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

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Emergency Response Division
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.

### Environmental Fate Data

<table>
<thead>
<tr>
<th>Chemical Name</th>
<th>Benzenes</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Structure</strong></td>
<td><img src="image" alt="Structure" /></td>
</tr>
<tr>
<td><strong>Hazard of searched chemical</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Physical Properties Data</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Environmental Fate Data</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Environmental Explanations</strong></td>
<td></td>
</tr>
</tbody>
</table>

#### Environmental Explanations

- **Environmental Fate**

  If released to the environment, Benzenes is expected to be found predominantly in water (48.1%). It is also expected to be found in soil (14.1%), air (13.6%) and sediments (2.2%).

  **SOIL**

  - In soil, Benzenes are expected to have moderate mobility based on a KOC of 165.5 (estimated).
  - Benzenes may volatilize from dry soil surfaces based on a vapor pressure of 94.8 mm Hg (estimated).
  - Benzenes may volatilize from most soil surfaces based on a Henry’s Law constant of 0.0155 atm·m³/mol (estimated).

  **WATER**

  - Benzenes may volatilize slowly from water surfaces, with an important rate process based on a Henry’s Law constant of 0.0155 atm·m³/mol (estimated).
  - Estimated volatilization half-lives for a model river and model lake are 1 hour and 84.06 hours, respectively.

  - In water, Benzenes are not expected to adsorb to suspended solids and sediments based on a KOC of 165.5 (estimated).

  **Half-life**

  - Estimated half-life for Benzenes in soil is 165.5 days.
  - Estimated half-life for Benzenes in water is 84.96 days.
  - Estimated half-life for Benzenes in sediments is 1 hour and 40.66 hours, respectively.

  **Environmental Explanations**

  - The Aqueous Hydrolysis Rate Program (HYDROK) estimates aqueous hydrolysis rate constants for only certain chemical classes.
  - Estimation may be based on activity coefficients, solubilities, molecular weights, and selected alcohols.
  - HYDROK estimates acid and base-catalyzed rate constants; it does not estimate neutral hydrolysis rate constants.

  **HYDROK**

  - HYDROK was unable to estimate a hydrolysis half-life for Benzenes because the chemical may be stable with respect to hydrolysis. However, the inability of HYDROK to estimate a hydrolysis half-life does not necessarily mean that Benzenes is hydrolytically stable.
  - Benzenes 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 Benzenes with photochemically generated hydroxyl radicals is 5.46 days, assuming a hydroxyl radical concentration of 1.566×10⁶ OH (μg/mL) and a 12-hour day.

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6
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.

- **Select Life Stage(s)**
- **Select Endpoint(s)**
- **Select Water Type(s)**

At any point selections can be cleared.

Summary of all the parameters selected.
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\(^1\) (HC\(_1\) and HC\(_5\), 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.
- HC\(_1\) and HC\(_5\) 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 HC\(_5\) selected here was chosen because this is the most commonly used percentile, while a lower percentile (HC\(_1\)) 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.
• All final query plots can be printed.

Data Limitations

• This version of CAFÉ 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 CAFÉ 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 CAFÉ.
• The current version of CAFÉ 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.

2 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.
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 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:

![Alert]

New chemical name successfully added to database.

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.

![Graph showing toxicity data and shading by sources](image)

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

```
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.
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 (LC50 or EC50) 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:


⚠️ Users are highly encouraged to print the short exposure risk reports.
<table>
<thead>
<tr>
<th>Chemical Name</th>
<th>CAS Number</th>
<th>Voc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,1-Dimethylhydrazine</td>
<td>57147</td>
<td></td>
</tr>
<tr>
<td>1,1,2-Trichloroethane</td>
<td>79005</td>
<td></td>
</tr>
<tr>
<td>1,2,3,4,5,5-Hexachloro-1,2-cyclopentadiene</td>
<td>77474</td>
<td></td>
</tr>
<tr>
<td>2-Chloroethanol</td>
<td>107073</td>
<td></td>
</tr>
<tr>
<td>2-Furancarboxaldehyde</td>
<td>98011</td>
<td></td>
</tr>
<tr>
<td>2-Propanol</td>
<td>67630</td>
<td></td>
</tr>
<tr>
<td>2-Propanone</td>
<td>67641</td>
<td></td>
</tr>
<tr>
<td>2-Propanol</td>
<td>67641</td>
<td></td>
</tr>
<tr>
<td>2-Propanol</td>
<td>107028</td>
<td></td>
</tr>
<tr>
<td>2-Propanol</td>
<td>107131</td>
<td></td>
</tr>
<tr>
<td>2,4-Disocyanato-1-methylbenzene</td>
<td>584849</td>
<td></td>
</tr>
<tr>
<td>Acetic acid ethyl ester</td>
<td>141786</td>
<td></td>
</tr>
<tr>
<td>Ammonia</td>
<td>7664417</td>
<td></td>
</tr>
<tr>
<td>Benzene</td>
<td>71432</td>
<td></td>
</tr>
<tr>
<td>Bromine</td>
<td>7726555</td>
<td></td>
</tr>
<tr>
<td>Bromine chloride</td>
<td>13863417</td>
<td></td>
</tr>
<tr>
<td>Bromomethane</td>
<td>74839</td>
<td></td>
</tr>
<tr>
<td>Butyl benzyl phthalate</td>
<td>85687</td>
<td></td>
</tr>
<tr>
<td>Butyl ester, Acetic acid</td>
<td>125864</td>
<td></td>
</tr>
<tr>
<td>Cadmium</td>
<td>7440439</td>
<td></td>
</tr>
<tr>
<td>Cadmium Chloride</td>
<td>10108642</td>
<td></td>
</tr>
<tr>
<td>Chlorine</td>
<td>7782505</td>
<td></td>
</tr>
<tr>
<td>Chlorobenzene</td>
<td>108907</td>
<td></td>
</tr>
<tr>
<td>Chloromethyl benzene</td>
<td>100447</td>
<td></td>
</tr>
<tr>
<td>Chloromethyl oxirane</td>
<td>106898</td>
<td></td>
</tr>
<tr>
<td>[Dimethoxyphosphinolyl]butanedioic acid, Diethyl ester</td>
<td>121755</td>
<td></td>
</tr>
<tr>
<td>Ethanol</td>
<td>64175</td>
<td></td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>100414</td>
<td></td>
</tr>
</tbody>
</table>
### Benzene -- CAS# 71432

**Synonyms:** Cyclohexatriene, Benzole

#### Color key

<table>
<thead>
<tr>
<th>Color Scheme</th>
<th>Description</th>
<th>Color Scheme</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inherent acute toxicity</td>
<td>Moderately toxic</td>
<td>Yellow</td>
</tr>
<tr>
<td></td>
<td>Slightly toxic</td>
<td>Blue</td>
</tr>
<tr>
<td></td>
<td>Practically nontoxic</td>
<td>Green</td>
</tr>
<tr>
<td>Risk Estimate Reliability</td>
<td>Moderate</td>
<td>Gray</td>
</tr>
</tbody>
</table>

#### Table of 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.

<table>
<thead>
<tr>
<th>Exposure duration (h)</th>
<th>Number of Species</th>
<th>Species Group*</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>34</td>
<td>C=8, F=13, N=3, O=10</td>
</tr>
<tr>
<td>48</td>
<td>37</td>
<td>C=12, F=10, M=3, O=12</td>
</tr>
<tr>
<td>72</td>
<td>9</td>
<td>C=3, F=2, M=3, O=1</td>
</tr>
<tr>
<td>96</td>
<td>35</td>
<td>C=10, F=19, M=4, O=2</td>
</tr>
</tbody>
</table>

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

#### General Observations

- Most of the currently available acute toxicity data (LC50 and EC50) 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.

#### 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.

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

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

#### Observations about the data available

- Evaluation of data included in analysis

- Table of Data availability used in analysis
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 LC50 and EC50 data; therefore, these represent estimated LC50/EC50 values.

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

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

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

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

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

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

**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?*

<table>
<thead>
<tr>
<th>Fate Data - Physical Properties</th>
<th>Benzene</th>
</tr>
</thead>
<tbody>
<tr>
<td>Odor: Aromatic odor, Gasoline-like odor; rather pleasant aromatic odor</td>
<td></td>
</tr>
<tr>
<td>Color: Prismatic Colorless to light yellow liquid (a solid below 42°F)</td>
<td></td>
</tr>
<tr>
<td>Skin, eye, and skin irritant, respiratory: Severe eye and moderate skin irritant, irritation upon occupational exposures of &gt;60 ppm for three weeks.</td>
<td></td>
</tr>
<tr>
<td>Boiling Point (°C)</td>
<td>80°C (Experimental)</td>
</tr>
<tr>
<td>Melting Point (°C)</td>
<td>5.5°C (Experimental)</td>
</tr>
<tr>
<td>Density</td>
<td>0.687 g/cm³</td>
</tr>
<tr>
<td>Autoignition Temp.</td>
<td>928°F (497°C)</td>
</tr>
<tr>
<td>Vapor Density</td>
<td>2.8 (Ar=1)</td>
</tr>
<tr>
<td>Viscosity (cP)</td>
<td>0.604 cP at 25°C</td>
</tr>
<tr>
<td>Explosive/Flammable Limits</td>
<td>Lower: 1.4%; Upper: 8.0%</td>
</tr>
</tbody>
</table>

**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?**

**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 volatilize 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).