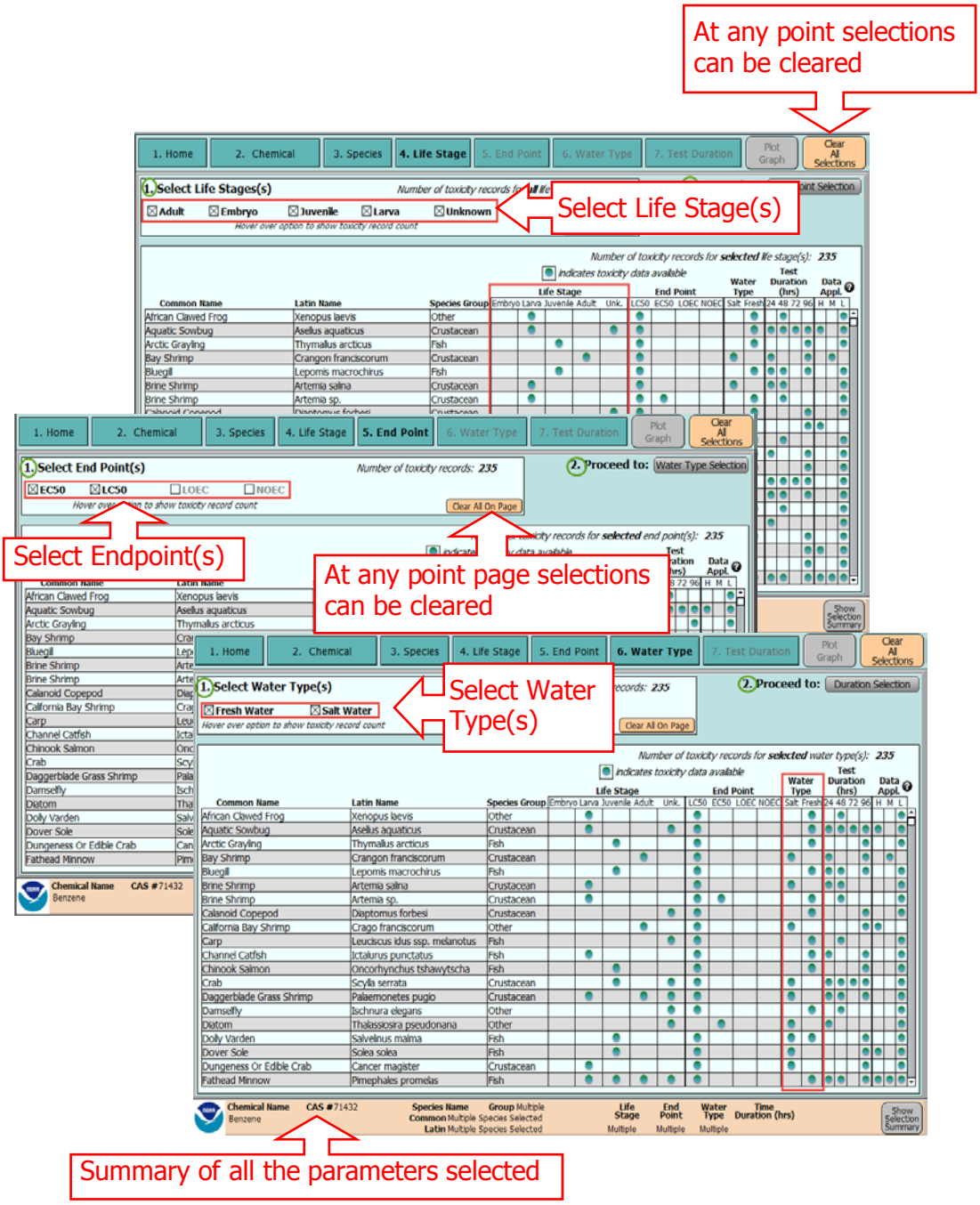
1. Select Species Groups to view which species in the selected groups are available.

2. Select all or individual species.

3. Click the button, Life Stage Selection, in the upper right to proceed to the next step.



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



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 ≥90% active ingredient purity

Moderate applicability

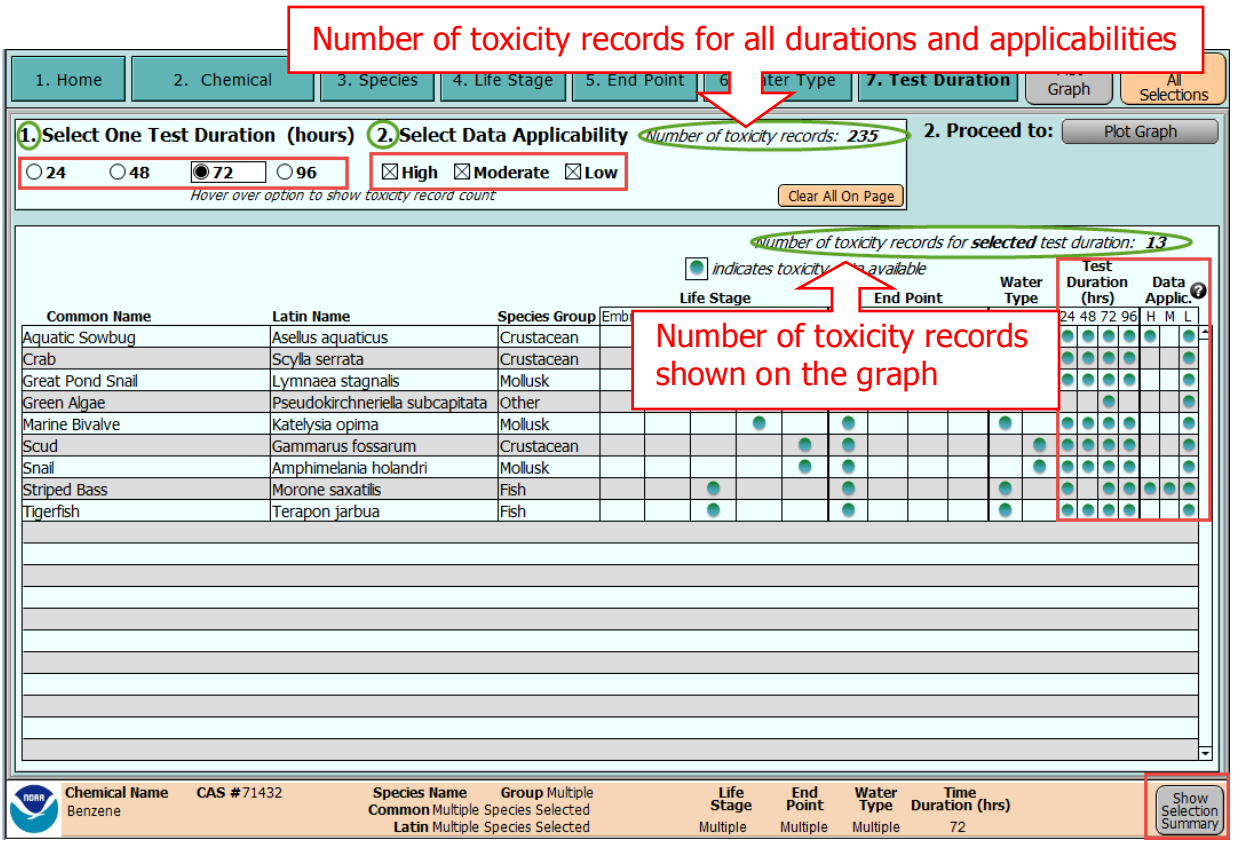
- Toxicity data with reported concentrations on the basis of measured concentrations (Test method: M)
- Toxicity data from laboratory setting performed under static or static renewal conditions (Exposure Type: S, R)
- Reported 75-<90% active ingredient purity

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.



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.

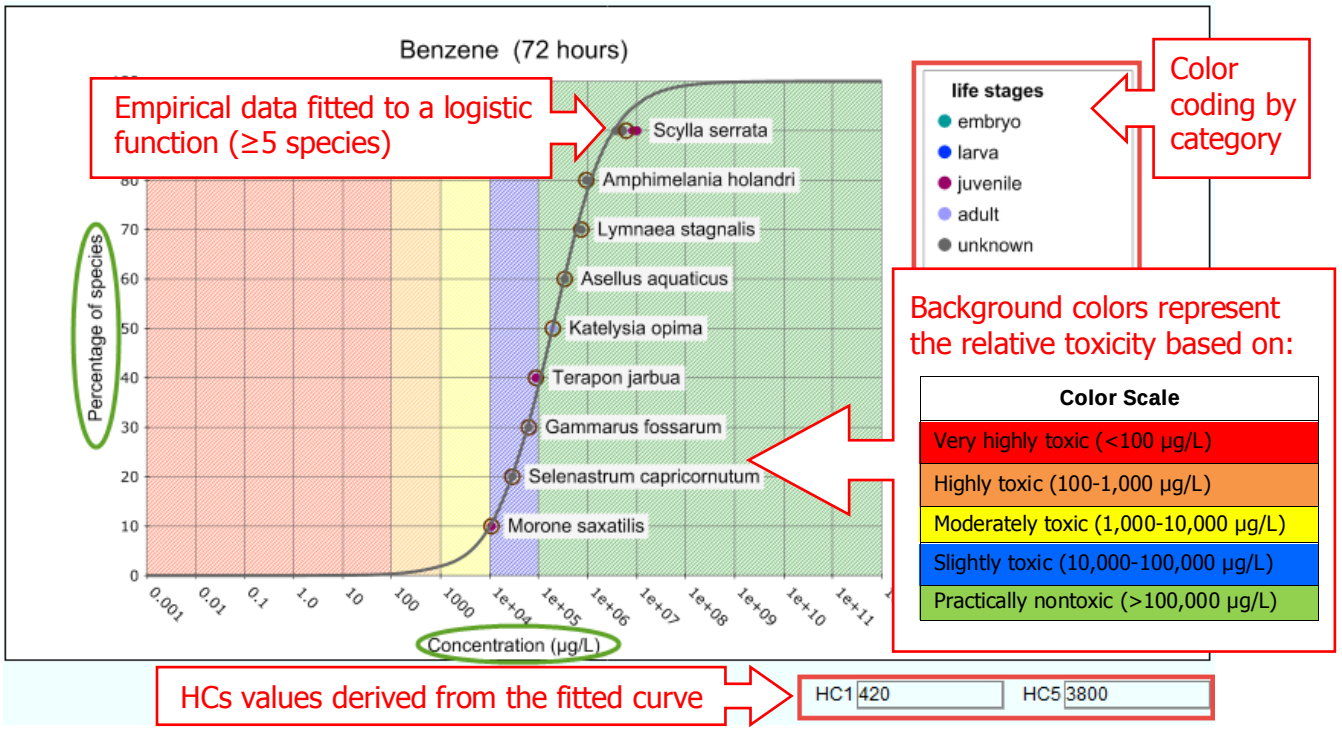
- The name of the chemical, oil or dispersant and the exposure duration (in parenthesis) are labeled as the title of the SSD
- The x-axis represents the concentration in µg/L (plotted on a log scale) required to adversely affect a unique species and the y-axis represents the percentage of species.
- 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[1] (HC1 and HC5, respectively; in µg/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.

[1] 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[2].
- All final query plots can be printed.

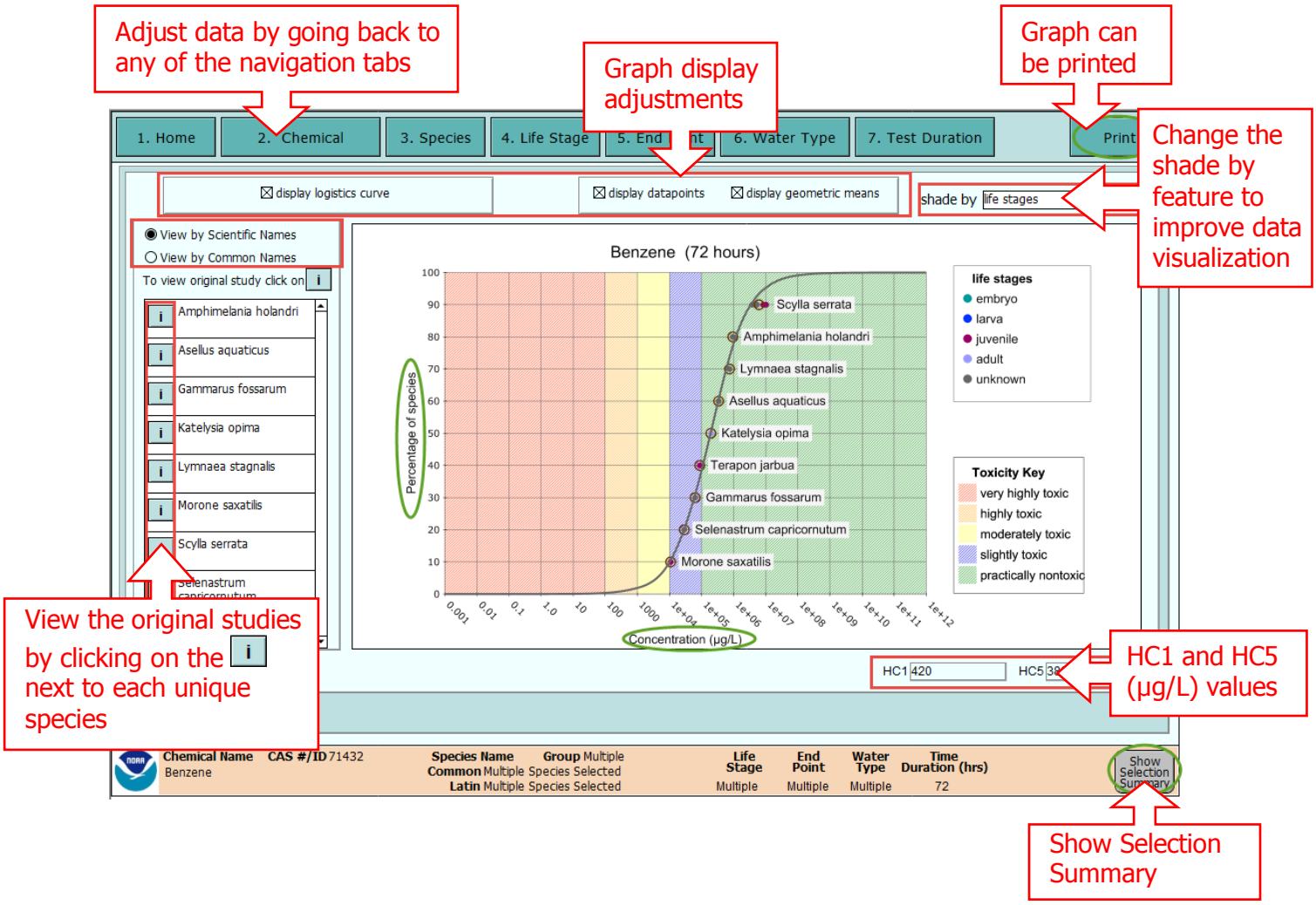
Data Limitations

- 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 indented 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.

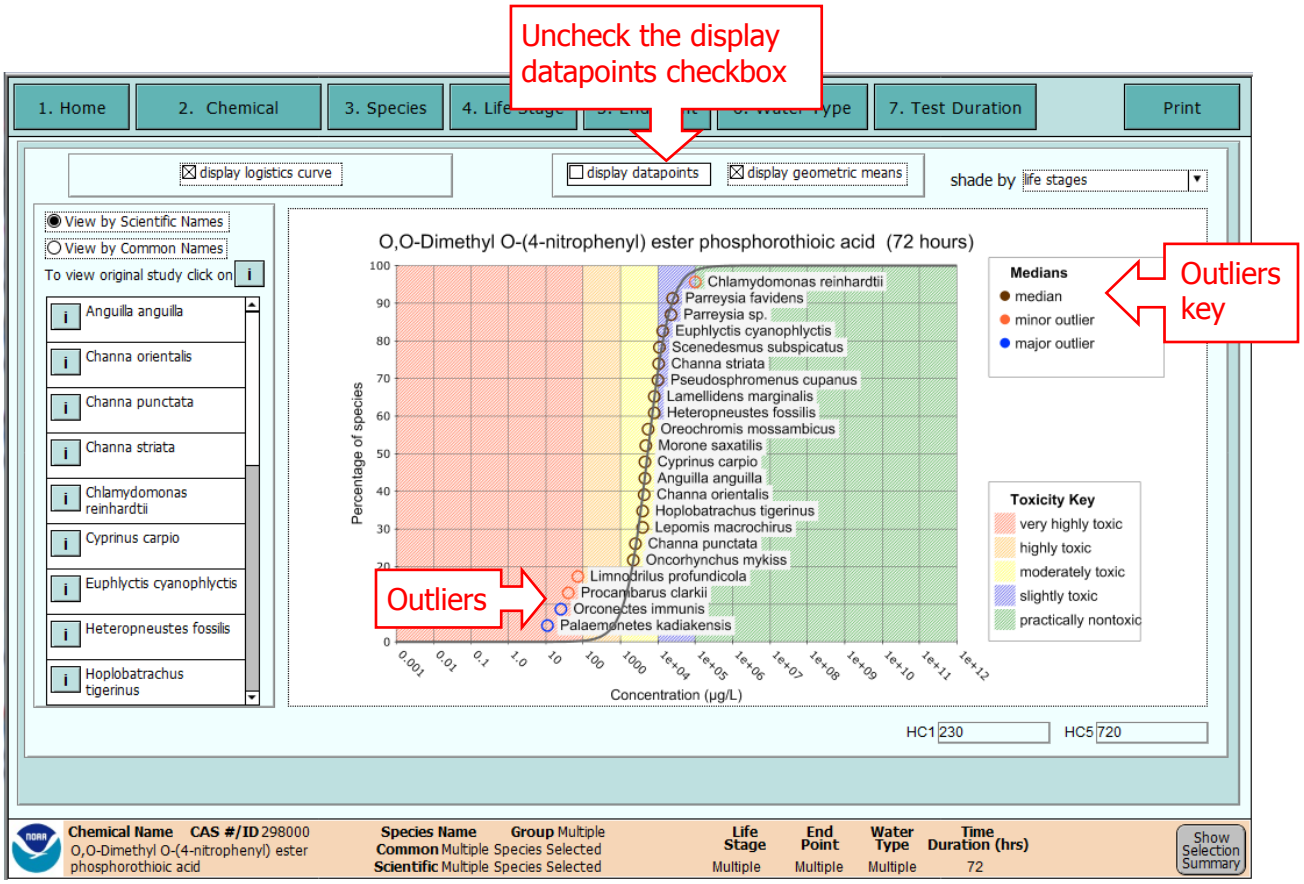


[2] Source: http://www.epa.gov/oppefed1/ecorisk_ders/toera_analysis_eco.htm#Ecotox

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.

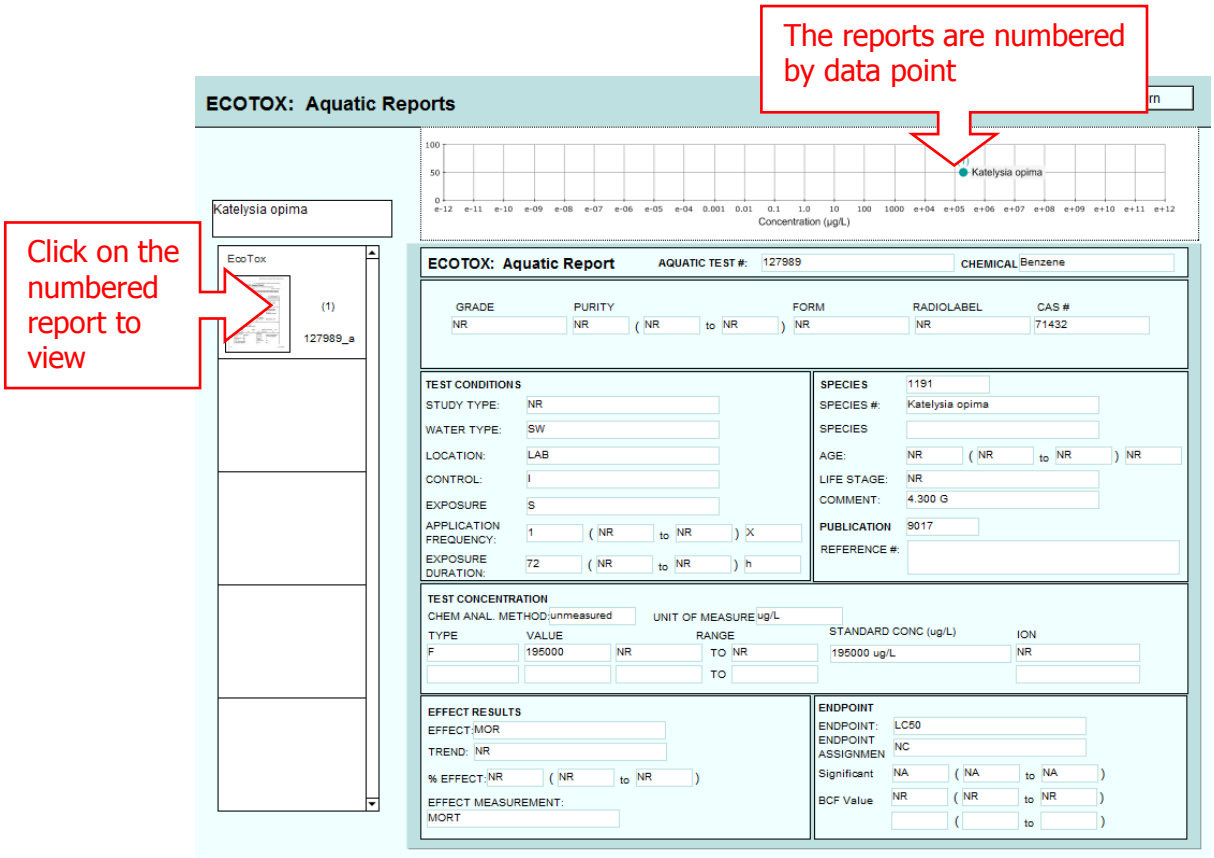


You can also shade by outliers. The logistics curves are computed using the geometric means. In certain cases, the curves were being skewed by outlier geometric means. The curves do not include these points in the computations, but the points are still displayed on the graph. When the user displays the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



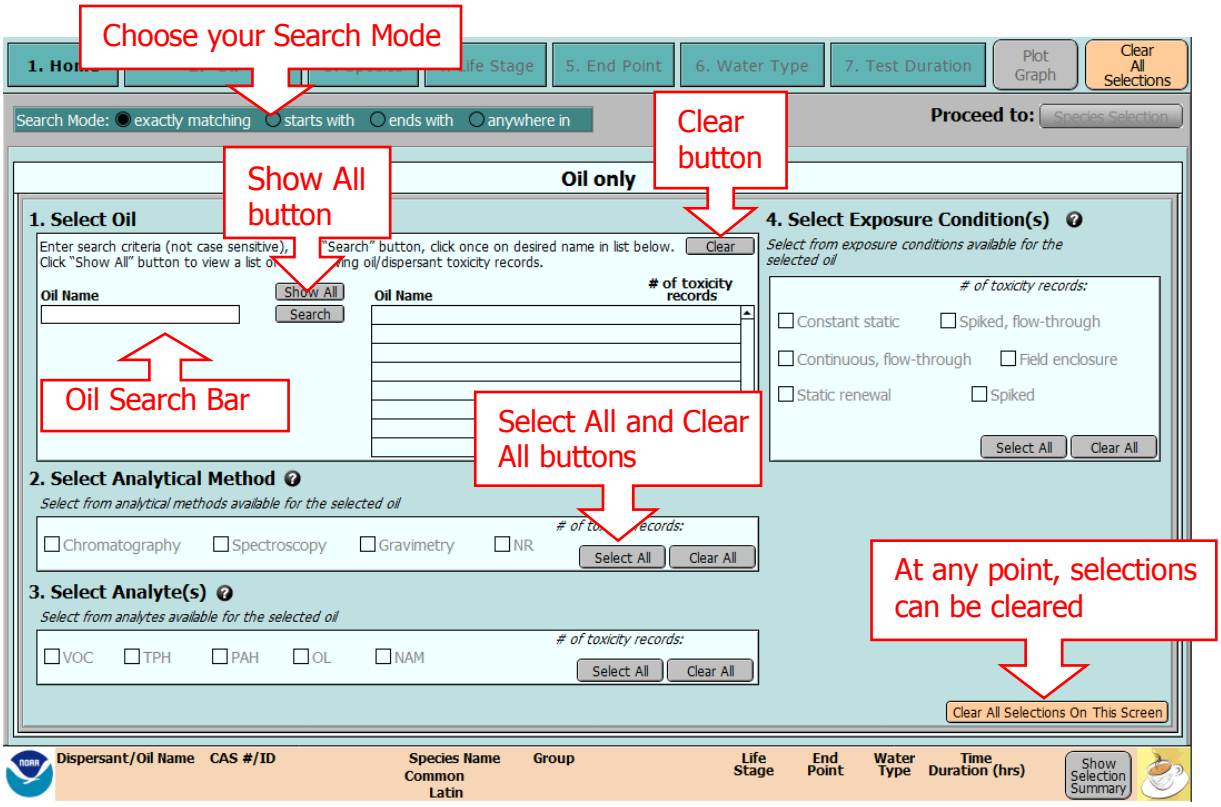
Each individual species plotted on the SSD has an associated report displaying important details from the original data source. Useful information includes chemical characteristics (e.g., grade, purity), test conditions (e.g., water type, exposure duration), species (e.g., scientific name, life stage 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.



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.

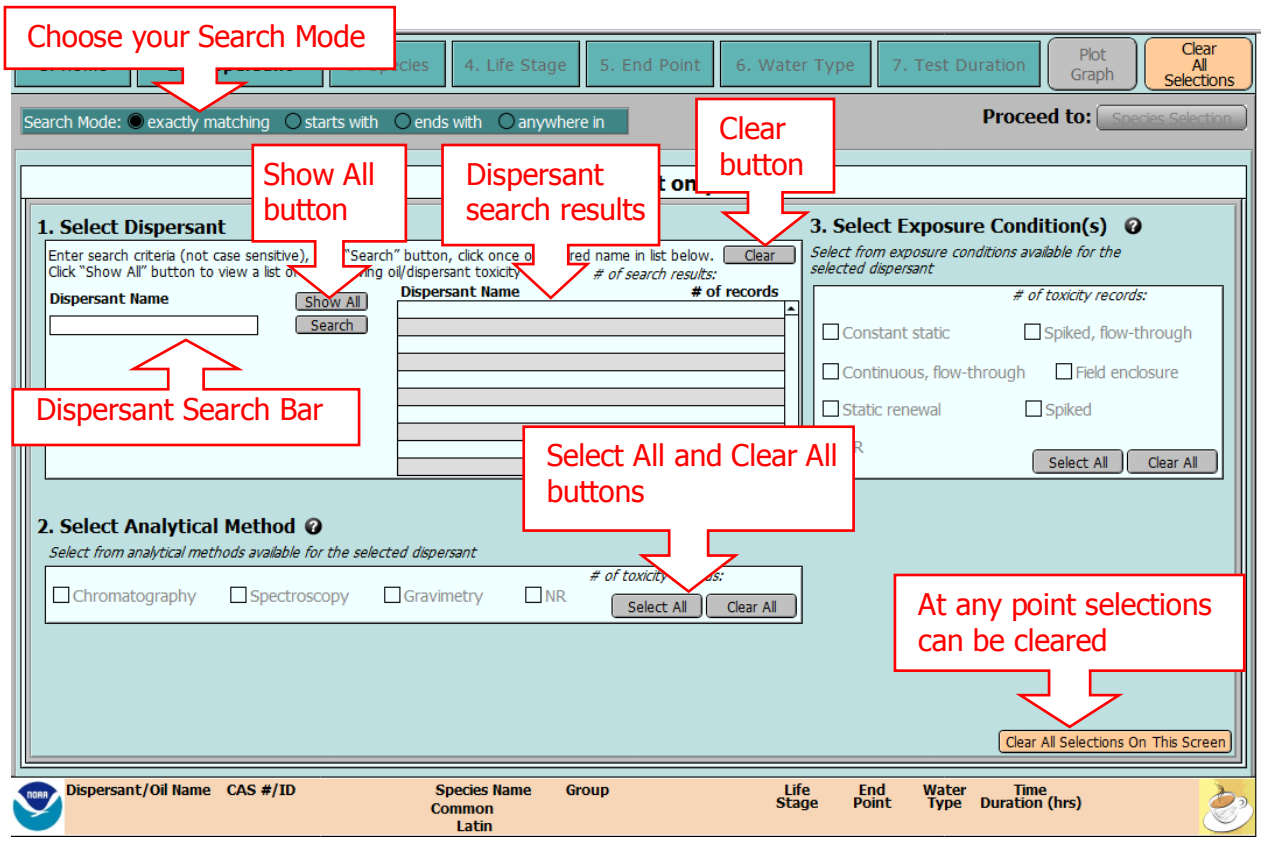
Analytical Method(s) – Select Analytical Method(s) used to quantify the oil. NR stands for Not Recorded.

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.



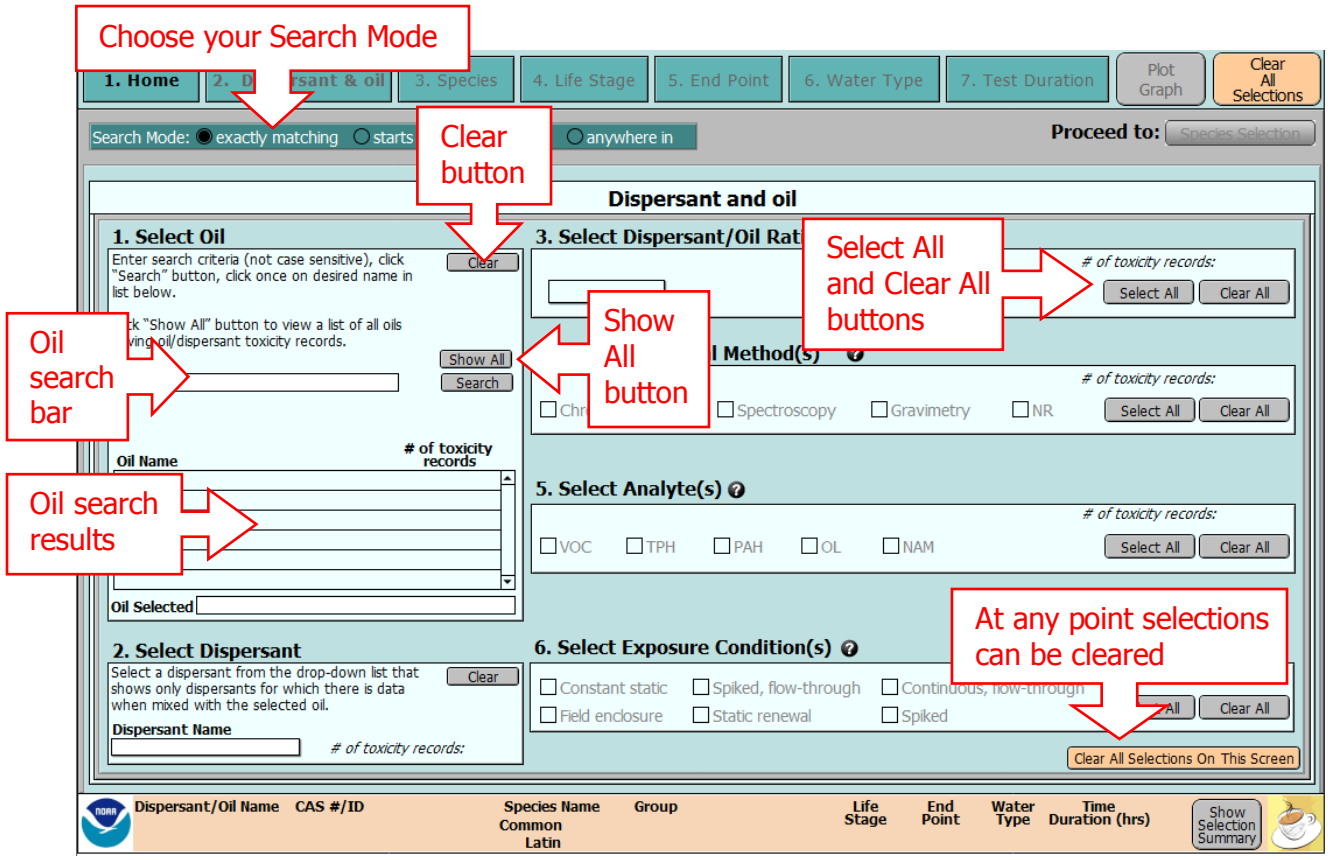
Dispersant – Search for the desired dispersant using the search bar. Click once on the desired name in the Search Results.

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).

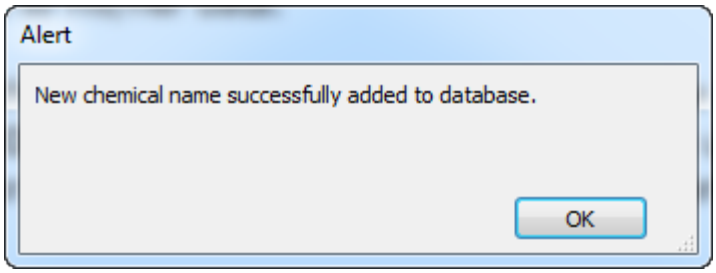
User-Added Data

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:

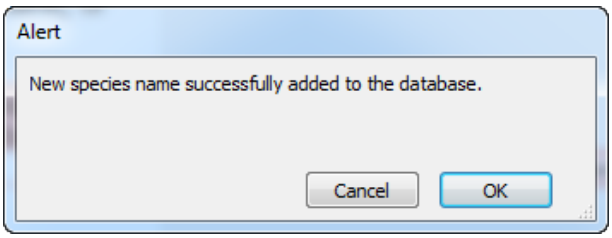


Your new chemical/dispersant/oil should also appear in the search results.

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.



Life Stage – Select Life Stage(s) (adult, embryo, juvenile, larva, or unknown) for which data are available.

Endpoint – Select Endpoint(s) (EC_{50}, LC_{50}, LOEC, or NOEC).

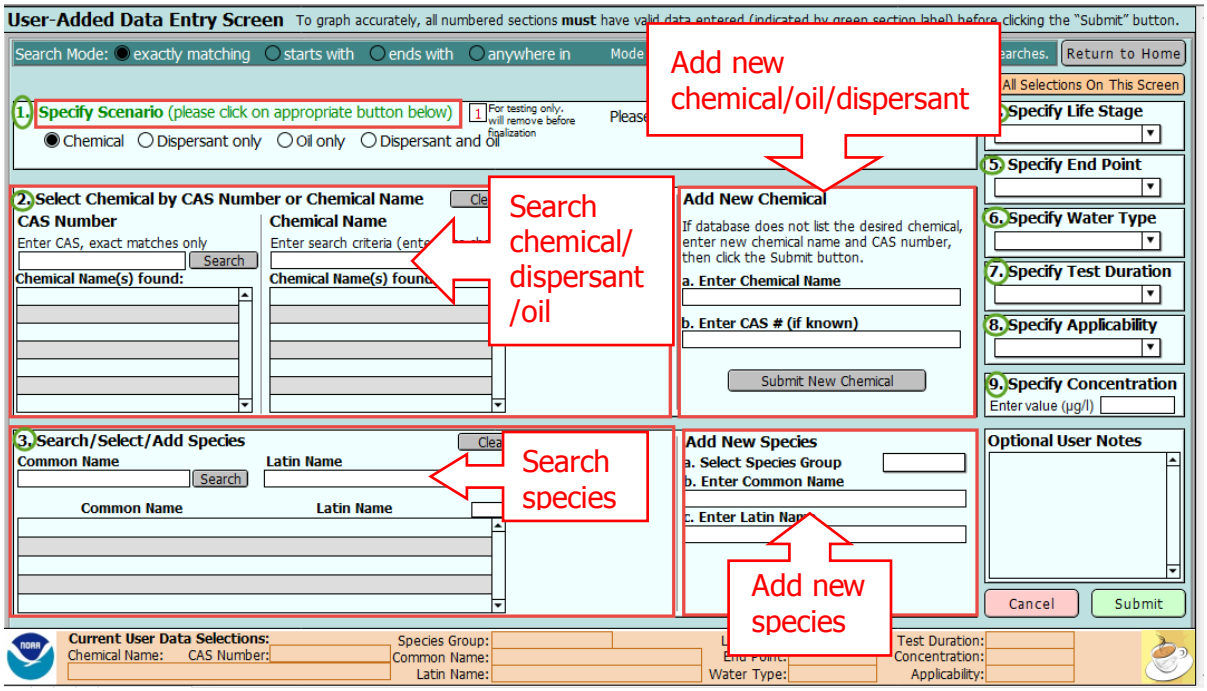
Water Type – Select Water Type(s) (fresh water or salt water).

Test Duration – Select a Test Duration (24, 48, 72, or 96 hours)

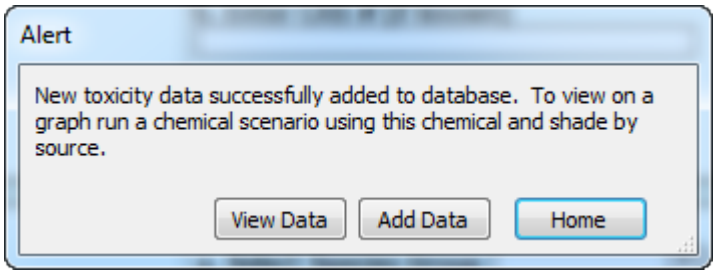
Applicability – Specify Applicability score(s) (high, moderate, or low), based on relevance of these data to spill response. See the CAFE User's Manual for criteria.

Concentration – Specify Concentration (µg/l). Enter the concentration in the space provided.

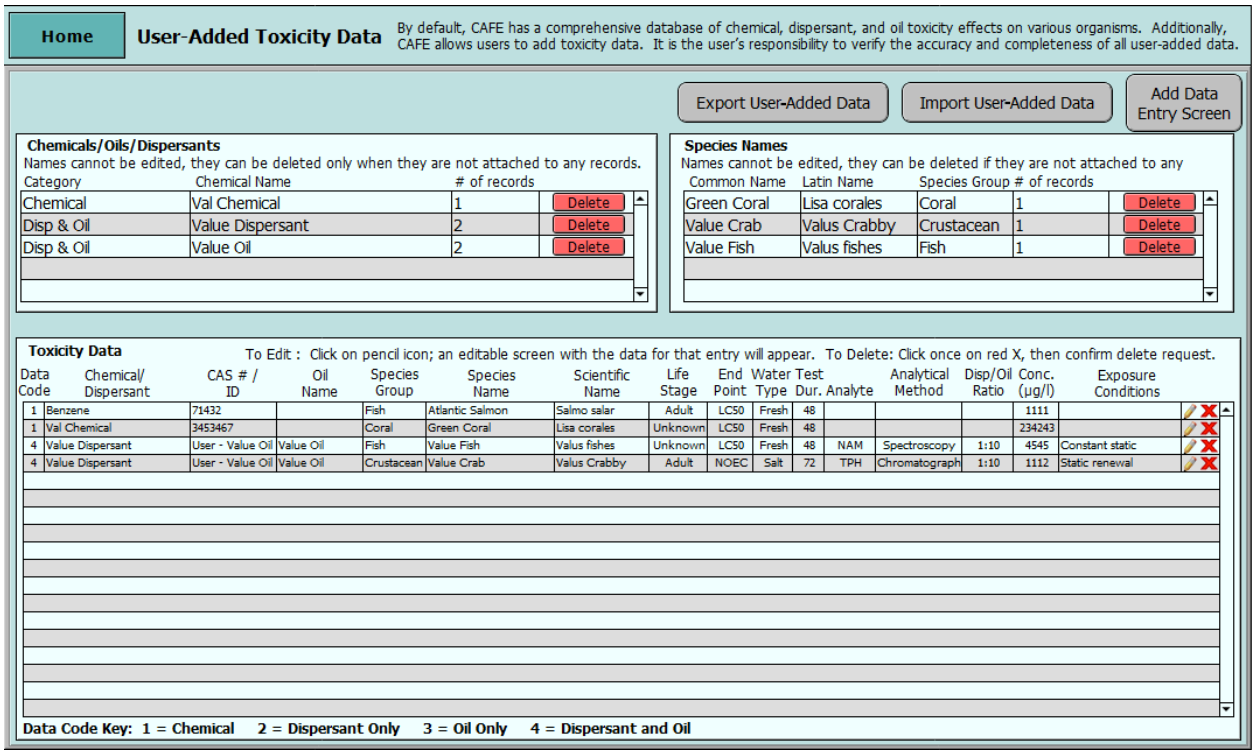
Others – Depending on the scenario you've chosen, specify Analytical Method, Analytes, Dispersant/Oil Ratio, or Exposure Condition(s) on their various dropdown menus and spaces provided.



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.



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

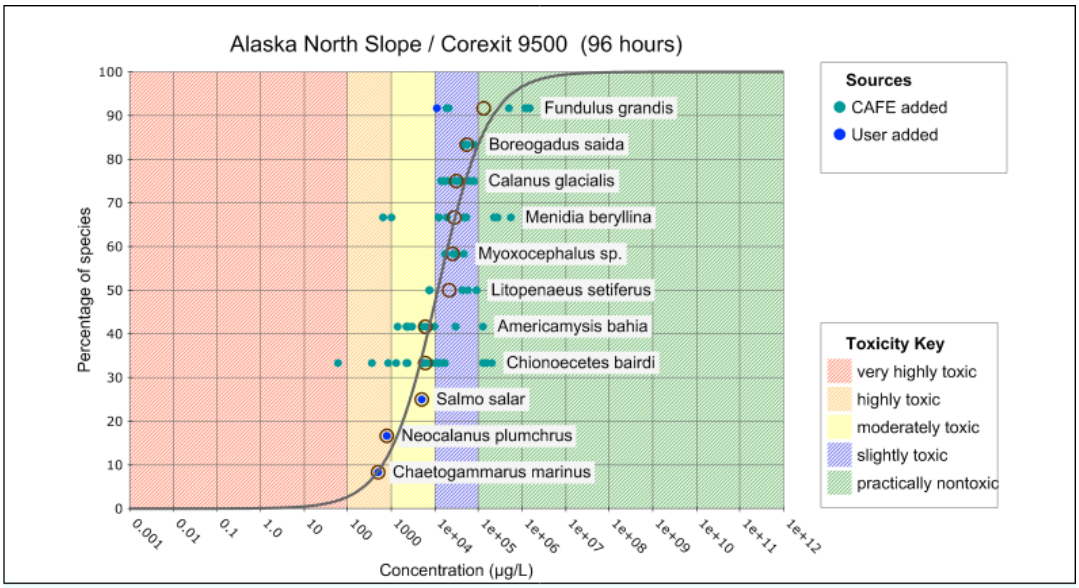
- These chemicals/oils/dispersants and species names can only be deleted when they do not have a complete record associated with them (e.g., a concentration, life stage, etc.). Otherwise, you would have to delete your individual record associated with the new chemical/oil/dispersant. The number of records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

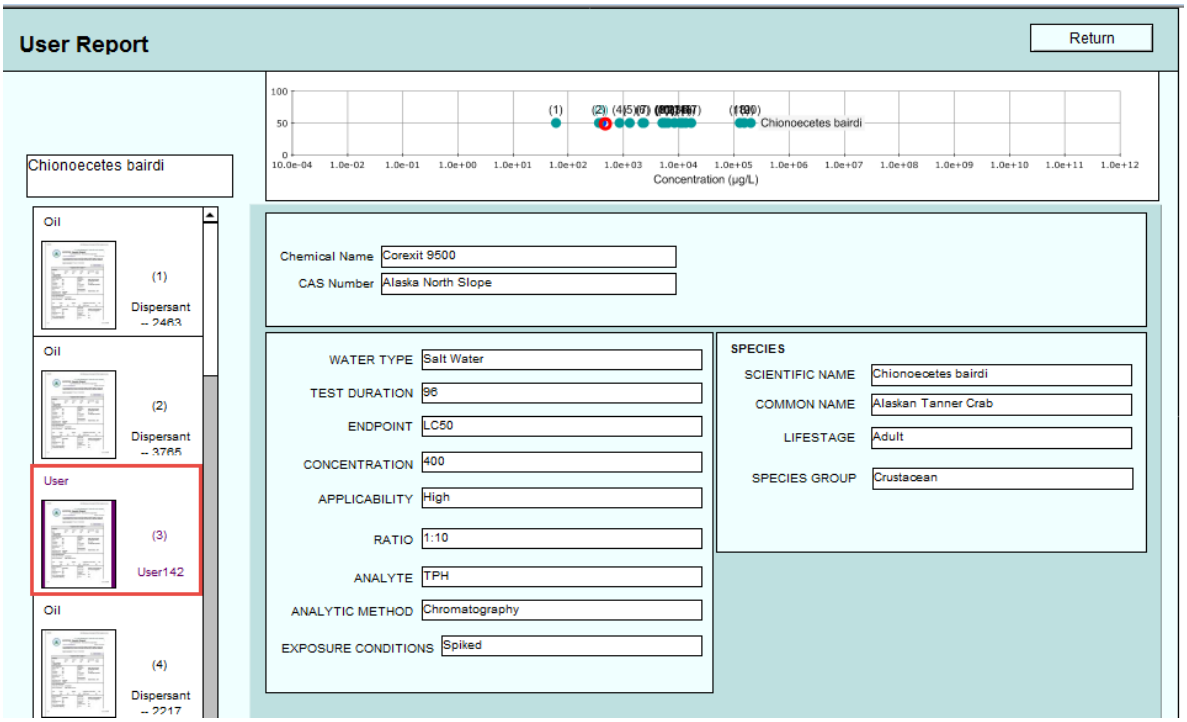
- Click on the pencil icon to edit a record.
- Click on the red X button to delete a record.
- Some toxicity parameters don't apply to a given scenario. For example, a chemical record would not have the following toxicity parameters: Analyte, Analytical Method, Dispersant, Oil Name, or Exposure Conditions.

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

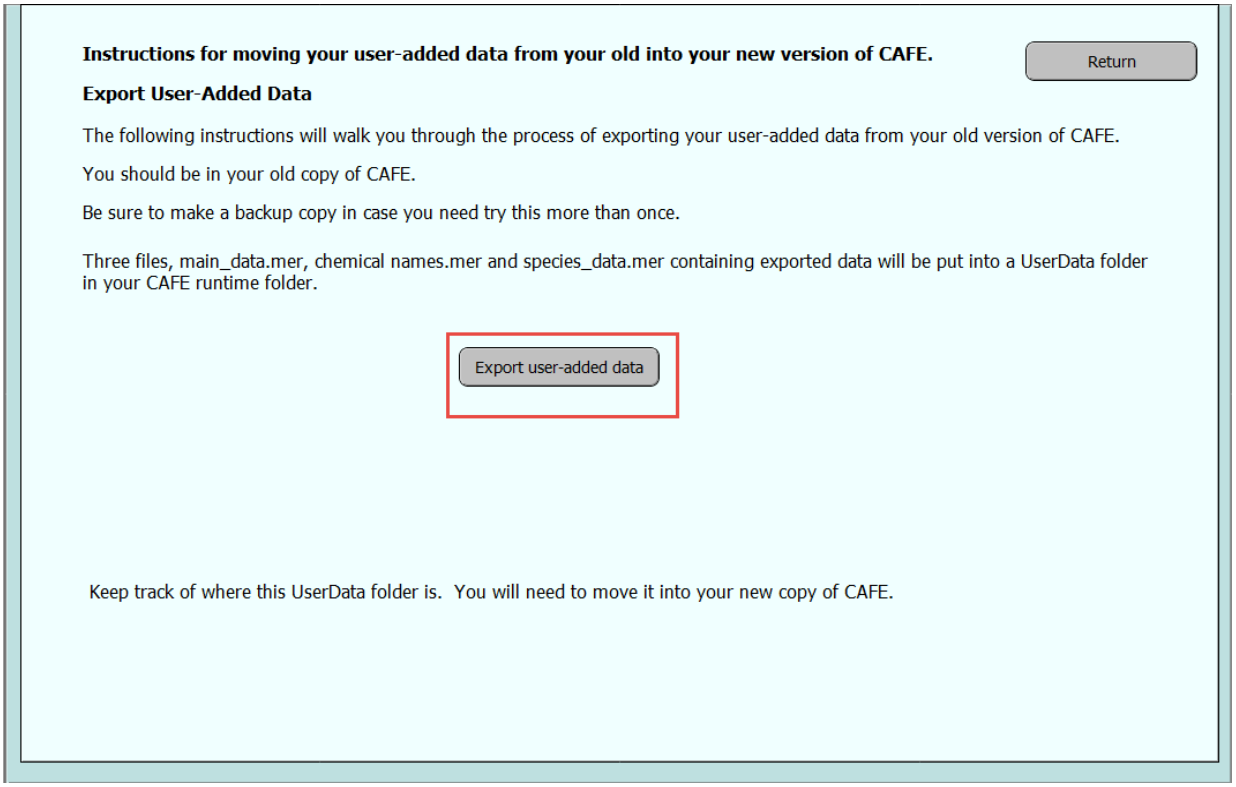
User-Added Data Import and Export

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

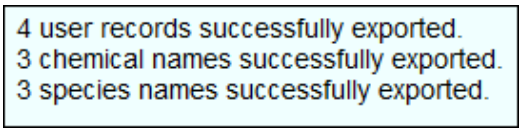
NOTE: You will not be able to import or export your user-added data from CAFE version 1.1. You will only be able to import and export your user-added data with version 1.2. or later.

Export User-Added Data

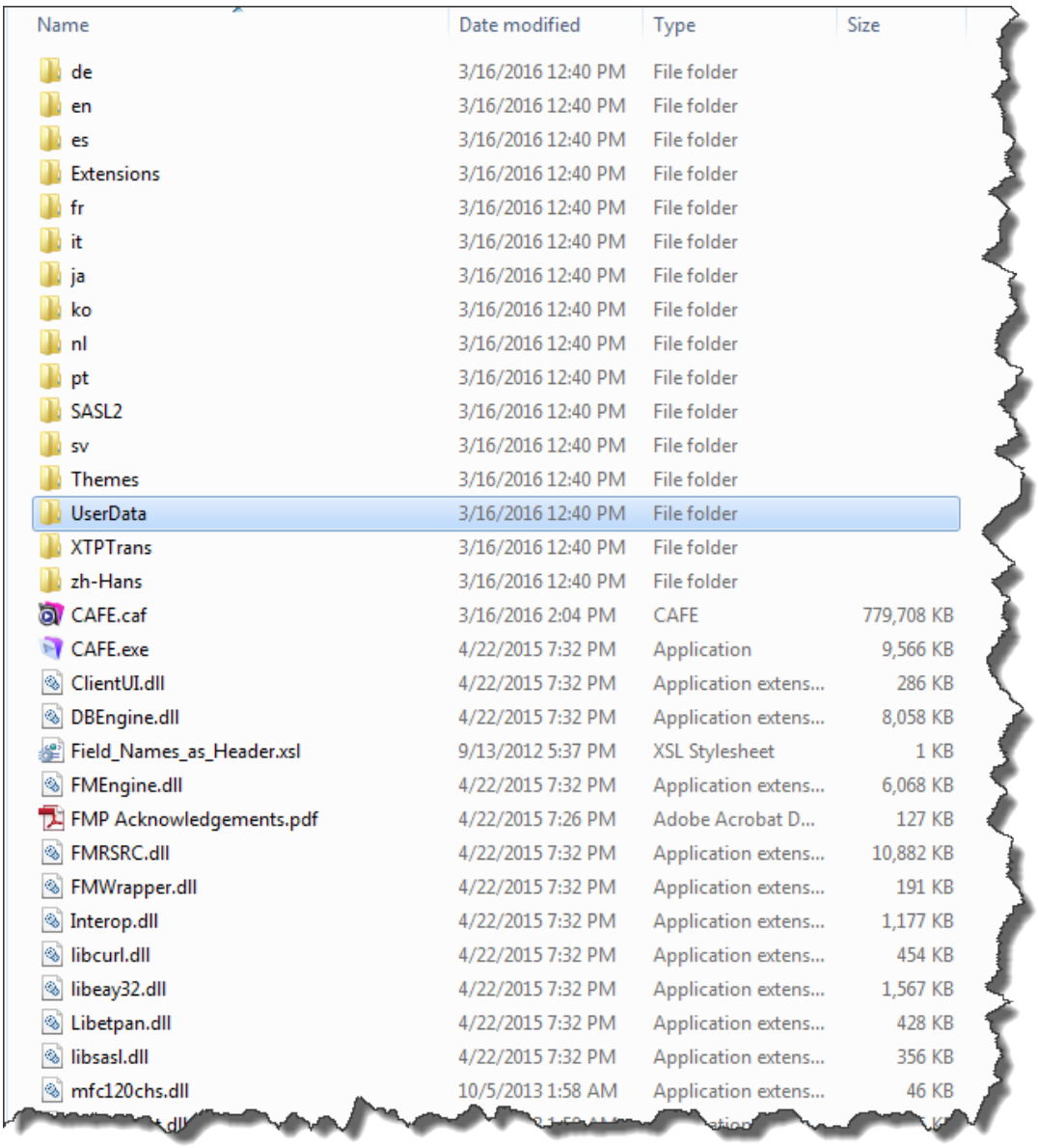
To export user-added data, first make a backup copy of CAFE. Then click the button below.



The export is confirmed with summary text



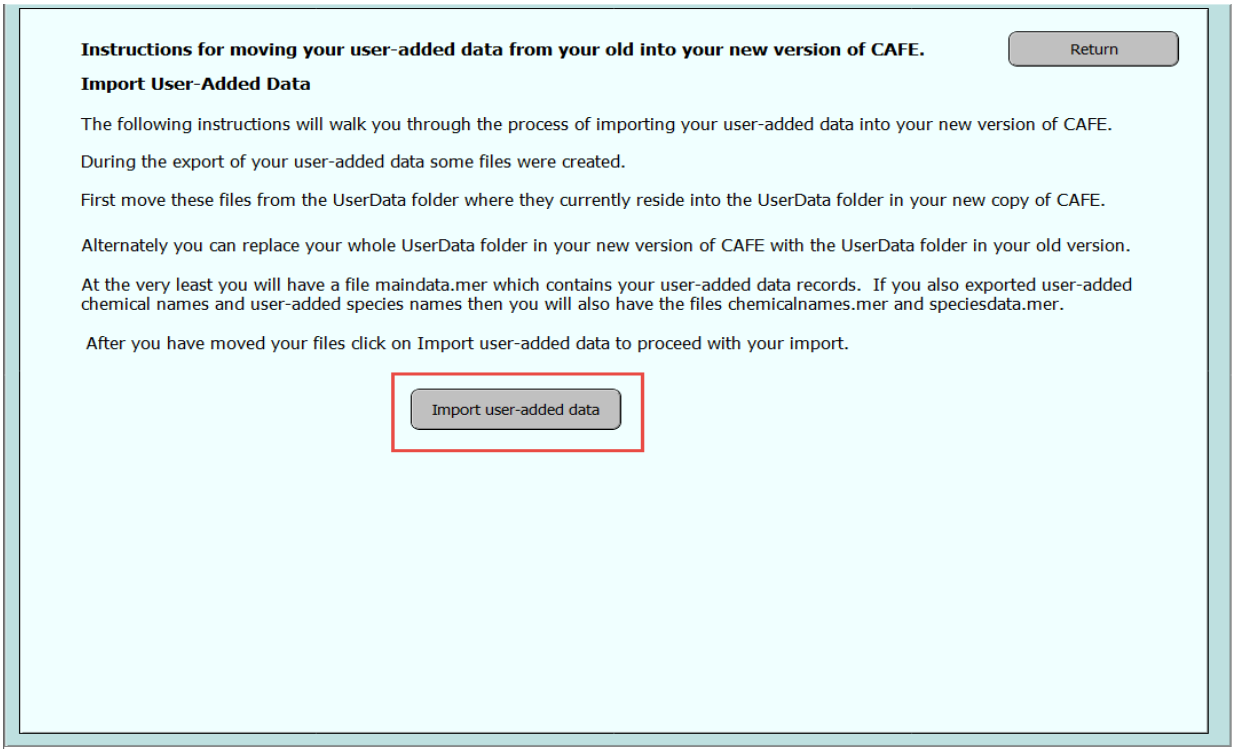
Three files are created with your export: main_data.mer, chemical_names.mer and species_data.mer containing the exported data. These files are placed in a folder called UserData in your CAFE folder. Make sure you make copy of your UserData folder. It contains the three files you need. Keep track of where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



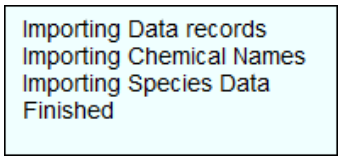
Import User-Added Data

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

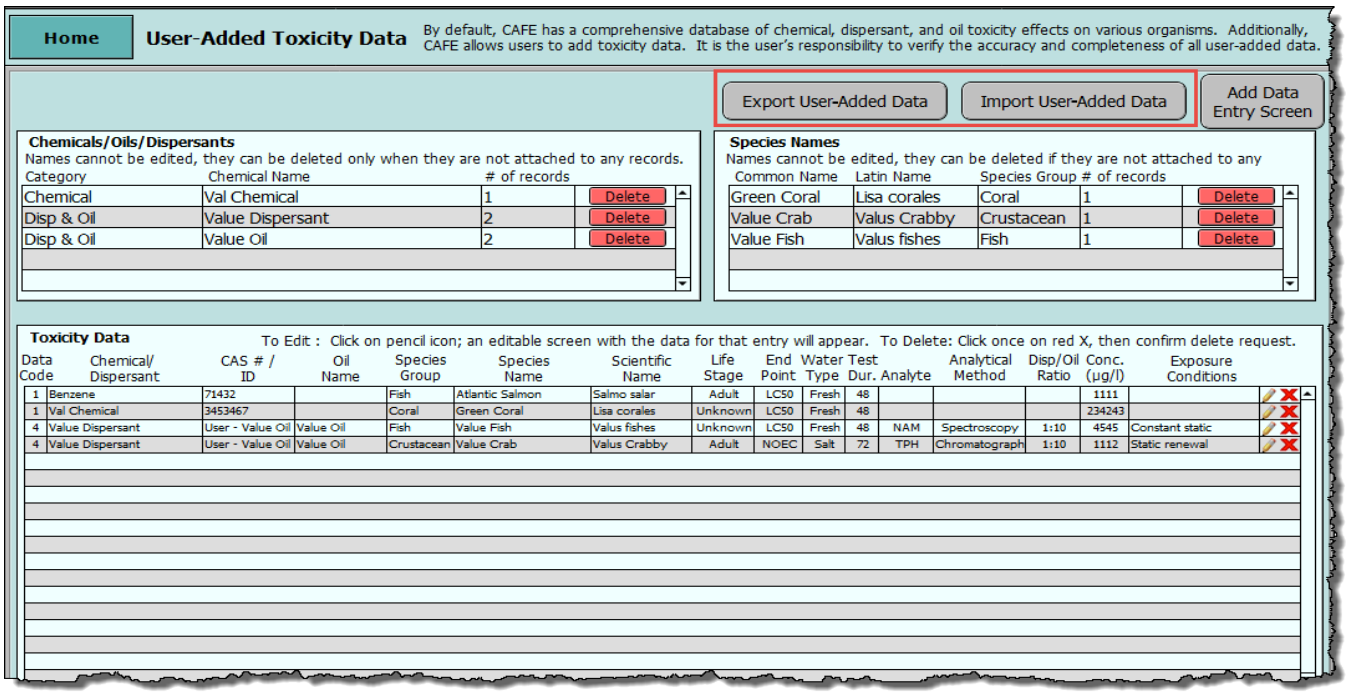
Once you have completed those steps, open your new copy of CAFE. Click the View User-Added Toxicity Data button then click the Import User-Added Data button.



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



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

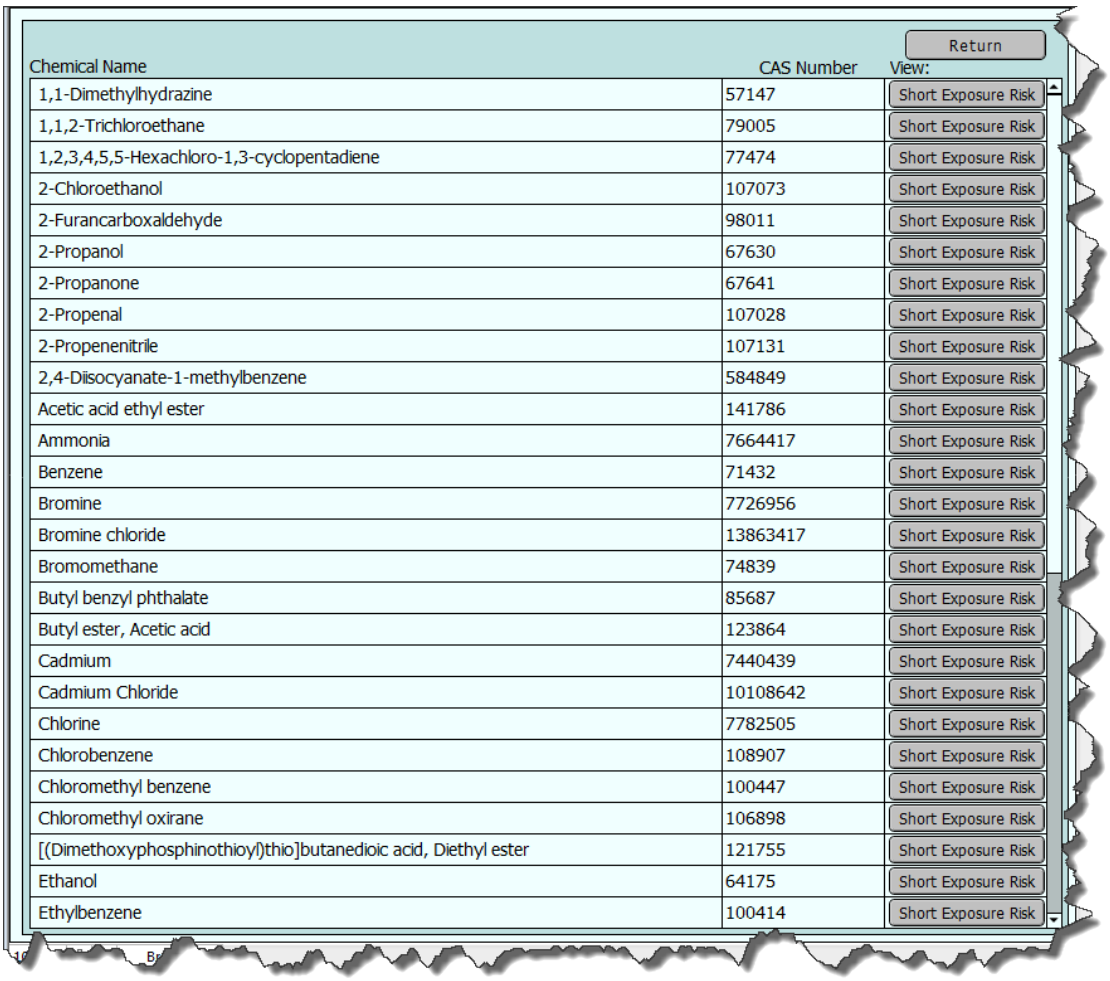


Short Exposure Risk Reports

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_{50} or EC_{50}) 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.



Return

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

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_{50} and EC_{50}) 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

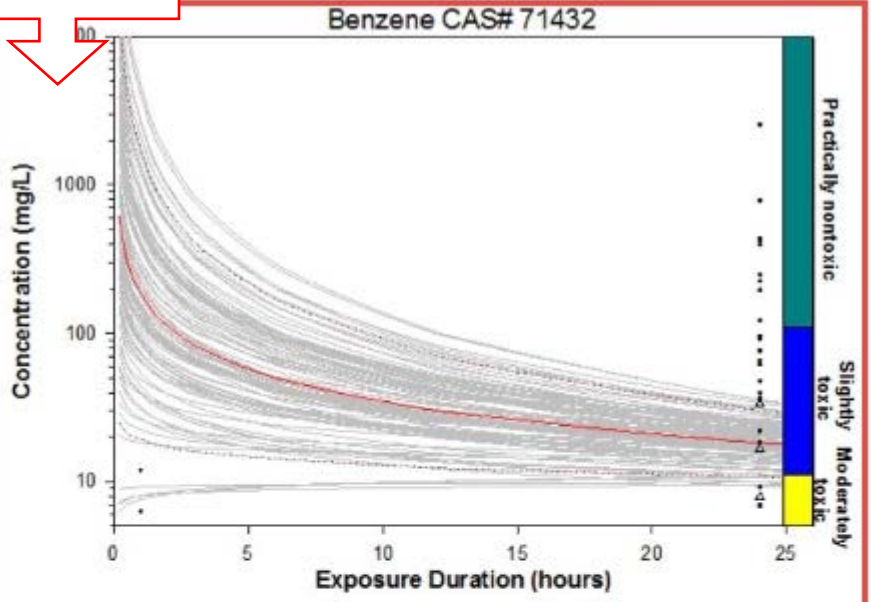
Evaluation of fish and crustacean aquatic toxicity data from CAFE (empirical) for benzene. Only curve with ≥5 species are shown. * Kolmogorov-Smirnov test only.

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: 5th 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_{50} and EC_{50} data; therefore, these represent estimated LC_{50}|EC_{50} 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.

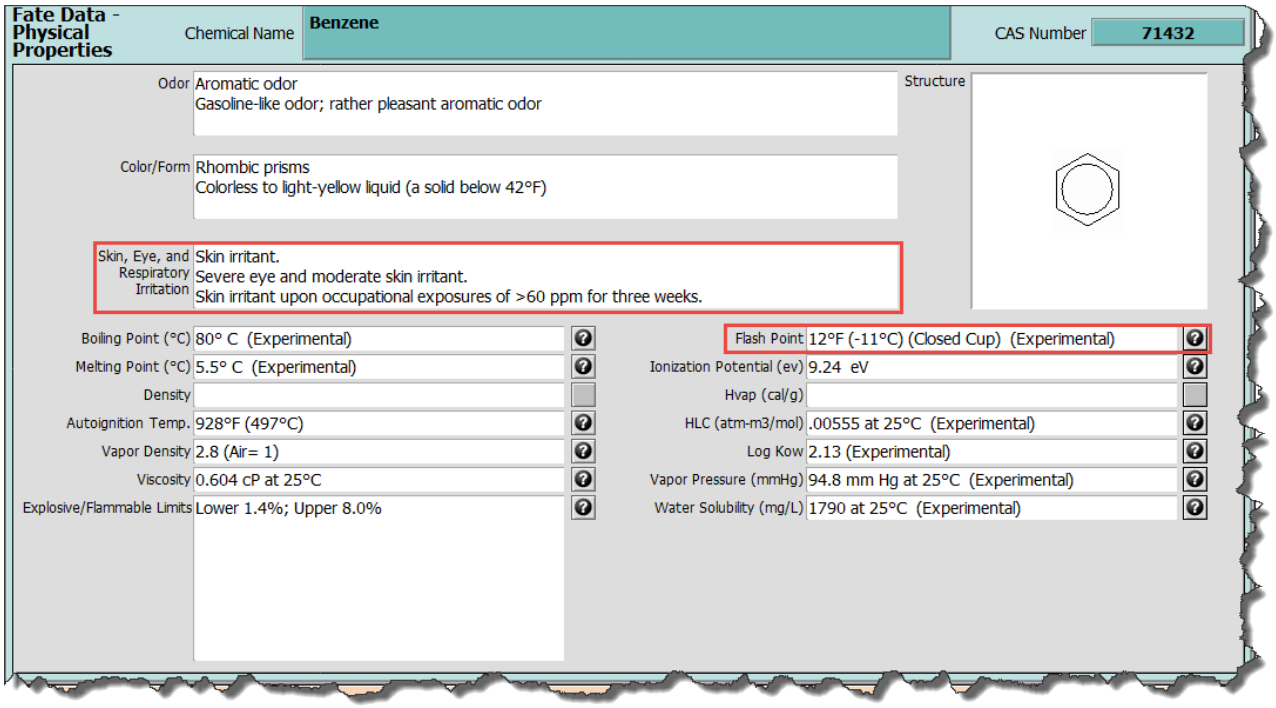
Review the following scenarios to help you use outputs from CAFE:

Scenario 1: Benzene (CAS No. 71432)

Incident Occurrence: Benzene Release, Parachute Creek, Colorado

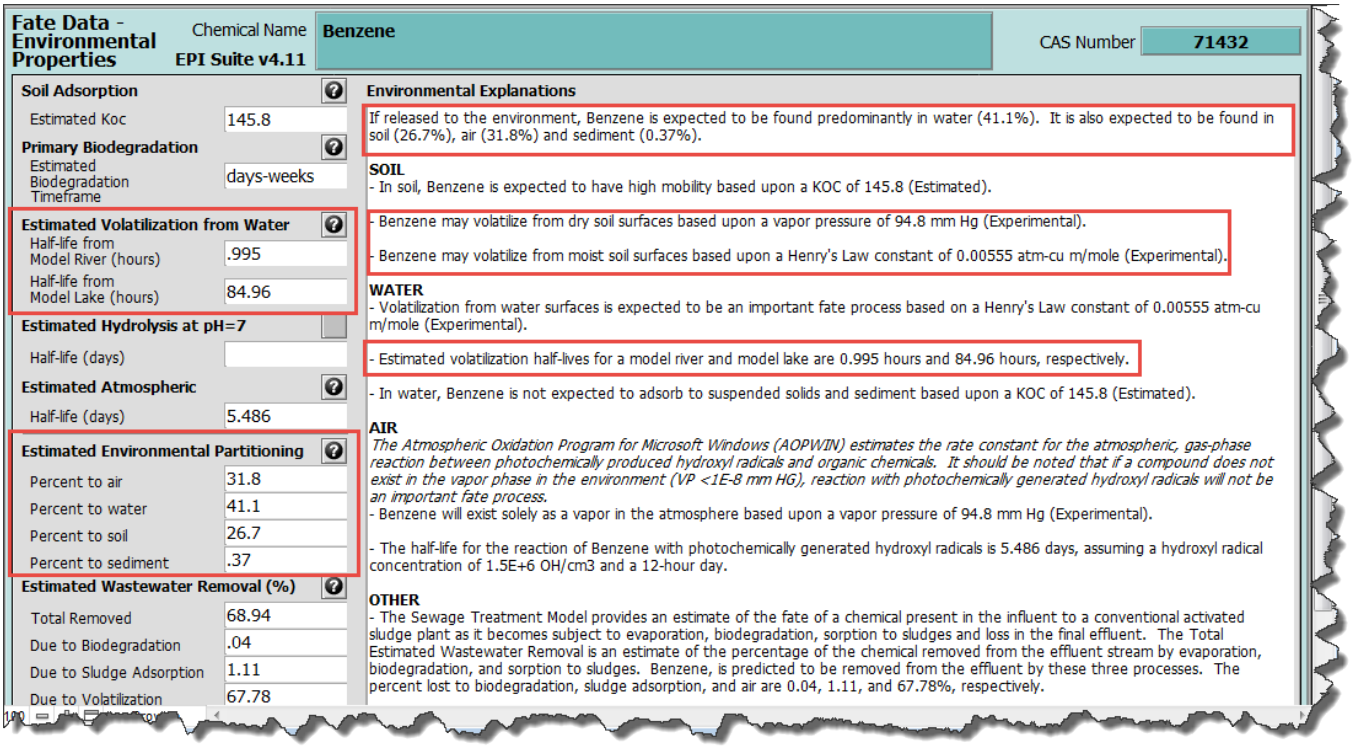
A fracking boom for fracked natural gas processor, Williams Energy, spilled an estimated 241 barrels of benzene (CAS No. 71432) into the ground, some of which eventually washed into Parachute Creek. Those responding to this incident would be seeking estimates for fate and effects of benzene.

Question 1: What are the hazards of the chemical?



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**

Soil Adsorption	
Estimated Koc	145.8
Primary Biodegradation	
Estimated Biodegradation Timeframe	days-weeks
Estimated Volatilization from Water	
Half-life from Model River (hours)	.995
Half-life from 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	31.8
Percent to water	41.1
Percent to soil	26.7
Percent to sediment	.37
Estimated Wastewater Removal (%)	
Total Removed	68.94
Due to Biodegradation	.04
Due to Sludge Adsorption	1.11
Due to Volatilization	67.78

Environmental Explanations

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%).

SOIL
- In soil, Benzene is expected to have high mobility based upon a KOC of 145.8 (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 0.00555 atm-cu m/mole (Experimental).

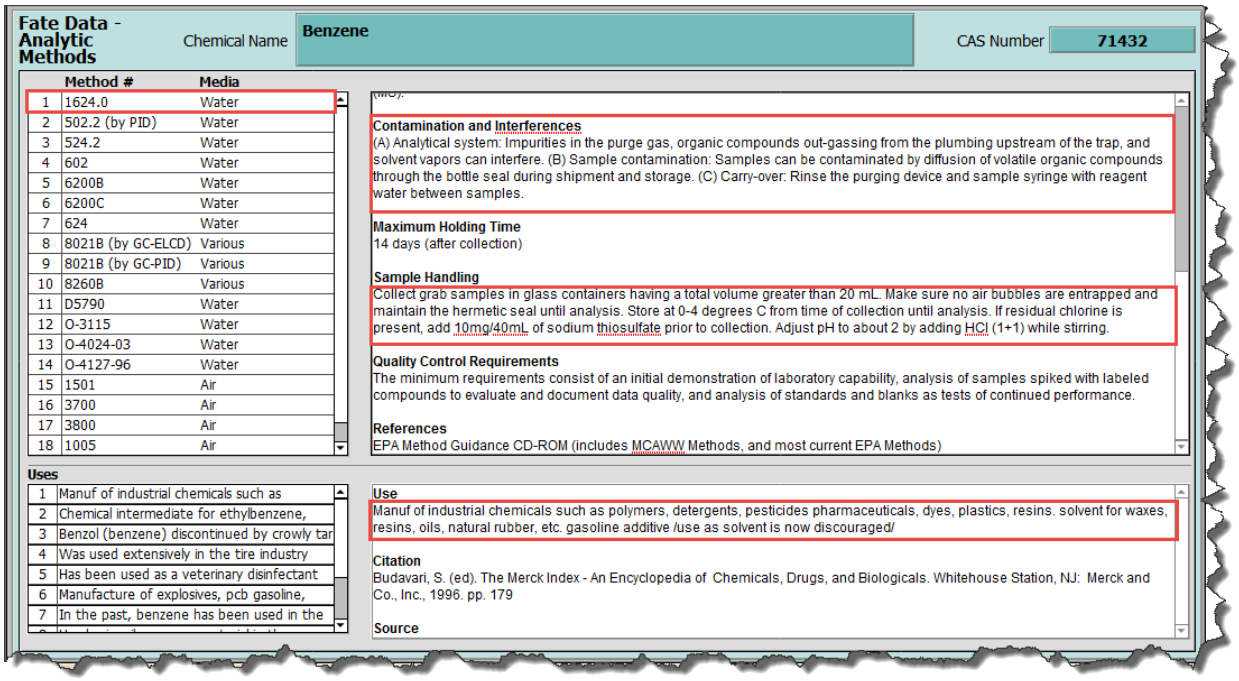
WATER
- Volatilization from water surfaces is expected to be an important fate process based on a Henry's Law constant of 0.00555 atm-cu m/mole (Experimental).
- Estimated volatilization half-lives for a model river and model lake are 0.995 hours and 84.96 hours, respectively.
- In water, Benzene is not expected to adsorb to suspended solids and sediment based upon a KOC of 145.8 (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.
- 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.

OTHER
- 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.

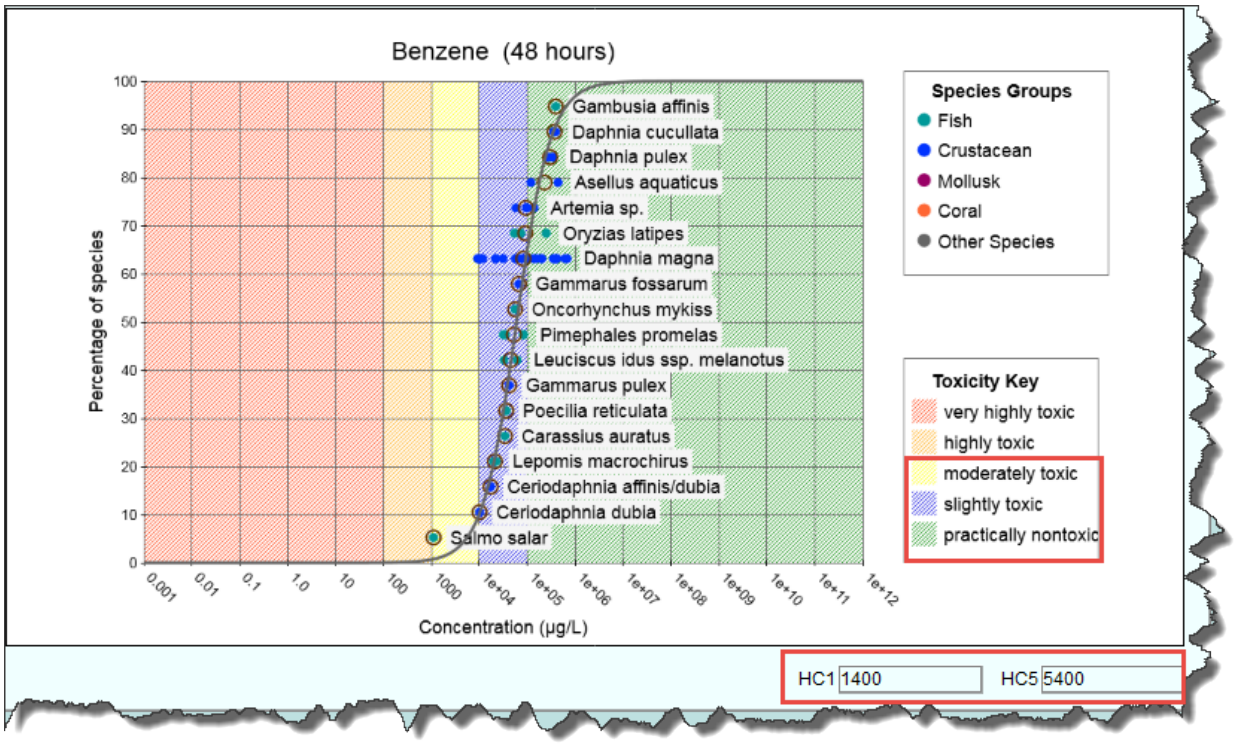
Answer: With a relatively high Henry's Law Constant (0.00555 atm-m^3/mol) and vapor pressure (94.8 mm Hg), benzene is moderately soluble in water and will volatilize easily. Estimated Environmental Partitioning by the fugacity model predicts that if released into the environment, benzene is expected 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 volatize at 0.995 and 84.96 hours, respectively.

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



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?



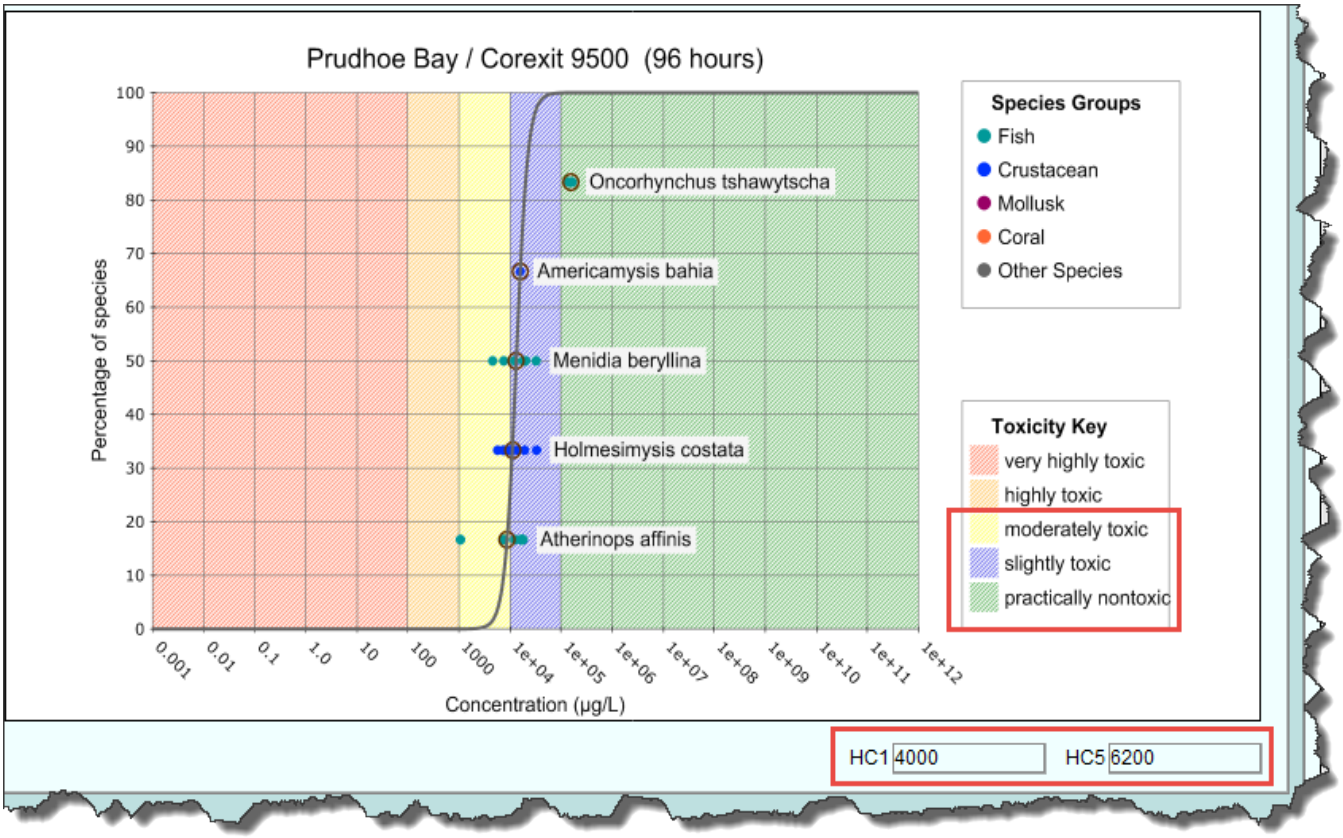
Answer: In an acute 48-hour exposure, benzene is moderately toxic to practically nontoxic to freshwater fish and crustaceans. The hazard concentrations indicate a HC5 protective value of 7,700 µg/L or 7.7 mg/L (7.7 ppm).

Scenario 2: Alaska North Slope Crude and Corexit 9500

Incident Occurrence: Oil Spill, Prince William Sound, Alaska

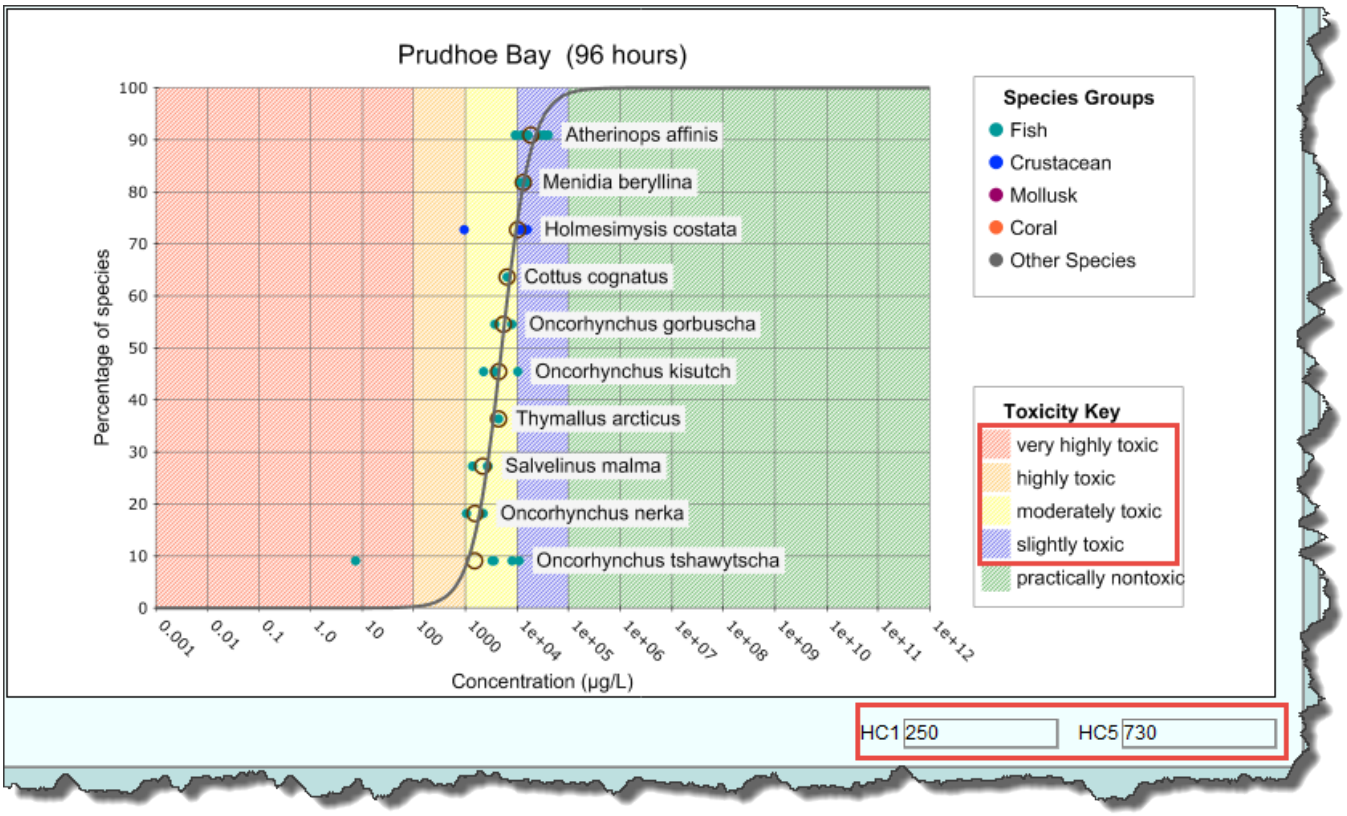
A barge collided near shore, spilling about 1,000 gallons of Prudhoe Bay crude in Prudhoe Bay, Alaska. Corexit 9500 was applied at the spill site at a 1:10 dispersant and oil ratio. The analytical methods used were chromatography. The analytes measured were TPHs and PAHs. Prudhoe Bay is a major fishing 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?



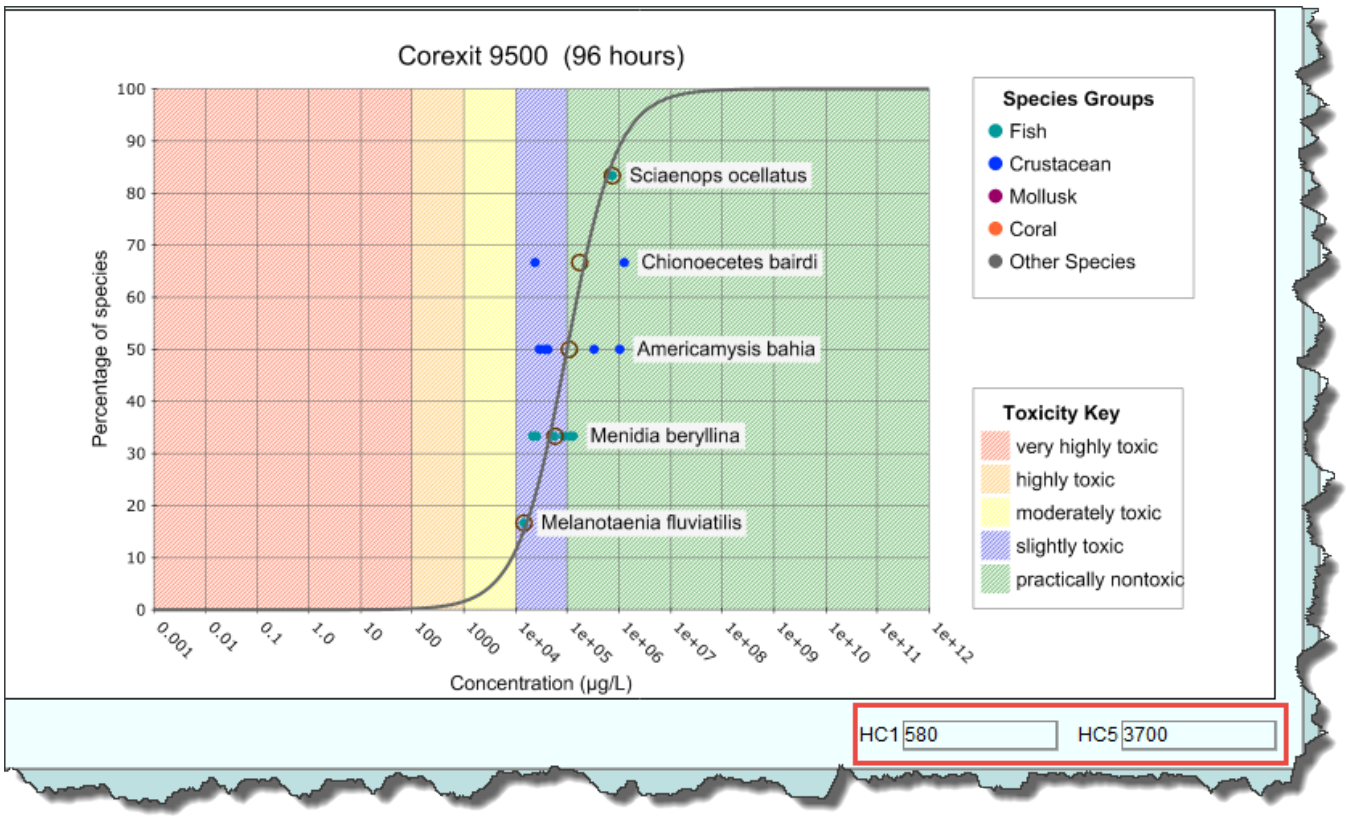
Answer: In an acute 96-hour exposure, Prudhoe Bay crude and Corexit 9500 together are moderately toxic to practically nontoxic to fish and crustaceans. The hazard concentrations indicate a HC5 protective value of 6,200 µg/L or 6.2 mg/L (6.2ppm).

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?



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).

U.S. DEPARTMENT OF COMMERCE
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Secretary, U.S. Department of Commerce

Dr. Kathryn D. Sullivan
Under Secretary of Commerce for Oceans & Atmosphere and
NOAA Administrator

Dr. W. Russell Callender
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May 2016