DTox: a Worldwide Quantitative Database of the Toxicity of Dispersants and Chemically Dispersed Oil

A Final Report Submitted to

The Coastal Response Research Center

Submitted by

Dr. Adriana C. Bejarano

Research Planning, Inc.
1121 Park Street
Columbia, SC 29201

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Abstract

The *Deepwater Horizon* oil spill revived much of the discussions on the use of dispersants as one of the tools considered in offshore oil spill response. Much of this discussion focused on concerns about the toxicity of dispersants and chemically dispersed oil to water column organisms. The ability to rapidly assess the toxicity of dispersants and chemically dispersed oil require unrestricted and rapid access to available toxicity data, a need shared by government, industry, consultants, and academic groups involved in oil spill response. While toxicity data on dispersants and both physically and chemically dispersed oil have been generated since the 1970s, the practical use of this information has been hindered by the lack of a centralized data repository. As a result, the Dispersant and Chemically Dispersed Oil Toxicity Database (DTox) is created to address that shared need of the oil spill community.

The main objectives of this project are to: 1) identify, evaluate, compile, and integrate all available toxicity data on dispersants and chemically dispersed oil, and 2) generate an interactive tool that can assist the oil spill response community in their assessments and management decisions regarding the use of dispersants. The ultimate goal of this effort is the synthesis of information in a meaningful way to improve scientific decision-making as well as to provide rapid access to centralized toxicity data. DTox includes information on over 35 data attributes (e.g., species scientific name, life stage tested, dispersant name, exposure type, oil weathering stage, exposure duration, etc.), compiled through a careful review of existing data extracted from the peer-review and gray literature. Data considered for inclusion in DTox are rigorously evaluated following a strict set of rules aimed at selecting the best available and suitable data that are further evaluated through detailed Quality Assurance/Quality Control (QA/QC) procedures, which included a review of at least 15% of all records in the database. Each data source in DTox is further evaluated and given an applicability score based on its relevance to oil spills, and not on its scientific merits. Key criteria in the determination of source applicability include exposure type, reported effects concentrations, and reported analytical chemistry. Data from 400 papers (peer-review and gray literature) were evaluated for their potential inclusion into the database, and data extracted from +160 of these sources. Information in DTox is integrated into a user-friendly tool that allows for on-the-fly data searches and data plotting in the form of Species Sensitivity Distributions, based on the specific needs of an end-user. This tool can assist with the development of risk estimates related to oil spills by allowing the selection of data that most closely match the needs of an end-user.

The effectiveness, usefulness, and transferability of DTox to oil spill response are evaluated through oil spill drills, dispersant-related workshops, and dispersant-related assessment. These exercises showed that, despite existing data limitations, DTox provides information that can be used to inform tradeoff decisions based on the current state of knowledge. Data in DTox have the potential to contribute to a better understanding of the biological effects of dispersants and oil in the aquatic environment, and can provided useful information to both environmental assessments and decision making efforts. Future efforts will focus on maintaining and updating DTox and expanding its use capabilities in oil spill response community.

Keywords: Dispersant, DTox, Oil spill response, Chemically dispersed oil, Species Sensitivity Distributions.

Acknowledgments

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1.0 Introduction

During the *Deepwater Horizon* oil spill an unprecedented volume of dispersants was used as a response tool to accelerate the natural biodegradation of oil and help minimize the impacts of oil on sensitive nearshore and shoreline habitats and resources (Lubchenco et al., 2012). This exceptional use of dispersants raised concerns among the public and many scientists about the toxicity of dispersant and chemically dispersed oil to water column organisms. While aquatic toxicity testing of dispersants and chemically dispersed oil has been conducted under laboratory and field conditions for at least four decades (e.g., NRC, 1989, 2005, and more recent studies) the practical use of this information, particularly to communicate risks and to address misconceptions about the use of dispersants, was limited by the lack of a centralized data repository (a data gap identified by CRRC et al., 2012). While aquatic toxicity databases contain toxicity data on dispersants and petroleum products (e.g., CAFÉ-NOAA/ERD, AQUIRE-USEPA), a database solely dedicated to consolidating in a meaningful way decades of existing toxicity data on dispersants and both physically and chemically dispersed oil was nonexistent at the time. As a result, Dispersant and Chemically Dispersed Oil Toxicity Database (DTox) is developed to address the shared need of the national and international oil spill community for access to toxicity data. The main objectives of this project are to review and integrate all available toxicity data on dispersants and chemically dispersed oil into an interactive tool that can assist the oil spill response community in their management decisions regarding the use of dispersants.

While it is clear that additional research is needed to improve our understanding of the biological, toxicological, and ecological effects of dispersants and chemically dispersed oil to a wide range of aquatic species (CRRC et al., 2012), and despite data limitations, decades of research in this field can provide valuable information to the oil spill response community and practitioners. As evident during the *Deepwater Horizon* oil spill, the ability to assess the toxicity of chemically dispersed oils is a goal shared by oil spill responders, where a common requirement is the unrestricted and rapid access to the available toxicity data, compiled following a detailed Quality Assurance/Quality Control plan.

2.0 Objectives

The main objectives of this project are to identify, evaluate, compile, and integrate all available toxicity data on dispersants and both physically and chemically dispersed oil generated under laboratory and field conditions, and to generate an interactive tool that can assist the oil spill response community in management decisions regarding the use of dispersants. The ultimate goal of this effort is the synthesis of information in a meaningful way to improve scientific decision-making as well as to provide rapid access to centralized toxicity data. The specific objectives of this project are to:

1. Identify documents and peer-review and gray literature (e.g., field, laboratory, mesocosm, accidental oil spills) reporting toxicity data (acute and chronic) of dispersants and chemically dispersed oil;
2. Rigorously evaluate each data source for quality and potential for inclusion in the DTox database;

3. Compile all quantitative information including all relevant fields (e.g., species, exposure conditions, oil type and weathering, etc.);
4. Integrate the above information into a tool that can be used by the end-user to guide management decisions regarding the use of dispersants; and
5. Test the suitability of the compiled quantitative data for use in spill response at two pilot study areas.

3.0 Methods

The identification of peer-review and gray literature documenting the toxicity of dispersants and physically and chemically dispersed oil was done via a combination of online searches, visits to web sites of government agencies, industry, and research institutions, and direct contact with leading researchers in the field. Hard copies or electronic versions of each data source were obtained and cataloged in EndNote® prior to their review. Each data source was rigorously evaluated for their potential for inclusion in DTox following the Quality Assurance/Quality Control (QA/QC) plan developed for this project (see Appendix A for details). Examples of data criteria are shown in Table 1.

Table 1. Examples of some of the criteria used to evaluate each data source for their potential inclusion in DTox. Studies not satisfying these requirements are not included.

Criteria	Requirement/Inclusions	Limitations/Exclusions
Dispersant	Documented commercial name	Not documented
Oil	Documented fresh/weathered oil name or source	Not documented
Species	Aquatic invertebrates, vertebrates, marine bacteria	Mammals, reptiles
	Documented taxonomic information verifiable against standard taxonomic sources	Species or common name not documented
Effect/ Response	Biological effect on live, whole organisms	Dead organisms; in-vitro studies
	Adverse acute or chronic effects	Beneficial, nutritional effects
Exposure conditions	Water only exposures	Sediment, other exposures
	Acceptable control survival (at least 70%), or acceptable control endpoints	Poor control survival or unacceptable control endpoints
	Documented experimental conditions (e.g., flow through, static)	Not documented
	Documented exposure durations conditions associated with biological effects (e.g., flow through, static)	Unverifiable duration, not reported
	Documented effects concentrations	Not documented

Data were entered into a carefully designed database template in a systematic and consistent fashion. Examples of database elements (see Appendix A for details) included: 1) species attributes: taxonomic group, common name, scientific name, life stage, species distribution; 2) experimental conditions and settings: study type, water type, oil name and weathering condition, dispersant name, dispersant-to-oil ratio, exposure type, exposure duration; 3) endpoints: acute, subacute, effects concentration, effects concentration units, analyte name, analytical methods; and 4) data source: author name, publication year, article title. Whenever possible, entries were standardized facilitating further sorting and treatment of the existing data. An additional field was created to score the applicability of each data source (e.g., High, Moderate, Low) to spill response. Source applicability is based on the relevance of each data source to oil spill response, and not on the overall scientific merit of individual sources (see Appendix A for details). Data entered into the database template went through several QA/QC evaluations to ensure that each record accurately represented the information and data of the original data source (see Appendix A for details). Critical steps of the QA/QC process included the review of currently accepted scientific species names, standardization of column content and applicability criteria, and identification of duplicate data (e.g., several papers by the same author(s) reported in several report/manuscripts). Identifying duplicate data is an important step because it affects the values per species plotted on Species Sensitivity Distributions (SSD) (see below). Consequently, duplicate data are not removed from the database, but are not used in SSD calculations. The revised dataset is then migrated into a database program (FileMaker® Pro 12) with expanded capabilities, allowing the development of an interactive, searchable, and user-friendly tool that allows for visual exploration and examination of data (suggested citation Bejarano and Dahlin, 2013).

4.0 Results

4.1 Compiled Toxicity Data

Over 400 papers from peer review and gray literature were initially screened for their potential inclusion into the database. The complete list of citations of all papers reviewed as part of this project was compiled into an EndNote® library. This library is available to the larger oil spill community through the PI and/or CRRC. Although many of the data sources originally reviewed contained important information, many are not included in DTox because these were not the original data source and, therefore, the quality of these papers could not be judged based on the information provided (see Appendix A for details). Of these initially screened papers, data were extracted from +160 sources amounting to +3500 rows of records. A graphic representation of the type of data currently in DTox is shown in Figure 1. To date, this database contains toxicity data for +100 oils, +120 dispersants, and +190 unique aquatic species, amounting to +3,500 toxicity records. The large majority of records are for species with subtropical distributions (+1,200 records), followed by temperate species (+900 records). Cold-water species and tropical species are the most underrepresented group by geography (+800 records combined). Most currently available toxicological records are for species (and life stages) found in the water column (+2,400 records), while a considerably lower number of records are available for species from the other two general habitats (benthos and epibenthos) (+1,500 records combined). When looking at the number of records by taxonomic group, most records are for fish (+1,500 records) followed by crustaceans (+1,400 records), while other groups, especially corals are underrepresented in the database. At least one third of all records are for 13 U.S. standard test species (+1,300 records), with data for mysid shrimp (*Americamysis bahia*) and inland silverside (*Menidia beryllina*) comprising nearly 50% of all standard test species records.

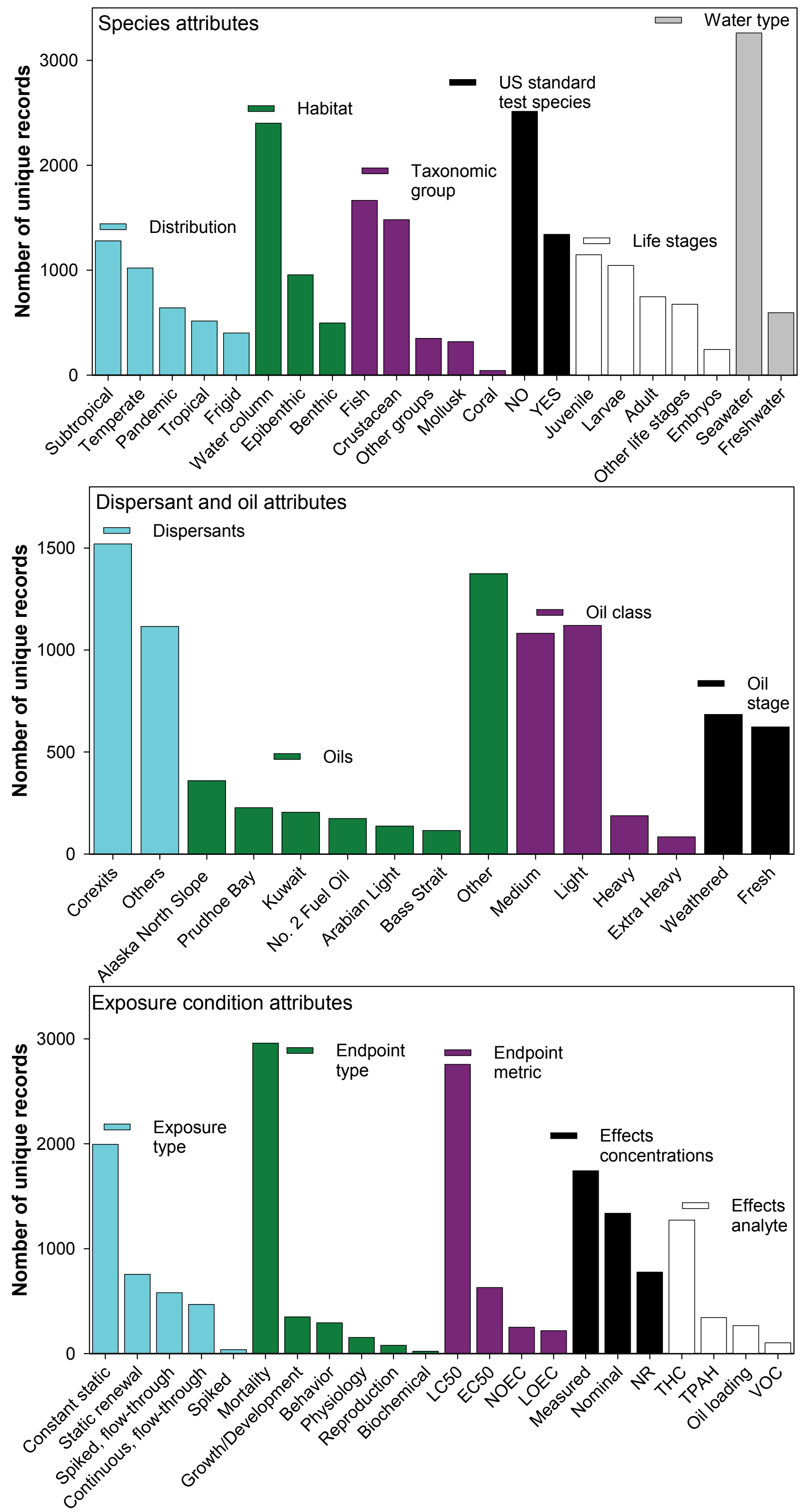

Figure 1. Breakdown of final QA/QC data and information currently in DTox by species attributes (top); oil/dispersant attributes (middle); and exposure conditions (bottom).

Based on the currently available information, it is clear that there was a surge of toxicity studies on dispersants and oil in the mid 1970s, declining drastically through the 1980s. Since the late 1980s, there have been a variable number of studies, as reflected in the number of records in DTox. Nearly one fifth of all records (+700 records) has been generated since 2010, likely driven by the *Deepwater Horizon* oil spill[1]. The most studied dispersants are the Corexits (+1,500 records; specifically Corexit 9500, Corexit 9527 and Corexit 7664), while the most studied oils are Alaska North Slope, Prudhoe Bay, and Kuwait oil (+700 records combined). The large majority of oil records (+2,000) are for light and medium oils (based on API gravity), while heavy and extra heavy oils are underrepresented in the database (+200 records combined). A large percentage of records (70%) are derived from 48- and 96-hour exposures (+2,500 records), and via static exposures (+2,400 records). Of the 171 peer-review and gray literature papers included in DTox, 37, 52, 72 were given High, Moderate and Low Applicability scores, respectively. Ten data sources were rejected.

It is important to note that there are additional data sources not currently in DTox (e.g., data currently under peer review, data unavailable because of confidentially agreements, data under litigation, older reports requiring company approval for release, etc.), and it is hoped that these data would be included in future updates of the existing database. Specifically, NOAA/BP data from the *Deepwater Horizon* oil spill are not currently available for inclusion into the database, but requests have been made to ensure that upon their release from embargo, these data will be entered into DTox following the same procedures and QA/QC plan developed during this project.

4.2 DTox-Version 1

The ultimate goal of this effort is the synthesis of information in a meaningful way to improve scientific decision-making as well as to provide rapid access to centralized toxicity data. As a result, a user-friendly tool was created to facilitate data querying. This tool is designed to allow the end-user to navigate through a series of screens where data selections can be made, narrowing the type and amount of information used in data plotting. Prior to the distribution of the first version of DTox to a selected number of end-users, a beta version of DTox was extensively tested both internally and externally by a number of individuals (testers). This step was critical to ensure that the tool met the requirements expected of an interactive tool. During the testing window, recommendations were made to improve the appearance and functionality of the tool, and a series of glitches and technical issues were identified and addressed. These early evaluations allowed the project team to address any outstanding issues and improve the presentation of the tool prior to its public release. The end-result is the production of a DTox-Version 1 tool (suggested citation Bejarano and Dahlin, 2013). Examples of the navigation windows of the first version of DTox are shown in Figure 2. Note that the first window includes a clear disclaimer, and a request for reporting of errors and inconsistencies. A window is also included to clearly acknowledge the funding source. More detailed information regarding DTox-Version 1 is provided in Appendix B, a document that is also included as a pdf within the interactive tool.

[1] Data generated through to support NRDA from the *Deepwater Horizon* oil spill are not currently included in the database.

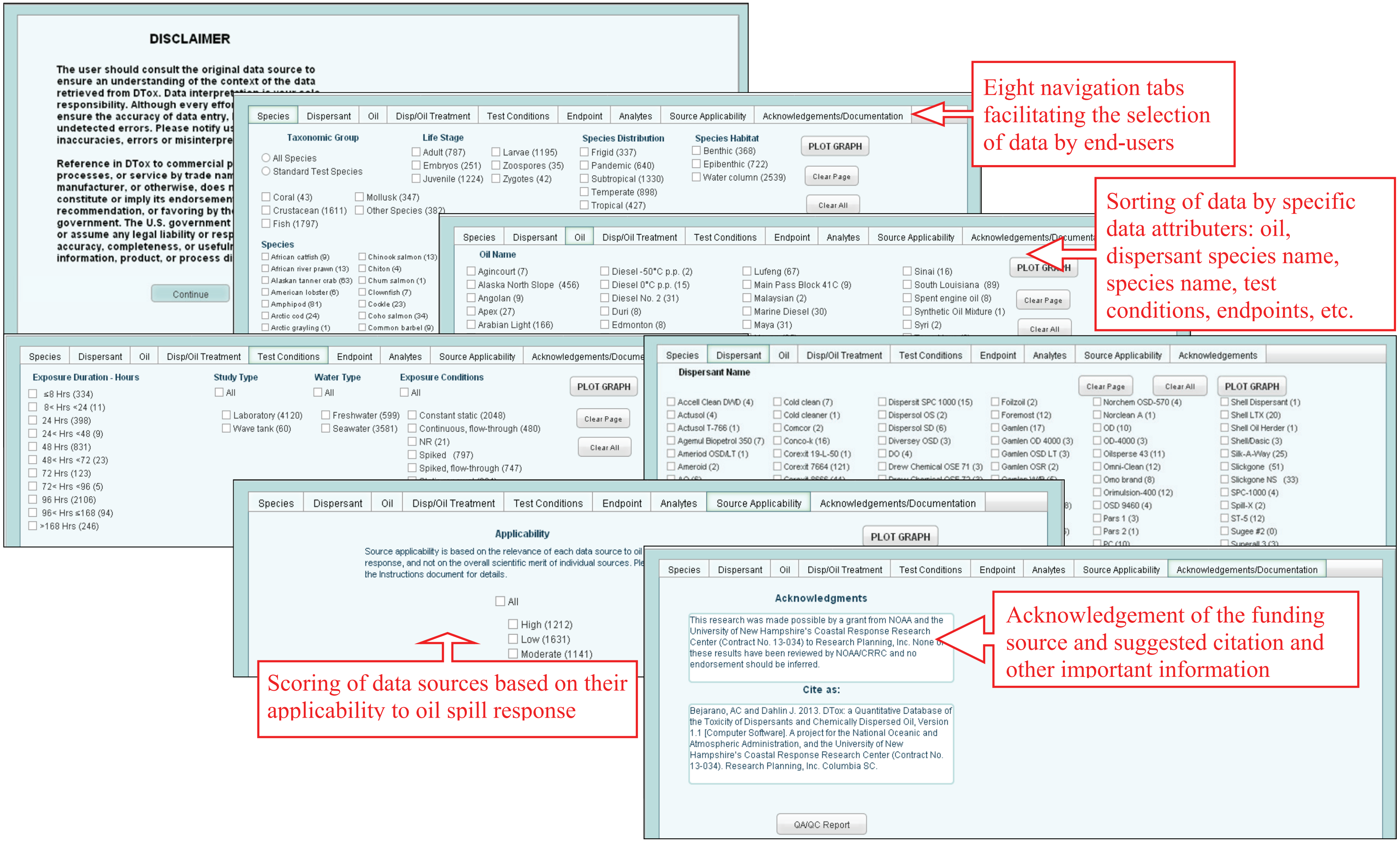

Figure 2. Examples of navigation tabs where the end-user can query the available data. A total of nine navigation tabs are currently available in DTox (Version 1).

Following data selection from the navigation windows, the remaining data are plotted in separate windows in the form of Species Sensitivity Distributions (SSDs) (Figure 3). SSDs are probabilistic models that describe the relative sensitivity of species to a particular compound or compound mixture (Posthuma et al., 2002), where species are ranked, based on their relative sensitivity, from the least to the most sensitive. As a result, each dot on a SSD represents a unique species, specifically the geometric mean of reported toxicity values. In DTox, SSDs are generated for datasets with a minimum of 5 species by fitting the empirical toxicity data to a logistic function defined by $F(\text{x})= \frac{e^{(\frac{\text{x}-\mu}{\sigma})}}{\sigma\,(1+e^{(\frac{\text{x}-\mu}{\sigma})})^2}$, x∈ R, with parameters μ(location) and σ (scale). SSDs are advantageous in that these allow for comparison of the sensitivity of different species to the same type of exposure (e.g., dispersant only, oil only, chemically dispersed oil), and can be used to derive benchmarks or hazard concentrations (HC) (Posthuma et al., 2002). Some of the most commonly used HCs are the HC1 and HC5 equivalent to the concentrations at which 1% and 5%, respectively, of the species in the SSD may not be protected. When enough data are available for curve fitting, the SSDs also display the estimated HC1 and HC5 values from the logistic curve.

The current version of DTox (Version 1) allows for up to two SSDs per display window (Dispersant Only, Dispersant and Oil, Oil Only) based on the following data fields: exposure duration, dispersant name, or oil name. When only one curve is plotted, common names are displayed to facilitate data interpretation. For better visualization and interpretation of data, the queried data are displayed based on color coding the selections (e.g., by taxonomic group; by species distribution). All SSDs are plotted over a colored background representing a common scale used to rank the relative toxicity of contaminants (http://www.epa.gov/oppefed1/ecorisk_ders/toera_analysis_eco.htm#Ecotox) (see Figure 3 for details). Other features of DTox include a selection criteria tab that displays the selections made through the navigation tabs, and a report tab displaying the information used to plot the SSDs with the option of exporting both SSDs and summary data to a pdf file. DTox also contains the complete QA/QC plan used in the development of the tool (Appendix A), and a "How To" document (Appendix B), guiding end-users how to navigate and understand navigation tabs and query options, and providing examples on how to use outputs generated from this tool. This document also highlights some of the existing limitation with the current version of DTox. DTox also contains the EndNote® library with the complete list of citations of all papers reviewed as part of this project.

Throughout the development of DTox, care was taken to address individuals with disabilities (Section 508 29 U.S.C. '749d) particularly by selecting color palettes (whenever possible) designed to be readable by individuals with color blindness. A stand-alone executable file of DTox (Versions 1), which can be run in desktop and laptop computers, was made available to a selected number of end-users. As mentioned previously, prior to the distribution of DTox (Version 1), the tool was extensively tested both internally and externally by a number of testers. While these early evaluations allowed the project team to address issues prior to its public release, it is acknowledged that the organization of copious amounts of toxicity data into a practical, versatile, and logical system was challenging. However, the tool may still contain issues not currently identified. During training sessions with end-users (see Section 7.1) the PI encouraged participants to report any issues with the tool so that these can be addressed in future iterations of DTox. To date, comments have been provided which are summarized in Table 2. Development of additional access forms (e.g., html) may be developed in consultation with NOAA, as this agency may be in charge of the long-term maintenance and future updates of this database.

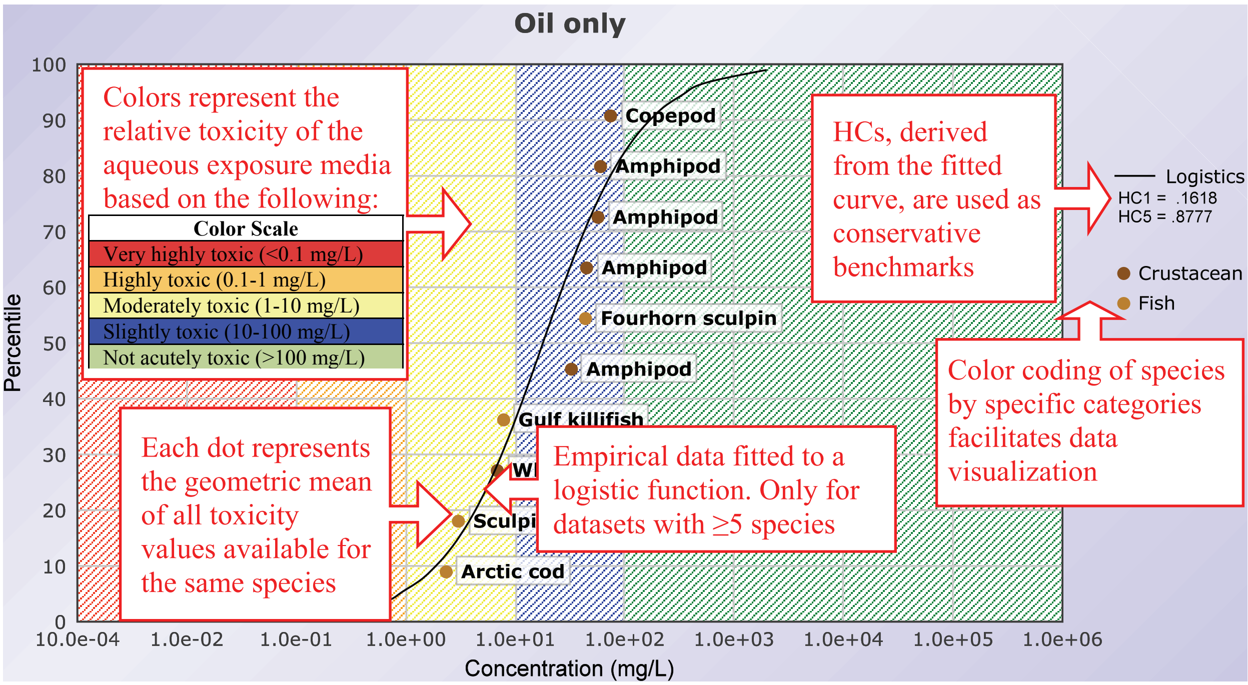

Figure 3. Example of a SSD generated following data queries, where dots represent the empirical data. Hazard Concentrations, HC1 and HC5, represent the benchmark concentrations assumed to be protective of 99% and 95%, respectively, of the species in the SSD.

Table 2. Strengths and limitation of DTox (Version 1) based on feedback provided by end-users.

Strengths
• Easy to use (e.g., check boxes, tabs) and intuitive design • Clear display of data in separate tabs according to attributes • Total count of records (in parentheses) are informative • Helpful "Clear Page" and "Clear All" button on each tab • Warning appears when there are not enough data • Single and double plots are informative and well designed • The summary query tab is helpful, particularly when many data selections are made • Both plots and raw data used in plots are easily exported • Well documented tool (complete QA/QC and Instructions documents)
Limitations
• Too many selection options • Applicability and life stage are not a shading options • Only common names are displayed. Scientific names should be an option • Names do not appear in double plots • Not enough information displayed on graph output section • Goodness of fit tests are not available (as pointed out by the authors)

4.2.1 DTox-Query Demonstration

In this section a series of queries are performed to demonstrate the usability of DTox (additional queries are presented in Section 4.3).

- Query 1a: Dispersant – Corexit 9500 and Corexit EC9500A; Oil – Prudhoe Bay and Alaska North Slope; Exposure conditions – Constant static, Flow through, Static renewal; Exposure duration – 96-hours; Endpoint metric– LC50, EC50; Concentration – Measured; Analyte – All options containing Total Hydrocarbon Content (THC); Applicability – Moderate, High.
- Query 1b: Identical as Query 1a, but without dispersant selection.
- Query 1c: Identical as Query 1a, but changing Exposure conditions to – Spiked, Spiked-flow-through.

As shown in Figure 4 (Top), the concentration assumed to be protective of 95% of the species in the SSD (HC5) is 0.1 milligrams of total hydrocarbons per liter (mg THC/L) in aqueous exposures to Prudhoe Bay and Alaska North Slope oils that were chemically dispersed with Corexit 9500 and Corexit EC9500A. By comparison, aqueous exposures to the same physically dispersed oils (without dispersants) (Figure 4, Middle) produce an HC5 of 0.3 mg THC/L. While the estimated HC5 values from aqueous exposures to chemically dispersed oil are smaller than those from physically dispersed oil, these two curves are likely not different from each other. These results are consistent with previous conclusions (NRC, 1989, 2005) indicating that there is no strong scientific evidence that the toxicity of chemically dispersed oil is substantially greater than that of physically dispersed oil. Note that Figure 4 (Middle) displays several amphipod species. A tab within DTox (not shown) allows the end-user to determine which amphipod species (scientific name) are included. In this case, *Anonyx nugax*, *Boeckosimus edwardsi*, *Gammarus setosus* and *Onisimus littoralis*.

Data in DTox are also queried to compare the impact of exposure conditions (static-Query1a vs. spiked-Query1b) on toxicity values. As shown in Figure 4 (Bottom), the concentration assumed to be protective of 95% of the species in the SSD (HC5) is 1.66 mg THC/L for spiked exposures, which is an order of magnitude larger (less toxic) than the HC5 value from constant exposures (0.1 mg THC/L). As a result, assessments based on toxicity data from tests performed under constant static exposures may overestimate toxicity, when compared to assessments based on spiked exposures. The latter type of laboratory settings represents more realistic field environmental exposures because these address the dilution that occurs in open waters by reproducing under laboratory conditions rapid changes in concentrations in the water column (Aurand and Coelho, 2005; Clark et al., 2001; George-Ares et al., 1999; NRC, 1989, 2005; Singer et al., 1995).

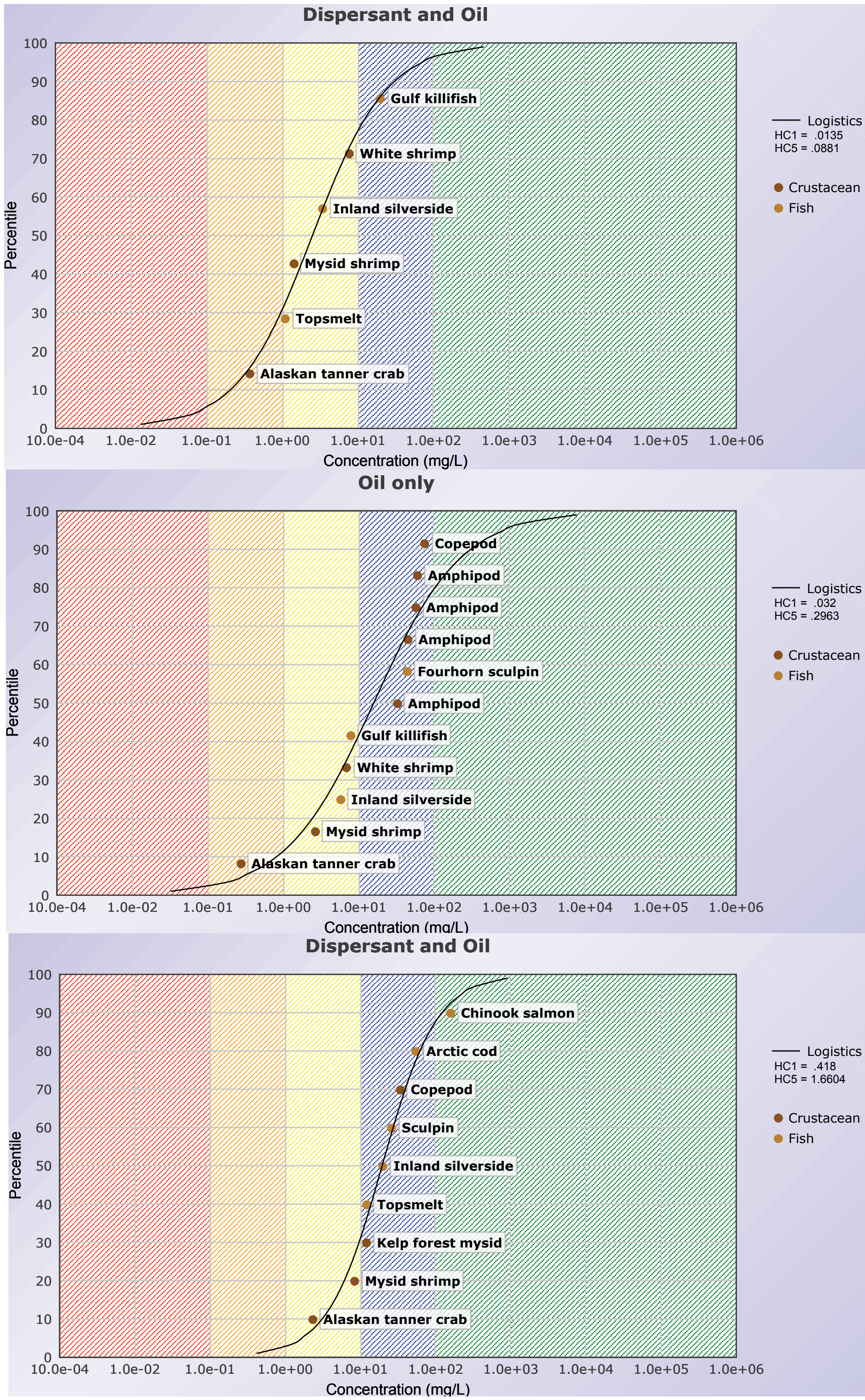

Figure 4. Example of a SSD generated following data queries in DTox. Dots represent the available empirical data. Hazard concentrations, HC1 and HC5, represent the benchmark concentrations assumed to be protective of 99% and 95%, respectively, of the species in the SSD. Top: Query 1a; Middle Query 1b; Bottom: Query 1c. See text for details.

4.3 DTox Applicability to Oil Spill Response and Planning

A database is only useful for storing information if people can correctly and efficiently query, update, and manipulate existing data to inform decisions or to perform assessments. Consequently, critical steps in assessing the effectiveness and usefulness of DTox dealt with its transferability to drills, or real oil spill situations, as well as its ability to provide information that can help inform decisions based on the current state of knowledge. To assess the applicability and transferability of this tool in spill response, two scenarios with different biological and oceanographic conditions are used to test the usefulness of DTox. The location and oil spill volume associated with each of these scenarios was provided by NOAA/ERD, and were based on either planned or past oil spill drills. Testing the applicability and transferability of DTox consists of performing data queries and selecting the appropriate receptor species with associated toxicological data, or user-specified query criteria, from which levels of concern for representative groups of species in these two areas are derived.

Steps involved in assessing the suitability of this database include:

1. Describing a spill scenario, including the location of the spill;
2. Determining the species/groups of species at risk, or species of concern;
3. Selecting the appropriate environmental and search criteria;
4. Conducting data query/queries considering Steps 1-3;
5. Deriving potential levels of concern or risk estimates; and
6. Describing data gaps and sources of uncertainty.

Note: The drills below are for demonstration purposes only and should not be taken out of context. Results and conclusions should not be used beyond the scope of this exercise, which is intended to demonstrate the applicability of DTox in oil spill response and planning.

4.3.1 Drill 1: Bay of Fundy, Maine

Spill scenario (Drill). "At 1200 ADT on Tuesday, June 18, 2013, the tank vessel *M/T NERITINA*, with a full cargo of 1,092,000 barrels (bbl) of Kuwait crude oil is transiting inbound in the Bay of Fundy collided with a cargo vessel. This collision resulted in spill of 35,000 bbl (~4,775 tonnes/1.47 million US gallons) of crude from the *M/T NERITINA*, with a potential secondary release of 50,000 bbl." This scenario is identical to the Canadian/U.S. Joint Response Team full scale exercise for the Atlantic Region (CANUSLANT) (June 17-20, 2013).

Resources at Risk. The islands of coastal Maine support a high diversity and abundance of marine life including birds and marine mammals. Nearshore areas also support productive commercial fisheries for fish and invertebrate species. Because of the ecological importance of nearshore waters to numerous marine species, the use of dispersants is not taken lightly as there are several federally threatened and endangered species (protected under the Endangered Species Act), as well as species of special concern, and species of local significance. A summary of these biological resources of concern is summarized in Table 3.

Table 3. Biological resources at risk from a release of oil from the *M/T NERITINA*, with focus on nearshore/offshore waters. U.S. Status: FT = Federal threatened; FE = Federal endangered; ST = State threatened; SE = State endangered, SC= State species of special concern. Canada Status: CA-FE = federal endangered; CA-FSC: federal species of special concern.

Species Group	Species Subgroup (Status)	Seasonal Presence	Comments
Birds	Arctic terns (ST)	Nests May-Jun	
	Atlantic puffin (ST)	Nests Apr-Aug	
	Double-crested cormorant	Nests Apr-Jul	
	Harlequin ducks (ST)	Wintering Oct-Mar	
	Leach's storm petrel (SC)		
	Least tern (FE, SE)	Nests May-Aug	
	Piping plover (FT; CA-FT; SE)	Nests May-Aug	
	Razorbill (ST)	Mar-Sep; nests May-Jun	
	Red knot	Migration Jun-Jul	
	Roseate tern	Nests May-Aug	
Marine mammals	Atlantic white-sided dolphin	Calve Jun-Jul	
	Fin whale (FE; CA-FSC)	Peak abundance Apr-Oct	Most frequently found in waters over the continental shelf
	Gray seals	Pup Dec-Feb	
	Harbor porpoise	Calve May-Jun	Found throughout the Bay of Fundy
	Harbor seals	Pup May-Jun	
	Harp seals	Jan-May	
	Humpback whale (FE; CA-FSC)	Moderate abundance Summer	Most frequently found in waters over the continental shelf
	Minke whale		
	North Atlantic right whale (FE, CA-FE)	Peak abundance May-Sep	Found in shallow nearshore waters
	Sei whale (FE, CA-FE)	Peak abundance May-Sep	Most frequently found in waters over the continental shelf
Fish	American plaice		
	Atlantic cod		
	Atlantic halibut		
	Atlantic herring		Offshore spawning areas
	Atlantic salmon (FE; CA-FE)	Apr-Nov	Coastal/inland Maine critical habitat for this species under ESA. Present in the outer Bay of Fundy
	Bluefin tuna	Migration July	
	Halibut		
	Winter and Witch flounder		
Invertebrates	American lobster	Inshore migration Summer	Species of local economic importance
	Northern shrimp	Spawn Nov-May	
	Rock crabs		
	Sea scallop		

One of the main resources of concern in the area is the American lobster (*Homarus americanus*), which is an iconic commercial species harvested since the 18th century. While most life stages of this species are associated with the substrate (benthic), three of the four stages of lobster larvae are found in the water column (pelagic) between late spring to early fall (May to October), where they are transported by surface water from offshore to coastal waters before settling to the bottom (MacKenzie and Moring, 1985). Recent work by Incze (2010) reported, based on a spatially explicit population model, that larvae stages I-III are generally found in the top 15 meters (m) of the water column concentrating in the coastal shelf (<50 m to 100 m isobaths), with vertical distribution varying depending on water column stratification. A related paper (Annis, 2005) also documented that post-larvae (stage IV) concentrate in the upper 2 m of the water column, spending the large majority of their time near the surface (0-0.5 m) closer to shore. Consequently, an oil spill of large magnitude coinciding with peak distributions of larvae in the top few meters of the water column may have impacts on a fraction of the lobster population. While there are reasonable concerns regarding the potential impact of oil to early life stages of lobster, only a small number of studies (Capuzzo et al., 1984; Wells, 1972; Wells and Sprague, 1976) have documented their sensitivity to physically dispersed oil.

Modeled Expected Environmental Concentrations. For the purpose of this exercise, two scenarios for this ***drill*** are run to characterized potential oil concentrations associated with this release using the General NOAA Operational Modeling Environment (GNOME) (Beegle-Krause, 2001; NOAA/ERD, 2013): 1) a scenario allowing the released oil to disperse physically without the use of dispersants; and 2) a scenario treating the released oil with dispersants, under the assumption that 50% of the oil is effectively dispersed. Note that this is an ***extreme*** case of dispersant effectiveness, and is intended here to provide a worst-case exposure condition of aquatic organisms to chemically dispersed oil. While dispersant effectiveness under field conditions is highly variable, dispersant effectiveness has been reported to vary between 5% and 30% (NRC, 2005). The hypothetical spill of Kuwait oil is assumed to take place offshore in an area between the 60 and 200 m isobaths.

GNOME was run under the following environmental conditions.

- Light to Medium crude (API 34)
- Environmental conditions:
    - Wind: variable, range 2 to 12 knots from various directions
    - Mixed layer: 10 m depth
    - Breaking wave height: variable, range 0.009 to 0.33 m
    - Contour depth: 0 to 5 m

GNOME modeled oil trajectories (Figures 5 and 6) showed that physically dispersed oil would impact coastal shorelines north east of Blacks Harbour within 48 hours post release, with large quantities of oil entering the western section of Bay of Fundy 48 to 96 hours post release. At 96 hours post release, oil would reach south eastern sections of the Bay (e.g., Roosevelt Campobello International Park, Clark Gregory Nature Preserve). By comparison, modeled trajectories of the oil chemically treated with dispersants showed generally the same trends, except that the extent of shoreline oiling would be substantially lower. However, larger amounts of oil are entrained in the top few meters of the water column. Under the chemically dispersed scenario, peak oil concentrations in the water column would be localized north of Grand Manan Island.

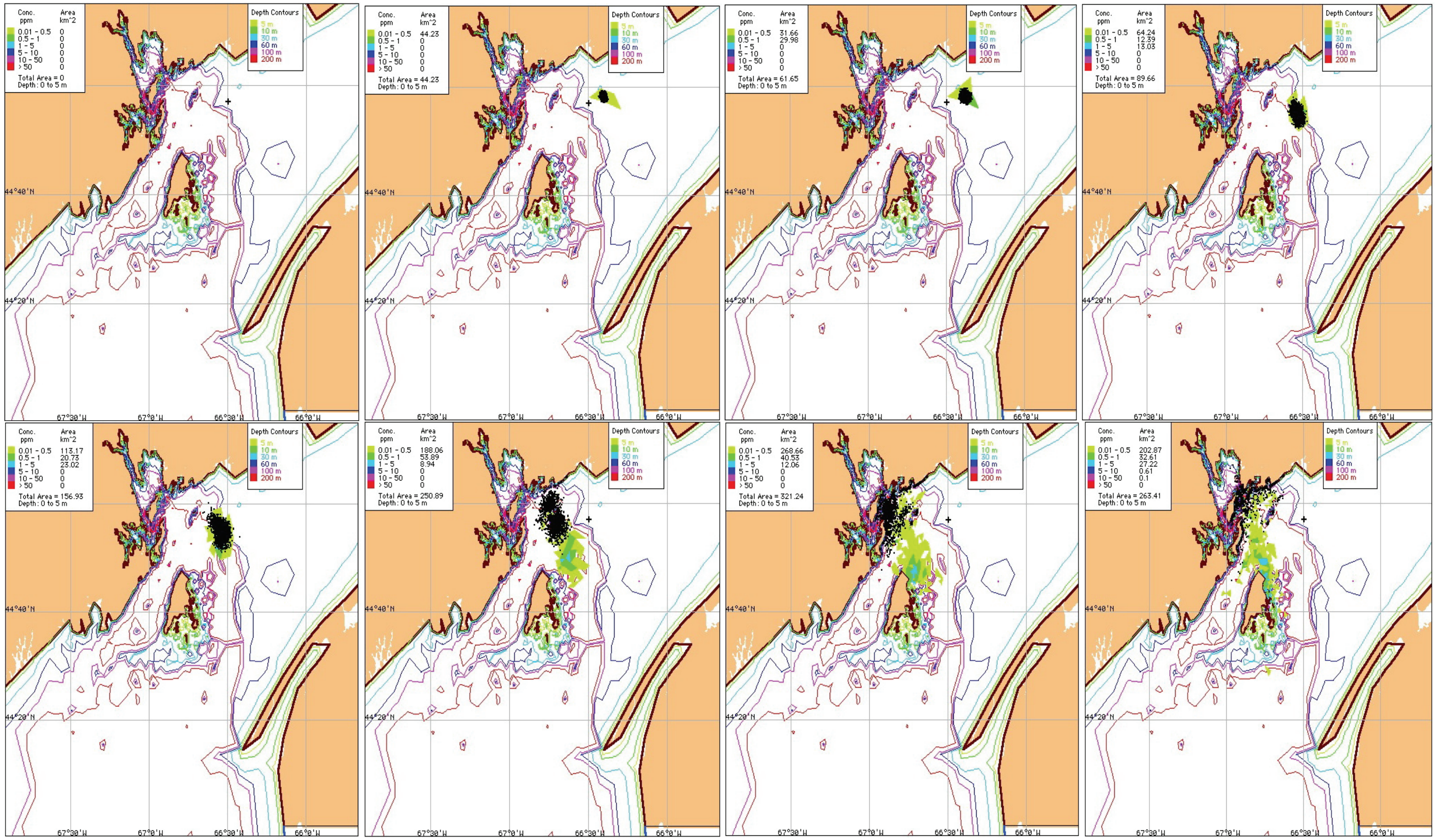

Figure 5. Spill trajectory snap shots of a physically dispersed plume of Kuwait crude oil (1.47 million gal) released into Bay of Fundy by the tank vessel *M/T NERITINA* ***(drill)***. Top and bottom, and left to right, represent GNOME model outputs 0, 3, 6, 12, 24, 48, 72, and 96 hours post release. Colors represent modeled oil concentrations in the top 5 m of the water column. Data provided by A. Mearns, NOAA ERD.

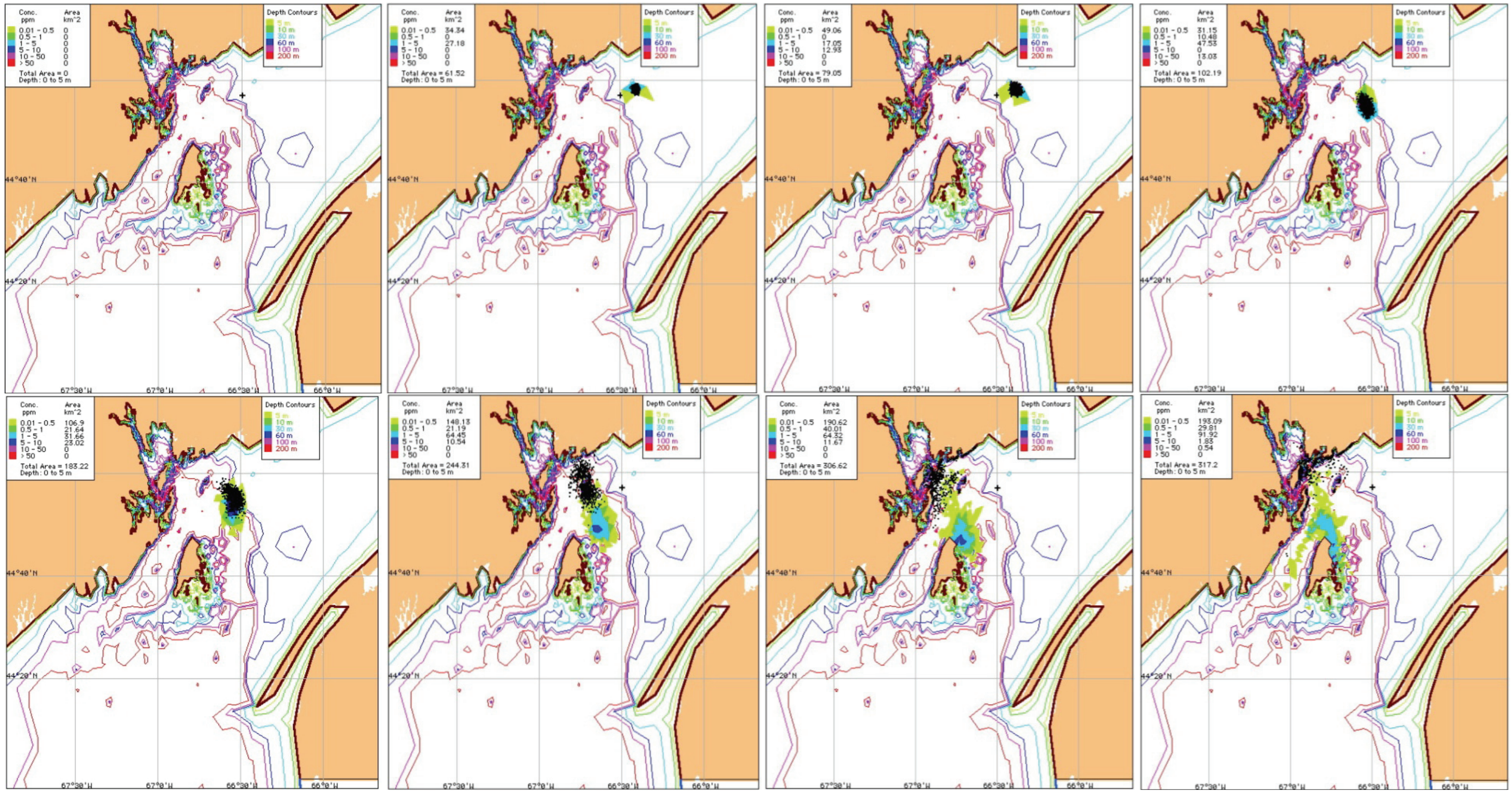

Figure 6. Spill trajectory snap shots of a chemically dispersed plume of Kuwait crude oil (1.47 million gal) released into Bay of Fundy by the tank vessel *M/T NERITINA* ***(drill)***. Top and bottom, and left to right, represent GNOME model outputs 0, 3, 6, 12, 24, 48, 72, and 96 hours post release. Colors represent modeled oil concentrations in the top 5 m of the water column. Data provided by A. Mearns, NOAA ERD.

Oil budgets for the two scenarios of this ***drill*** (Figures 7) indicated that physically dispersed oil would remain in large quantities floating on the water surface during the first 24 hours post release (48% of the oil released), following by large quantities of oil stranding on shoreline habitats (up to 25% of the oil released) between 48 and 96 hours post release. Under this scenario, 37% of the oil would evaporate, and up to 30% would be physically dispersed into the water column. By comparison, a relatively small amount of the released oil (4%) would be present on the water surface following chemical treatment of oil slicks. Under this scenario, a large proportion of the released oil (60%) would disperse into the water column (mostly into the top 10 m of the water column) within the 24 hours post release, but a relatively small proportion (13%) would impact coastal shorelines. Under this scenario, 19% of the oil would dissipate via evaporation.

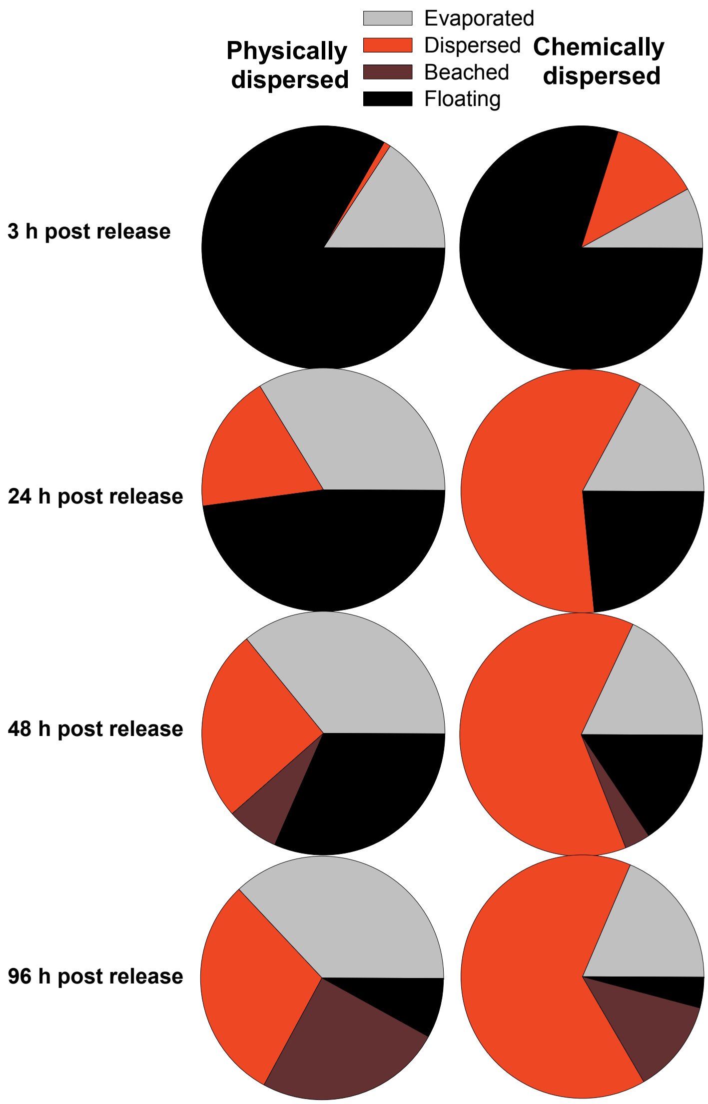

Figure 7. Oil budgets comparison as a function of time between the physically and chemically dispersed scenarios from a release of Kuwait crude oil (1.47 million gal) into Bay of Fundy by the tank vessel *M/T NERITINA* ***(drill)***. Note that the chemically dispersed scenario assumes an extremely high dispersant effectiveness (50%), which is intended here to provide a worst-case exposure condition to aquatic organisms. Data from GNOME provided by A. Mearns, NOAA ERD.

Two summary statistics are obtained from GNOME to characterize oil concentrations for this ***drill***. These are the average and maximum (worst-case) concentrations in the top 5 m of the water column for each 30 min interval over the entire model run period (0 to 96 hours). Average and maximum (worst-case) modeled oil concentrations in the water column (covered in detail in a later section) under the physically dispersed scenario are generally low (Figure 8) (Average: mean 0.29 mg/L, median, 0.30 mg/L, maximum 0.43 mg/L; Maximum (worst-case): mean 1.29 mg/L, median, 1.54 mg/L, maximum 2.19 mg/L). By comparison, the average and maximum modeled oil concentrations in the water column under the chemically dispersed scenario are in the 1.5- 3 mg/L range, with some exceptions (Average: mean 0.79 mg/L, median, 0.89 mg/L, maximum 1.97 mg/L; Maximum: mean 2.39 mg/L, median, 2.56 mg/L, maximum 3.62 mg/L).

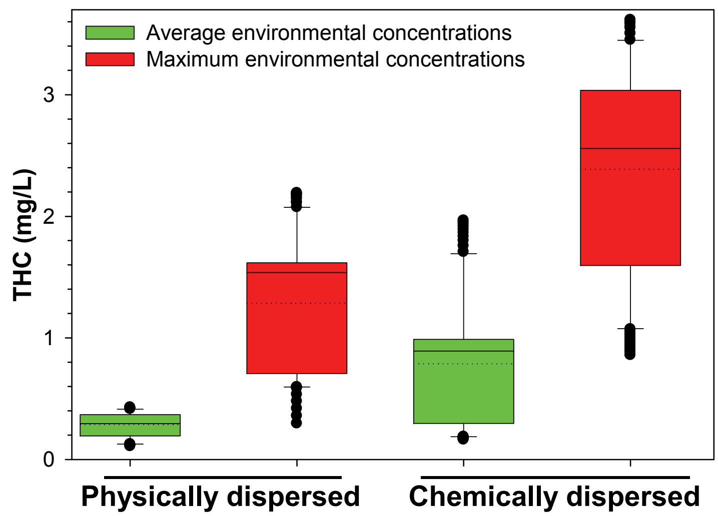

Figure 8. General box-plot overview of the expected oil concentrations of physically and chemically dispersed scenarios from a release of Kuwait crude oil (1.47 million gal) into Bay of Fundy by the tank vessel *M/T NERITINA* ***(drill)***. Data from GNOME. Note that the chemically dispersed scenario assumes an ***extremely high*** dispersant effectiveness (50%), and intended here to provide a worst-case exposure condition to aquatic organisms. Oil concentrations are the average and maximum concentrations in the top 5 m of the water column for each 30 min interval over the entire model run period (0 to 96 hours). The length of the box represents the distance between the 25th and the 75th percentile concentrations, while the whiskers represent the 5th and 95th percentile concentrations. The solid and dashed horizontal lines in the box represents the median and mean respectively. The closed circles indicate outliers.

Estimated Environmental Concentrations of Concern. A query was performed in DTox to facilitate the understanding of the potential impact of physically and chemically dispersed oil on lobster larvae. To ensure reproducibility of the analyses presented here, a complete list of relevant fields queried and selected in DTox is provided below (Figure 9):

- Query #1: Life stage – embryos, larvae, juvenile; Habitat – water column; Taxonomic group – fish and crustaceans; Dispersant/Oil Treatment – Oil only, and Dispersant and Oil; Exposure duration – 96-hours (*assumed to be a worst case exposure*); Exposure conditions – Spiked, Spiked-flow-through; Endpoint metric – LC50, EC50; Effects concentration analyte – All options containing Total Hydrocarbon Content (THC); Concentration –Measured; Paper Applicability– Moderate, High

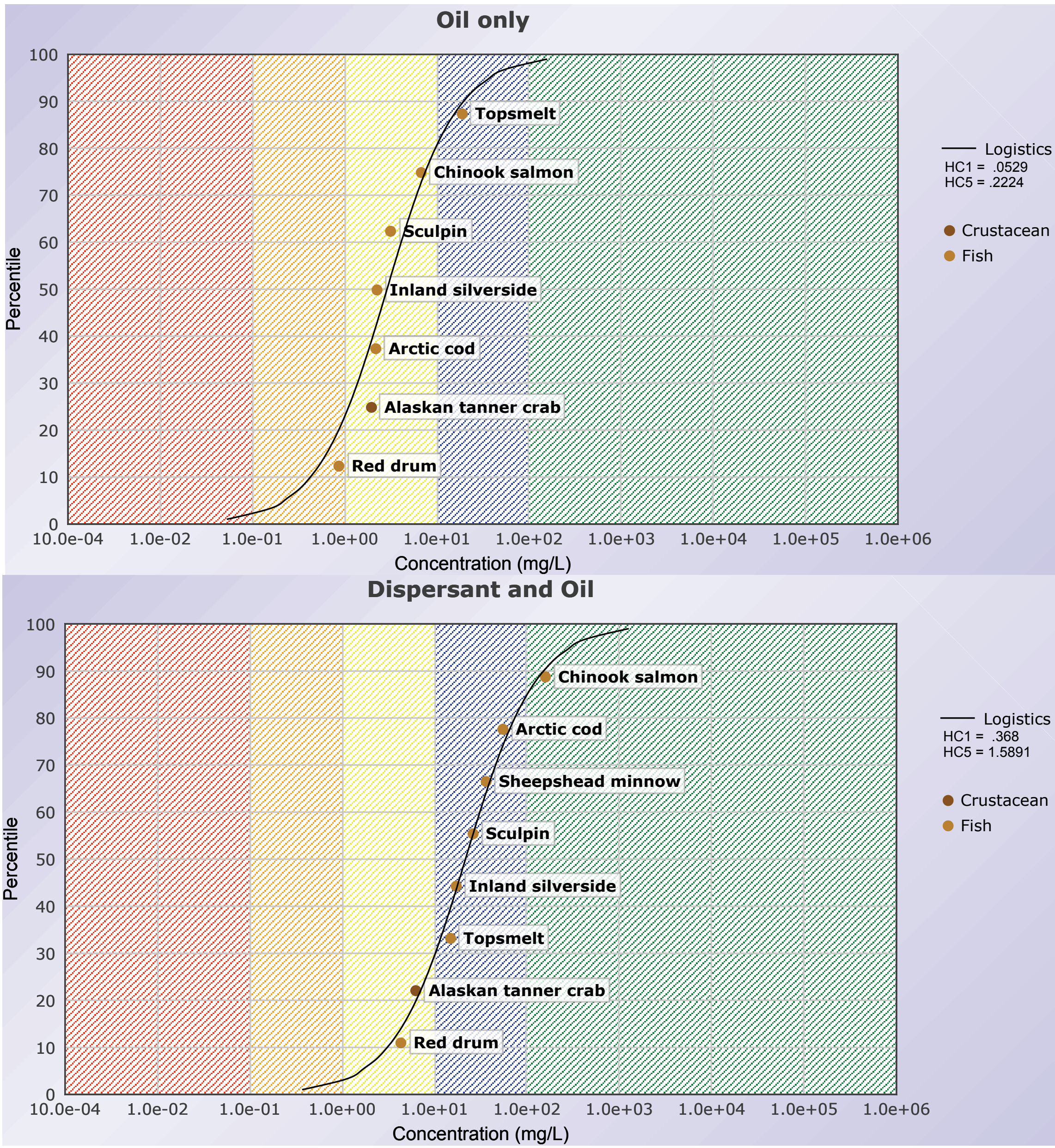

Figure 9. SSD generated following a data query in DTox for the ***drill*** in Bay of Fundy involving the tank vessel *M/T NERITINA*.

For the purpose of this ***drill***, the SSD with the most conservative 5 percentile hazard concentration (HC5=0.22 mg/L) (Figure 9, top) is used in further interpretations. Note that the only toxicity data available for larvae of the American lobster are from Wells and Sprague (1976) who reported a 96-h LC50 (based on measured reported concentrations) of 0.86 mg/L to first-stage larvae. HC values of the most conservative plot are also protective of first-stage larvae.

Potential Environmental Impacts. Average and maximum (worst-case) oil concentrations for the physically dispersed ***drill*** scenario overlap 5% and 40%, respectively, of the most conservative 96h-SSD (Figure 10). A different pattern is observed with the ***drill*** scenario involving chemical dispersion of the released oil. Average and maximum (worst-case) oil concentrations for the chemically dispersed scenario overlap 20% and 60%, respectively, of the most conservative 96h-SSD. Under the chemical dispersion scenario, 60% and 97% of the average and maximum (worst-case) oil concentrations, respectively, exceeded the HC5. Exposures above the HC5 are limited to the first 60-70 hours post release for the average scenario, and >90 hours post spill for the maximum oil concentrations scenario. All of these exceedances are limited to the top 10 m of the water column, mostly within the top 2 m (data not shown).

While these comparisons are useful, without a spatial context these can lead to overestimation of risks. The areal extent of the water surface with modeled oil concentrations is also further analyzed for the chemically dispersed scenario. As shown in Figure 11, the areal extent of the concentration bracket exceeding the HC5 (0.5-1 mg/L, 1-5 mg/L and >5 mg/L) grew from 27.18 km^2 3 hours post release to 124 km^2 120 hours post release. By contrast, most of the areal extent of the impacted water surface had concentrations in the 0.01-0.5 mg/L range (range: 34 km^2 3 hours post release to 193 km^2 120 hours post release). As shown in this exercise, the area of potential impact is relatively small (0.07% of the Gulf of Maine/Bay of Fundy system, 180,000 km^2) and concentrated into an area 24 times the size of a standard football field. This information (and Figure 7) demonstrate that while there is an increased risk to water column organisms from dispersant use to mitigate the impacts of this particular ***drill*** (albeit concentrated into a relatively small area and to depths <10 m), the greatest environmental tradeoff is the reduced impact to shoreline habitats (physically vs. chemically dispersed oil on shorelines, 368,088 gal vs. 183,456 gal, respectively), and reduced amounts of floating oil (physically vs. chemically dispersed oil on water surface 117,306 gal vs. 60,270 gal, respectively) which can pose adverse risks to surface marine species (e.g., birds and marine mammals).

As mentioned before, one of the main resources of concern is the American lobster, which under this spill scenario may be exposed to potentially toxic oil concentrations in the top few meters of the water column. The extent of potential adverse lethal and sublethal effects to this species and its local population depends on both the encounter rate of oil at concentrations above those assume to cause adverse effects, and exposure duration to those oil concentrations. Under the assumption that larvae are evenly distributed in the top 10 m of the entire Bay of Fundy area, and assuming that the entire area with concentrations ≥0.01 mg/L (physically dispersed scenario1,188 km^2; chemically dispersed scenario 1,294 km^2) would overlap the distribution of larvae, an estimated 0.7% of the lobster larvae in the entire Bay of Fundy would encounter oil in the water column.

While potential toxicological consequences to water column organisms may be expected, these assessments are conservative as the benchmark used here is biased towards overprotection or marine species (i.e., based on 96-h exposure toxicity data). This degree of conservatism added to the fact that oil biodegradation is not taken into account suggests that oil concentrations would likely be lower than those predicted by the GNOME model.

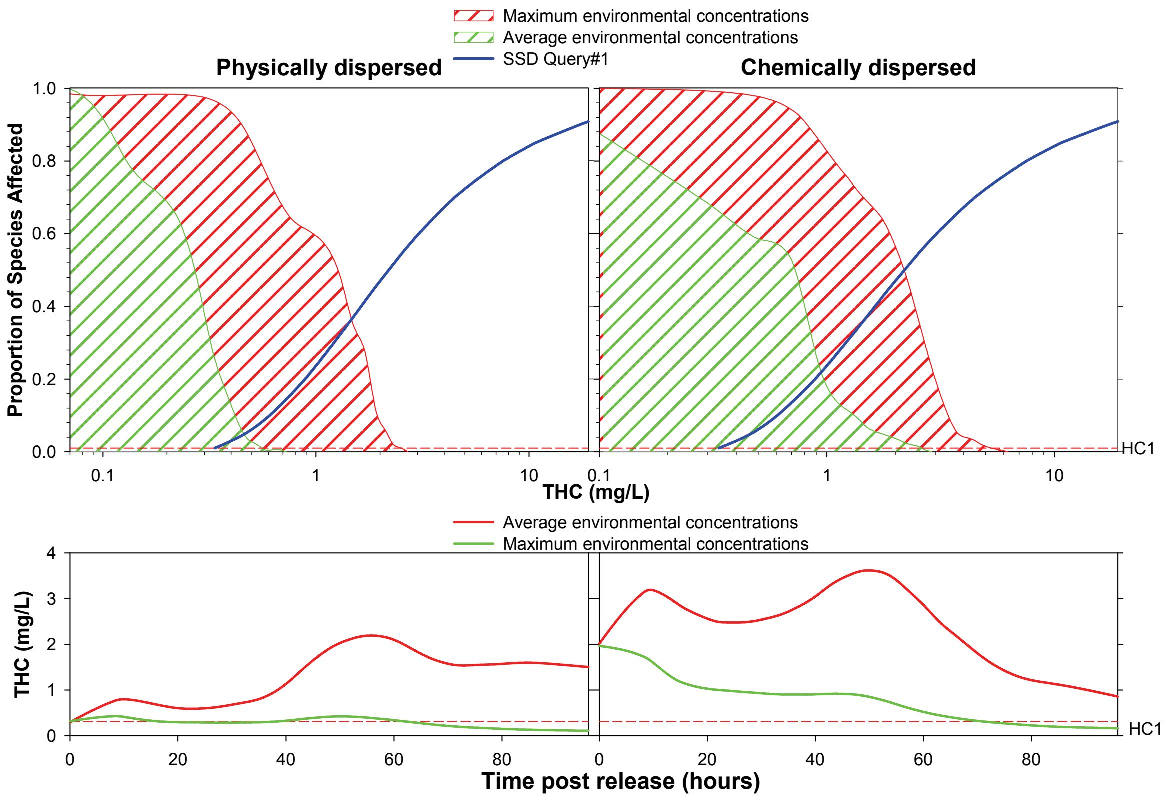

Figure 10. Cumulative average and maximum (worst-case) modeled oil concentrations relative to 96 h-SSDs (top), and average and maximum modeled oil concentrations as a function of time post release for a physically (left) and chemically dispersed (right) plume of a Kuwait crude oil into Bay of Fundy by the tank vessel M/T NERITINA (***drill***). As a reference, the benchmark for this drill is HC5=0.22 mg/L

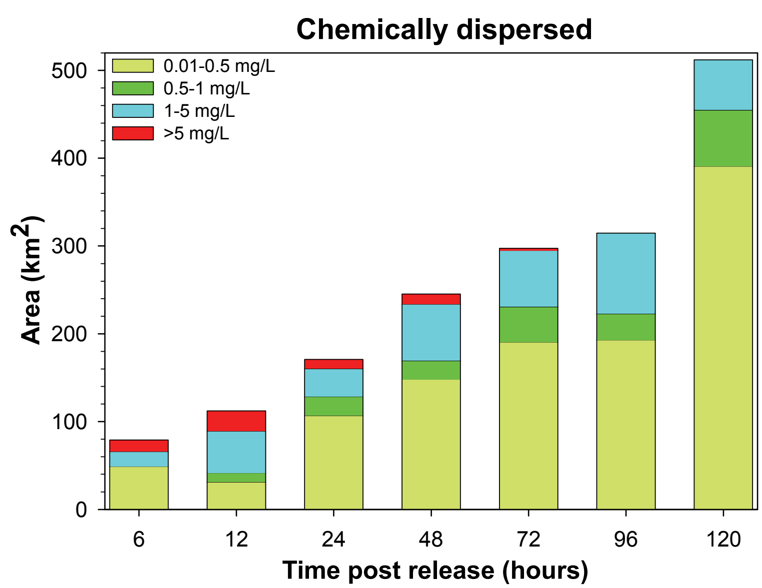

Figure 11. Water surface area impacted by a spill of Kuwait crude oil (1.47 million gal) into Bay of Fundy (***drill***), as a function of time post release (hours), and average oil concentrations. As a reference, the benchmark for this drill is HC5=0.22 mg/L.

4.3.2 Drill 2: Area offshore from Charleston Harbor, South Carolina

Spill scenario (Drill). On May 23, 2013 at 5:00 pm EDT a spill of 5,000 bbl (210,000 gal) of Qua Iboe Nigerian Crude is released offshore from Charleston Harbor, South Carolina. Qua Iboe Nigerian Crude (API 34) is a light to medium weight crude oil, which may coat intertidal habitats, as well as wildlife on the water surface. The oil may also result in water column and benthic impacts if mixed into the water column by waves, or if it strands in large amounts in shallow, sheltered areas with limited water exchange.

Resources at Risk. During spring and summer, shoreline habitats along the South Carolina coast support a high number of nesting seabirds, and beaches provide nesting habitat for several species of sea turtles. Marshes in the area provide important habitat for a variety of shorebirds, as well as terrestrial and aquatic mammals (mink, river otter, beaver, and raccoon). Nearshore and offshore areas also support productive commercial fisheries for fish and invertebrate species. Because of the ecological importance of nearshore waters to numerous marine species, the use of dispersants is not taken lightly as there are several federally threatened and endangered species (protected under the Endangered Species Act), as well as species of special concern, and species of local significance. These biological resources of concern are summarized in Table 4.

Table 4. Biological resources at risk from a release of oil off Charleston Harbor, South Carolina, with focus on nearshore/offshore waters. U.S. Status: FT = Federal threatened; FE = Federal endangered; ST = State threatened; SE = State endangered, SC= State species of special concern.

Species Group	Species Subgroup (Status)	Seasonal Presence	Comments
Birds	American oystercatchers		Largest wintering concentration on the east coast
	Bufflehead		Present in coastal and offshore areas
	Brown pelicans		Present in coastal and nearshore areas
	Cormorants		
	Great blue heron	Nesting peak May-Aug	
	Gull-billed terns and	Nesting peak Apr-Aug	
	Black skimmers	Nesting peak Apr-Aug	
	Least tern (FE; ST)		Present in marshes, and on tidal flats in the area
	Piping plover (FT; ST)		Most frequently found during winter
Reptiles	Green sea turtle (FE; SE)	Present year-round, peak Apr-Dec Nesting May-Aug Hatching July-Oct	Found in offshore waters
	Leatherback sea turtle (FE; SE)	Present year-round, peak Apr-Dec Nesting Mar-Jul Hatching May-Oct	Present in nearshore and offshore waters
	Loggerhead sea turtle (FT; ST)	Present year-round, peak Apr-Dec	Present in nearshore and offshore waters

Species Group	Species Subgroup (Status)	Seasonal Presence	Comments
		Nesting Jun-Nov Hatching Jul-Dec	
Marine mammals	Bottlenose dolphin	Present year-round, Breeds year-round	Found in shallow nearshore waters and offshore waters
	Mink whale		Most frequently found in waters over the continental shelf. Occasionally present
	Humpback whale (FE; SE)		Most frequently found in waters over the continental shelf. Occasionally present
	North Atlantic right whale (FE)	Calving Nov-Mar	Found in shallow nearshore waters
Fish	Atlantic croaker	Larvae and juveniles may be present	Most frequently found in tidal creeks
	Atlantic menhaden	Eggs/larvae/post-larvae may be present	Adults most frequently found in offshore waters throughout the water column
	Red drum	Larvae and juveniles may be present	Adults most frequently found in coastal waters
	Red snapper	Eggs/larvae Jun-Oct Juveniles may be present	
	Shortnose sturgeon (FE)		Found in coastal rivers
	Spanish mackerel		Most frequently found in coastal and offshore waters
	Summer flounder	Larvae and juveniles may be present	Adults most frequently found in coastal waters
	Southern flounder	Larvae and juveniles may be present	Adults most frequently found in coastal waters
	Spot	Larvae and juveniles may be present	Adults most frequently found in coastal waters
Invertebrates	American oysters		Spawn in tidal creeks and on sheltered tidal flats
	Blue crab	Larvae and juveniles may be present	Found in offshore waters
	Brown shrimp	Eggs/larvae may be present Spawning Jan-Dec	Found in offshore waters
	Pink shrimp		Found in offshore waters. Not very common.
	Spiny lobster		Found in offshore waters
	Stone crab	Spawning Mar-Oct, peak May-Aug Larvae and juveniles may be present	Adult oyster, including females incubating eggs, found on bars and mud flats
	White shrimp	Spawning May-Jun	Found in offshore waters
		Larvae/juveniles may be present	

While the area off South Carolina harbors a high diversity of aquatic species, their exposure to physically and chemically dispersed oil depends on their spatial distribution and on their habitat distribution within the water column. Consequently, the primary resources of concern are those commonly found offshore at the water surface or in the upper few meters of the water column. Specific examples include adults and early life stages of commercially important free-swimming shellfish (brown shrimp, white shrimp, and blue crab), and fishery resources that spawn in the water column (e.g., Atlantic menhaden).

Modeled Expected Environmental Concentrations. For the purpose of this exercise, two scenarios for this ***drill*** are run to characterize potential oil concentrations associated with this release using GNOME) (Beegle-Krause, 2001; NOAA/ERD, 2013): 1) a scenario allowing the released oil to disperse physically without the use of dispersants; and 2) a scenario treating the released oil with dispersants, under the assumption that 80% of the oil is effectively dispersed. Note that this is an ***extremely high*** case of dispersant effectiveness, and is intended here to provide a worst-case exposure condition of aquatic organisms to chemically dispersed oil. While dispersant effectiveness under field conditions is highly variable, dispersant effectiveness has been reported to vary between 5% and 30% (NRC, 2005).

GNOME was run under the following environmental conditions.

- Light to Medium crude (API 34)
- Environmental conditions:
    - Wind: 15 knots from the South
    - Mixed layer: 5 m depth
    - Breaking Wave Height: 1 m
    - Contour depth: 0 to 5 m

GNOME modeled oil trajectories (Figures 12 and 13) showed that physically dispersed oil would impact coastal shorelines north east of the harbor (e.g., Sullivan's Island and Isle of Palms) within 24 hours post release, with large quantities of oil entering Charleston Harbor between 24 and 48 hours post release. Coastal habitats south west of the harbor (e.g., Morris Island and Folly Beach) would be oiled >24 hours post release. By comparison, modeled trajectories of the oil that is chemically treated with dispersants showed generally the same trends, except that the extent of shoreline oiling would be substantially lower. However, larger amounts of oil are entrained in the top few minutes of the water column.

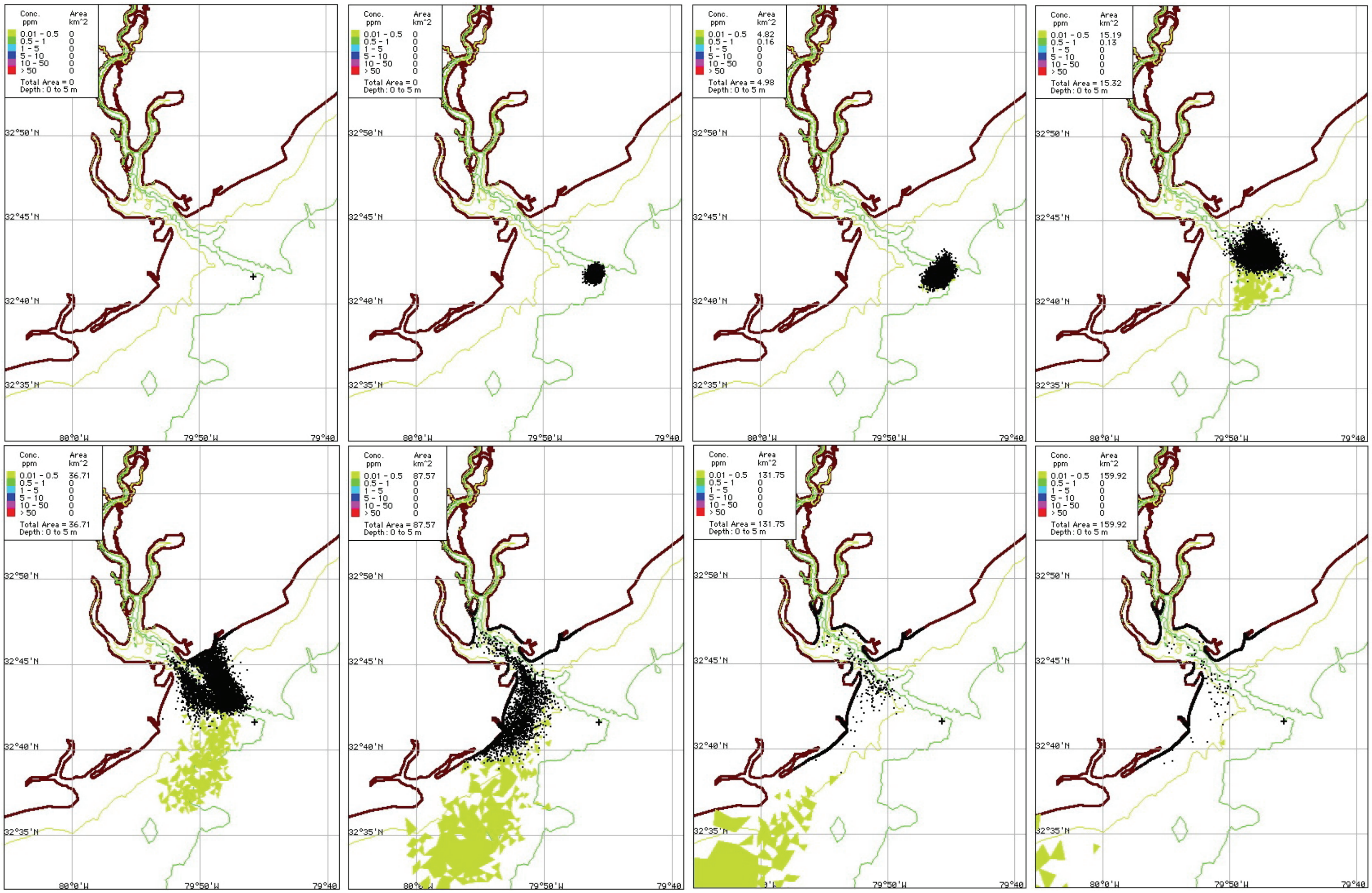

Figure 12. Spill trajectory snap shots of a physically dispersed plume of Qua Iboe Nigerian crude oil (210,000 gal) (***drill***) released offshore from Charleston Harbor. Top and bottom, and left to right, represent GNOME model outputs 0, 3, 6, 12, 24, 48, 72, and 96 hours post release. Colors represent modeled oil concentrations in the top 5 m of the water column. Data provided by A. Mearns, NOAA ERD.

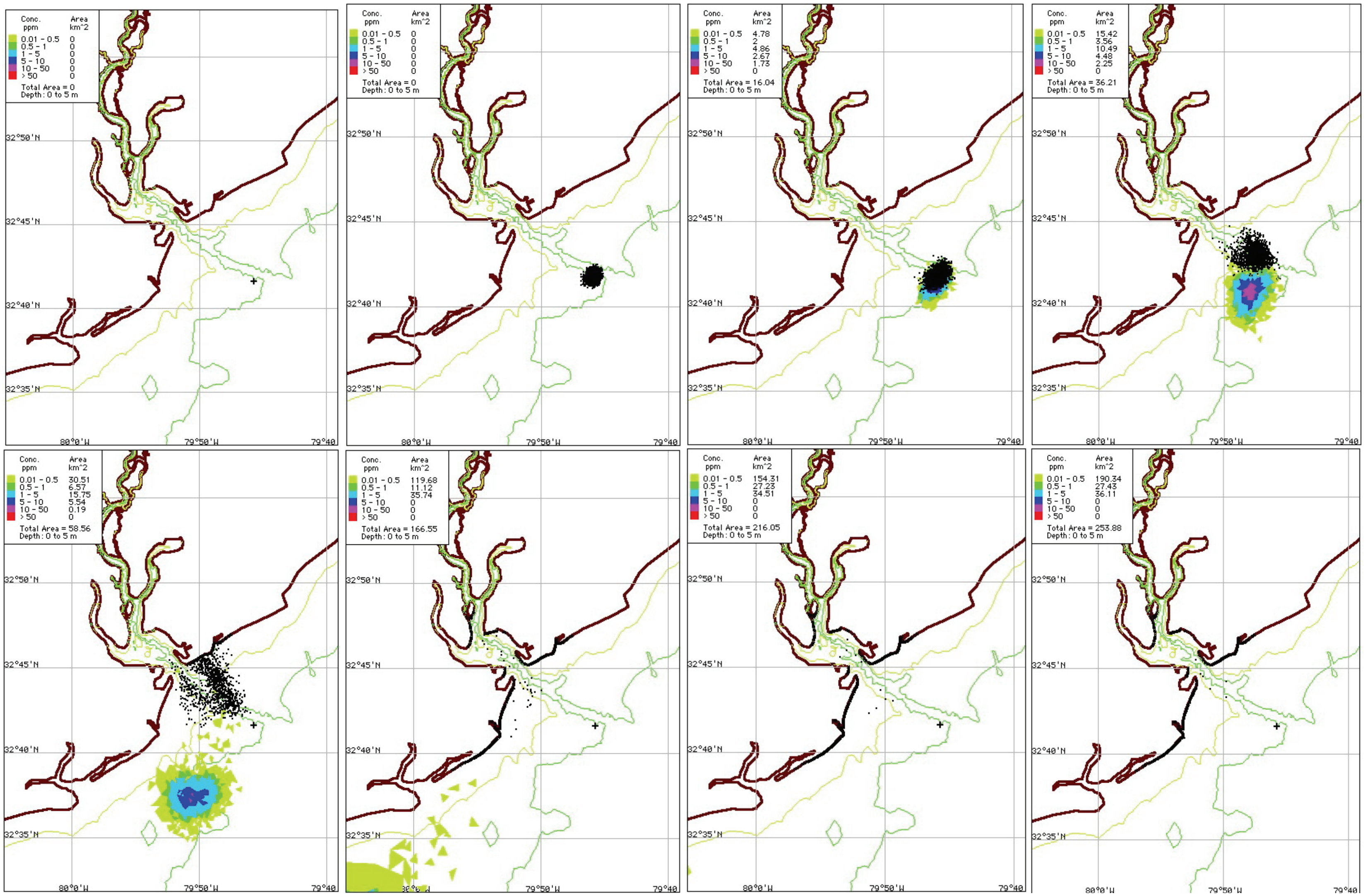

Figure 13. Spill trajectory snap shots of a chemically dispersed plume of Qua Iboe Nigerian crude oil (210,000 gal) (***drill***) released offshore from Charleston Harbor, assuming an extremely high dispersant effectiveness (80%). Top and bottom, and left to right plots represent GNOME model outputs 0, 3, 6, 12, 24, 48, 72, and 96 hours post release. Colors represent modeled oil concentrations in the top 5 m of the water column. Data provided by A. Mearns, NOAA ERD.

Oil budgets for the two scenarios of this ***drill*** (Figure 14) indicated that physically dispersed oil would remain in large quantities floating on the water surface during the first 24 hours post release (>50% of the oil released), following by large quantities of oil stranding on shoreline habitats (>30% of the oil released) between 48 and 96 hours post release. Under this scenario, 35% of the oil would evaporate, and <5% would be physically dispersed into the water column. By comparison, a relatively small amount of the released oil (14%) would be present on the water surface following chemical treatment of oil slicks. Under this scenario, a large proportion of the released oil (65%) would disperse into the water column (mostly into the top 5 m of the water column) within the 24 hours post release, but a relatively small proportion (11%) would impact coastal shorelines. Under this scenario, 20% of the oil would dissipate via evaporation.

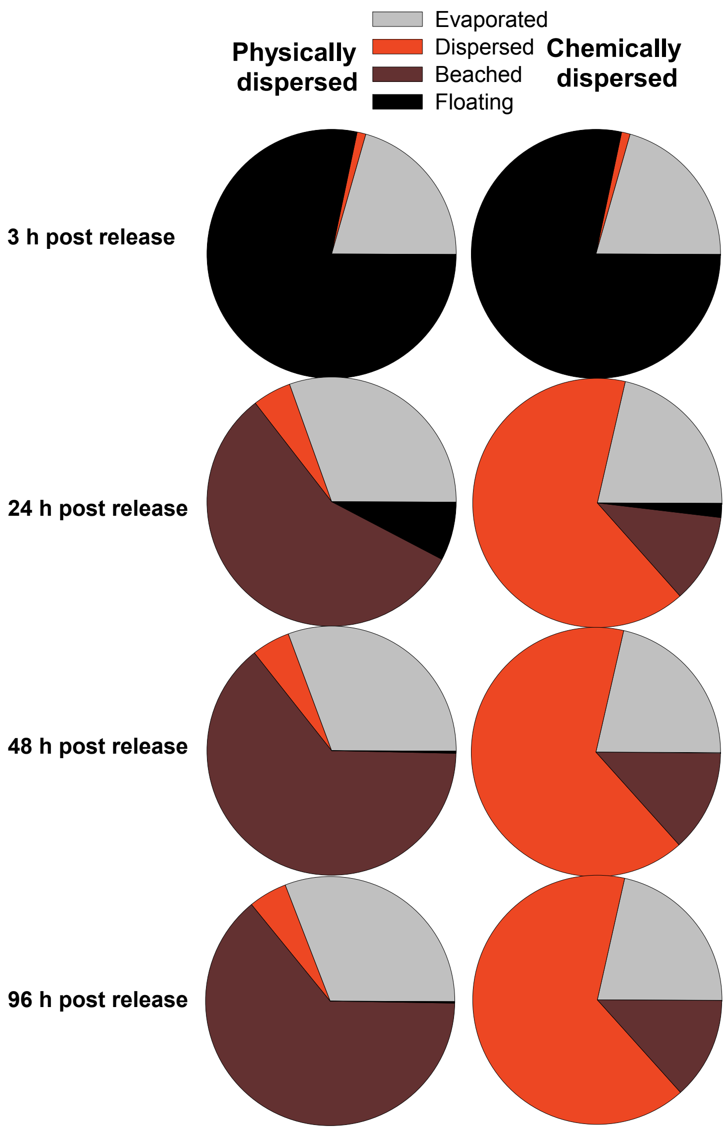

Figure 14. Oil budgets comparison as a function of time between the physically and chemically dispersed scenarios from a release of Qua Iboe Nigerian crude oil (210,000 gal) (***drill***) offshore from Charleston Harbor. Note that the chemically dispersed scenario assumes an extremely high dispersant effectiveness (80%)%), which is intended here to provide a worst-case exposure condition to aquatic organisms. Data from GNOME provided by A. Mearns, NOAA ERD.

Two summary statistics are obtained from GNOME to characterize oil concentrations of hydrocarbon for this ***drill***. These are the average and maximum (worst-case) concentrations in the top 5 m of the water column from each 30 min interval over the entire model run period (0 to 96 hours). Average and maximum (worst-case) modeled oil concentrations in the water column (cover on detailed in a later section) under the physically dispersed scenario are generally low (Figure 15) (Average: mean 0.07 mg/L, median, 0.05 mg/L, maximum 0.28 mg/L; Maximum (worst-case): mean 0.374 mg/L, median, 0.27 mg/L, maximum 0.73 mg/L). By comparison, the average and maximum (worst-case) modeled oil concentrations in the water column under the chemically dispersed scenario are in the 1- 3 mg/L range, with some exceptions (Average: mean 0.96 mg/L, median, 0.63 mg/L, maximum 3.2 mg/L; Maximum (worst-case): mean 2.92 mg/L, median, 1.59 mg/L, maximum 13.15 mg/L).

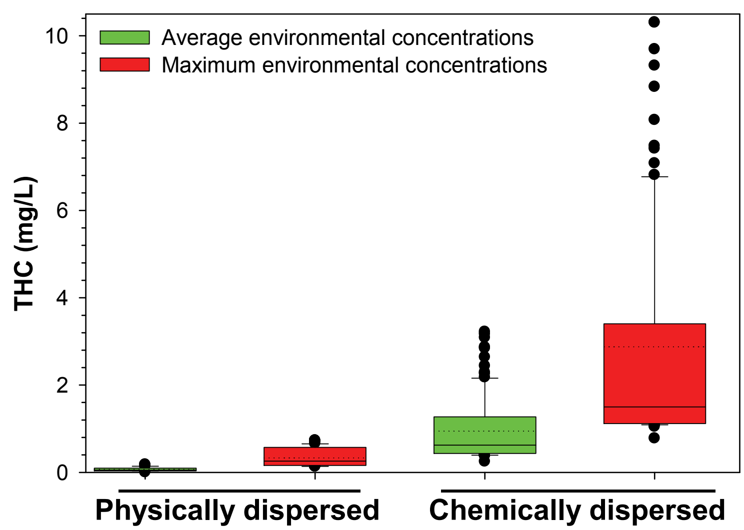

Figure 15. General box-plot overview of the expected oil concentrations physically and chemically dispersed scenarios from a release of Qua Iboe Nigerian crude oil (210,000 gal) (***drill***) offshore from Charleston Harbor. Note that the chemically dispersed scenario assumes an ***extremely high*** dispersant effectiveness (80%), and intended here to provide a worst-case exposure condition to aquatic organisms. Oil concentrations are the average and maximum concentrations in the top 5 m of the water column for each 30 min interval over the entire model run period (0 to 96 hours). The length of the box represents the distance between the 25th and the 75th percentile concentrations, while the whiskers represent the 5th and 95th percentile concentrations. The solid and dashed horizontal lines in the box represents the median and mean respectively. The closed circles indicate outliers.

Estimated Environmental Concentrations of Concern. Two queries are performed in DTox to facilitate the understanding of the potential impact of physically and chemically dispersed oil on species of interest off Charleston Harbor, South Carolina: selected species query, and shrimp query regardless of their global distribution. To ensure reproducibility of the analyses presented here, a complete list of relevant fields queried and selected in DTox is provided below (Figure 16):

- Query #1: Species – all shrimp-like species, plus sheepshead minnow, gulf killifish and longnose killifish (species of the genus, *Fundulus*), Inland silverside, and Red drum (25 species total); Exposure duration – 96-hours (*assumed to be a worst case exposure*); Endpoint metric – LC50; Oil name – All light and medium oils; Dispersant name – Corexit 9500, EC9500A, 9527, and EC9527A; Effects concentration analyte – all options containing Total Hydrocarbon Content (THC); Concentration – Measured; Paper Applicability – Moderate, High

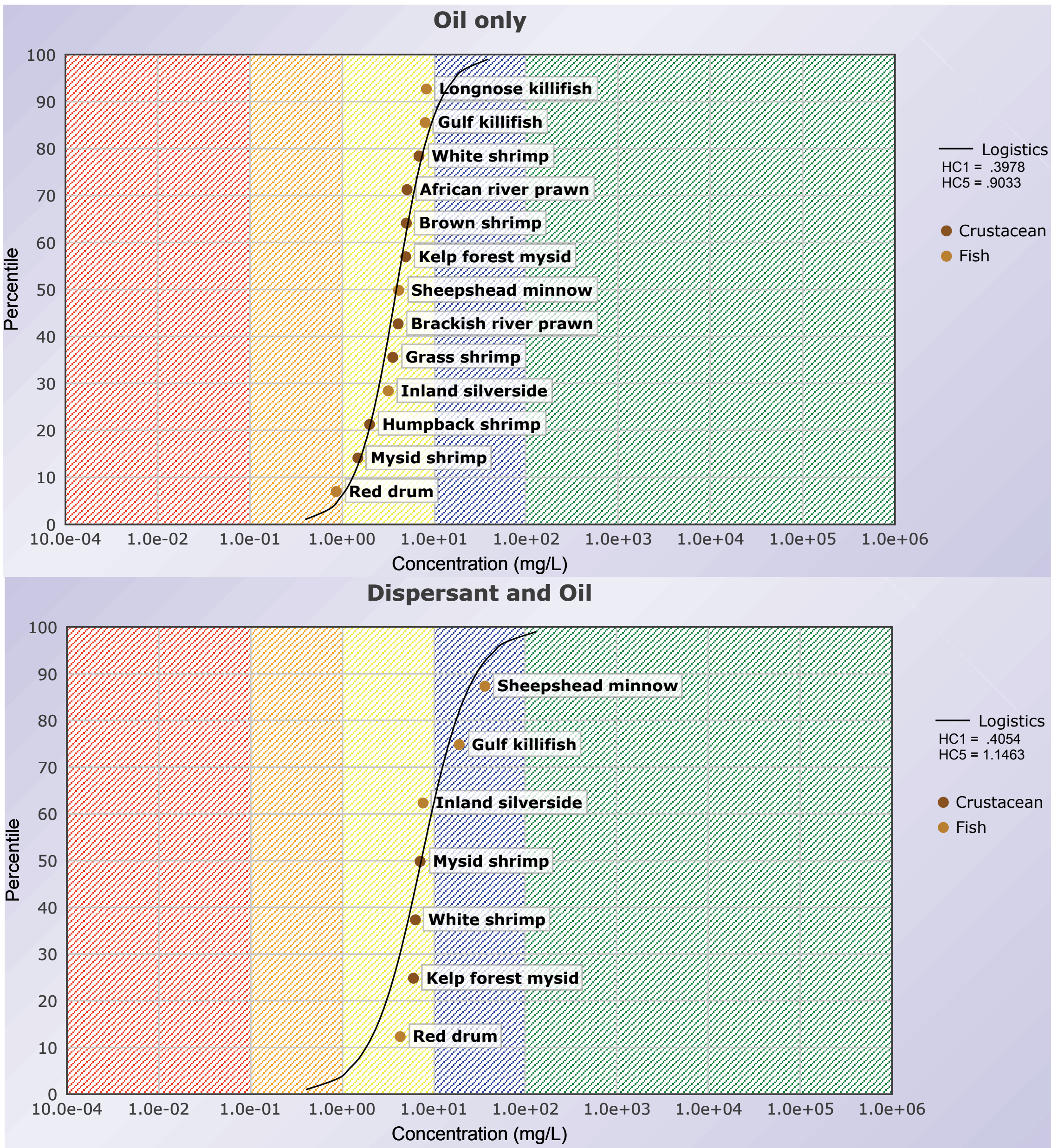

Figure 16. SSD generated following a data query in DTox for the ***drill*** off Charleston Harbor.

For the purpose of this ***drill***, the SSD with the most conservative hazard concentration (HC1=0.4 mg/L) (Figure 16, top) is used in further interpretations.

Potential Environmental Impacts. Average and maximum (worst case) oil concentrations for the physically dispersed ***drill*** scenario overlap 0% and 10%, respectively, of the most conservative 96h-SSD (Figure 17). A different pattern is observed with the ***drill*** scenario involving chemical dispersion of the released oil. Average and maximum (worst case) oil concentrations for the chemically dispersed scenario overlap 40% and 70%, respectively, of the most conservative 96h-SSD. Under the chemical dispersion scenario, 60% and 95% of the average and maximum (worst case) oil concentrations, respectively, exceeded the HC1. Exposures above the HC1 are limited to the first 40-50 hours post release for the average scenario, and >90 hours port spill for the maximum (worst case) oil concentrations scenario. All of these exceedances are limited to the top 5 m of the water columns (data not shown).

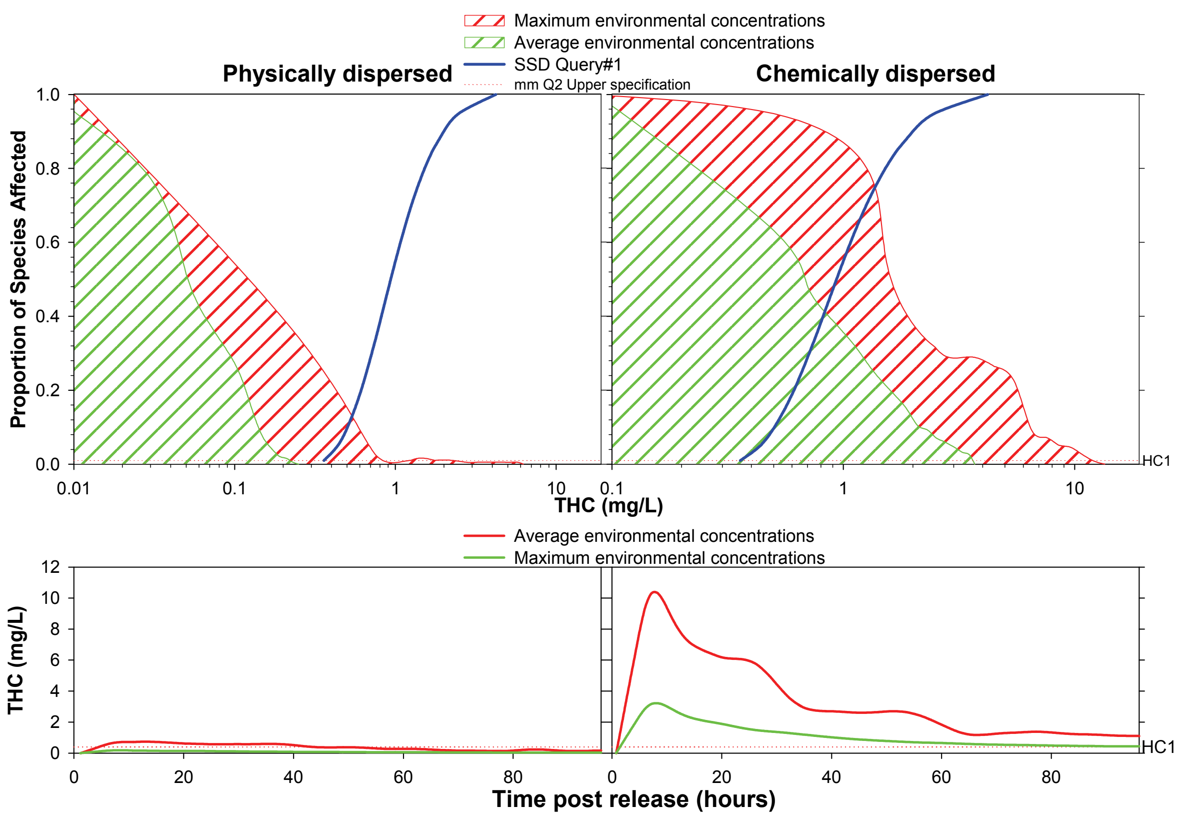

Figure 17. Cumulative average and maximum (worst-case) modeled oil concentrations relative to 96 h-SSDs (top), and average and maximum modeled oil concentrations as a function of time post release for a physically (left) and chemically dispersed (right) plume of a Qua Iboe Nigerian Crude spill off Charleston Harbor, SC (***drill***). As a reference, the benchmark for this drill is HC1=0.4 mg/L.

While these comparisons are useful, without a spatial context, these can lead to overestimation of risks. The areal extent of the water surface with modeled oil concentrations is also further analyzed for the chemically dispersed scenario. As shown in Figure 18, areal extent of the concentration bracket containing and exceeding the benchmarks (0.5-1 mg/L, 1-5 mg/L and >5 mg/L) grew from 11 km^2 6 hours post release to 63 km^2 120 hours post release. By contrast, most of the areal extent of the impacted water surface had concentrations in the 0.01-0.5

mg/L range (range: 5 km^2 6 hours post release to 190 km^2 120 hours post release). As shown in this exercise, the area of potential impact is relatively small and concentrated into an area 12 times the size of a standard football field. To put the information above into perspective (see also Figure 14) under the physical dispersion scenario, 85 km of coastal shoreline would be directly impacted, with maximum estimated oil stranded concentrations up to 47 gallons of oil per meter of shoreline (A. Mearns, pers. comm.). By comparison, under the chemical dispersion scenario, 64 km of coastal shoreline would be directly impacted, with maximum estimated oil stranded concentrations up to 10 gallons of oil per meter of shoreline. This information, and data presented in Figure 14, demonstrate that while there is an increased risk to water column organisms from dispersant use to mitigate the impacts of this particular spill (***drill***) (albeit concentrated into a relatively small area and to depths <5 m), the greatest environmental tradeoff is the reduced impact to shoreline habitats (both on extent and degree of oiling), and reduced amounts of floating oil which can pose adverse risks to surface marine species (e.g., birds and marine mammals).

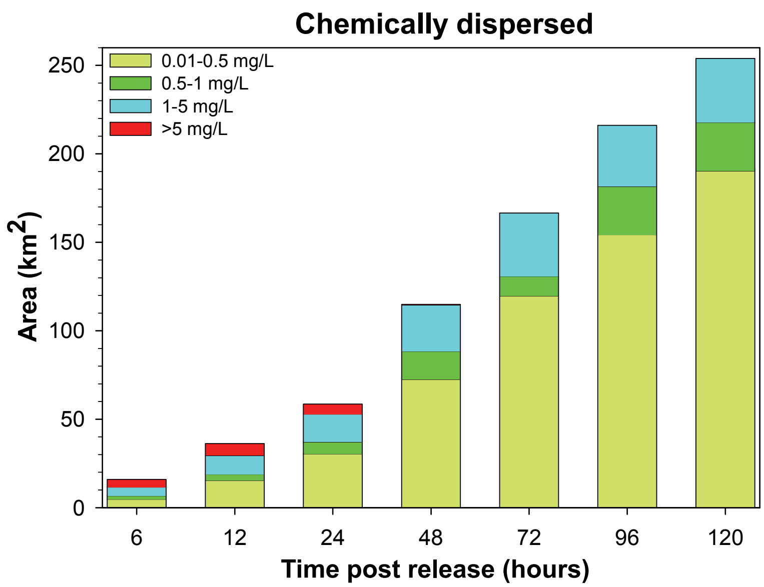

Figure 18. Water surface area impacted by a spill of Qua Iboe Nigerian Crude off Charleston Harbor, SC (***drill***), as a function of time post release (hours), and average oil concentrations. As a reference, the benchmark for this drill is HC1=0.4 mg/L.

While potential toxicological consequences may be expected from worst-case oil concentrations (e.g., maximum oil concentrations), these assessments are conservative as the benchmark used here is conservative and biased towards overprotection or marine species (i.e., based on 96 h exposure toxicity data). This degree of conservatism added to the fact that oil biodegradation is not taken into account suggests that oil concentrations would likely be lower than those predicted by the model.

5.0 Discussion and Importance to Oil Spill Response and Damage Assessment and Restoration

5.1 DTox - Data Compilation, Demonstration, and Application

The primary intent of the exercises presented in Section 4.3 is to demonstrate the applicability of DTox as a tool to aid assessment performed during an oil spill response (spills or drills), and not to support or discourage the use of dispersants as a countermeasure to respond to off shore oil spills. Important to note is the fact that both drill scenarios involved large releases of oil and high dispersant effectiveness, leading to exceedances of benchmark values. It is also important to note that a conservative approach is used, by deriving benchmark values derived from 96-h toxicity data, which is assumed to be a worst case exposure scenario. Specific data limitations identified though drills in Section 4.3 include:

Drill #1:

- Queried data does not contain data on the species of interest (American lobster)
- There are insufficient data for Kuwait crude oil and the queried data contain only a few records for a related oil (Forties)
- Larvae and other early life stages of crustaceans are underrepresented in the database

Drill #2:

- Queried data contained toxicity data for species found in the Charleston Harbor area, including species listed in Table 4. However, queried data does not contain toxicity data for other relevant species of concern
- There are insufficient data for Qua Iboe Nigerian Crude
- Larvae and other early life stages of crustaceans are underrepresented in the database

One of the greater limitations encountered during the development of SSDs to support decision-making for these two drills is the lack of toxicity data for shorter exposures (e.g., <24 hours). Data for spiked flow-through exposures, which are intended to address the dilution that occurs in field conditions, are also limiting. These types of information are important because oil concentrations are expected to peak immediately after release, especially immediately after chemical treatment with dispersants, and these conditions are not adequately addressed in most tests for which toxicity data are available. Another great limitation is that the large majority of studies on oil toxicity typically report measured concentrations of the exposure media on the basis of petroleum hydrocarbons, without providing a detailed chemical characterization of the fractions that most contribute to toxicity, polycyclic aromatic hydrocarbons (PAHs). Despite existing data limitations, the exercises about showed that DTox provides information that can be used to inform tradeoff decisions based on the current state of knowledge.

As discussed above, one of the greatest limitations of the existing toxicity data and, consequently, on the results and applicability of this project to oil spill response and damage assessment and restoration, deals with the lack of data derived from environmentally realistically exposures. This issue is not new and has been extensively discussed in the past (Aurand and Coelho, 2005; Barron and Ka'aihue, 2003; NRC, 2005; Singer et al., 1995). Consequently, deriving toxicity data from laboratory conditions that address dilution, water mixing, and changing exposure concentrations over time, continues to be a large data gap. Equally important is the reporting of toxicity data on the basis of measured exposure concentrations (specially for a complex mixture such as oil), instead of nominal concentrations, as this is the only reliable metric that allows for appropriate characterizations of potential risks (e.g., Coelho et al., 2013; NRC, 1989, 2005). The importance of reporting measured concentrations was not taken lightly during the development of DTox, as reflected in the applicability score given to each data source.

Another source of data uncertainty emerging from this project is related to toxicity of dispersants and physically and chemically dispersed oil to untested species (see for example Section 4.3), or to species protected under the Endangered Species Act. While lack of toxicity data on a number on important species or species of special interest is a source of concern, the approach implemented in DTox, namely the use of SSDs, can facilitate derivation of conservative benchmark values that may protect many of the untested species. As demonstrated here and in related studies using and applying SSDs in oil research (Barron et al., 2013; Bejarano et al., 2013; de Hoop et al., 2011), the use of these SSDs can provide a mechanism by which existing toxicity data can help assess risks to untested species. Another important use of SSDs (shown here and discussed in Barron et al., 2013) is that it allows for visualization of toxicity data for many standard test species, supporting the notion that these species are appropriate surrogate for many non-standard test species and untested species. However, future toxicity testing should not only focus on standard toxicity test species, but also on other test species easily reared and maintained under laboratory conditions. Additional toxicity data of value to the oil spill community and of interest for future updates of DTox also include toxicity testing on different life stages of the same species. In addition and as discussed above, toxicity data for short exposures is lacking in the literature. In Dtox, <10% of all records are derived from exposures <8 hours, while 83% of all records came from standard exposure durations used in toxicity testing (24, 48, 72, and 96 hours combined), mostly from 96 hour exposures (50% of all records).

Despite data deficiencies and uncertainties, existing toxicity data now compiled in DTox provide useful information to end-users and oil spill practitioners, so long as this information is used within the context of what is environmentally realistic to occur under field conditions. With that caveat in mind, the existing knowledge on the toxicity of dispersants and chemically dispersed oil can be useful in informing assessments and decisions regarding dispersant use.

The effectiveness, usefulness, and transferability of DTox to oil spill response are evaluated through two oil spill drills (Section 4.3), dispersant-related workshops, and dispersant-related assessment (Section 7). These exercises show that, despite existing data limitations, DTox provides information that can be used to inform tradeoff decisions based on the current state of knowledge. The data in DTox have the potential to contributed to a better understanding of the biological effects of dispersants and oil in the aquatic environment, and can provided useful information to both, environmental assessment and decision making efforts. Future efforts will focus on maintaining and updating data in DTox, and on expanding its capabilities for use by the oil spill community.

6.0 Technology Transfer

A critical step that facilitated the success of this project was the engagement of industry, government agencies, and academia in contributing to the development of this database, as well as to their transferability to several related purposes. Data currently in DTox were used to support two NOAA efforts. The first effort involved a dispersant workshop where there were discussions on the current state of knowledge regarding the toxicity of dispersants and chemically dispersed oil. Through several examples and using data primarily from DTox, concerns regarding potential toxicological effects were addressed. The second effort involved data compilation to support an oil spill drill between Canada and the U.S. (CANUSLANT, June

17-20, 2013). Data from Dtox were used to compare the relative sensitivity of American lobster larvae to naturally and chemically dispersed oil, relative to the sensitivity of other species for which larvae data are available in DTox. This analysis showed that American lobster larvae are relatively sensitive, compared to other species of larvae, as it falls within the lower end of the SSD curve. This information was used during internal discussions within the Unified Command during the drill. Data from DTox have also been used to support the preparation of a biological assessment on the pre-approved use of dispersants. These data, transferred in the form of data summaries and figures, provided some of the scientific bases for assessments of potential adverse effects to aquatic species, included those under the Endangered Species Act. Additional efforts were undertaken to transfer this wealth of knowledge to oil spill responders including the government, industry, and academics via web-based seminars (three in total), and presentations at national conferences (see Section 7).

As discussed above, DTox has been used to facilitate the communication of risks with the public and the scientific community concerned about the use of dispersants. DTox also has the potential to contribute to discussions taking place during consensus Ecological Risk Assessment (ERA) workshops where agency scientists and responders discuss the tradeoffs of the use of dispersant and other response options. In past ERA workshops, participants had to rely on adhoc compilations of toxicity data for oil and dispersed oil.

The results of this project and the practical application of information gathered through this effort are currently being prepared in the form of manuscripts to be published in peer-review journals. Run-time versions of DTox were distributed to end-users (in the form of a downloadable file) engaged with oil spill research and response.

7.0 Achievement and Dissemination

7.1 Workshops

Bejarano A.C. and A. Mearns. The Toxicological Effects of Dispersant Use in Oil Spill Response: Facts versus Fiction. Hawaii Dispersant Workshop. Honolulu, May 5, 2013. *Number of attendees: 20.*

7.2 Off-Site Training Seminars

Bejarano A.C. DTox for Scientific Support Coordinators (NOAA, Emergency Response Division). November 5, 2013. *Number of attendees*: 10.

Bejarano A.C. DTox for End-Users (Federal and State Agencies, Industry, Academics, International end-users). December 18, 2013. *Number of attendees*: 10.

Bejarano A.C. DTox for Scientists (NOAA, Assessment and Restoration Division). January 6, 2014. *Number of attendees*: 9.

7.3 Presentation

Bejarano, A.C, V. Chu, J. Dahlin, J. Farr. 2013. DTox: A Quantitative Database of the Toxicity of Dispersants and Chemically Dispersed Oil. SETAC. Nashville, TN, USA. (Poster)

Bejarano, A.C, V. Chu, J. Dahlin, J. Farr. 2014. DTox: A Quantitative Database of the Toxicity of Dispersants and Chemically Dispersed Oil. 2014 International Oil Spill Conference. Savannah, GA, USA. (Oral; accepted February, 2014)

7.4 Publication

Bejarano, A.C., J. Clark, G.M. Coelho. 2014. Issues and Challenges with Oil Toxicity Data and Implications for their Use in Decision Making: a Quantitative Review (accepted in *Environmental Toxicology and Chemistry*)

Bejarano, A.C, V. Chu, J. Dahlin, J. Farr. 2014. DTox: A Quantitative Database of the Toxicity of Dispersants and Chemically Dispersed Oil. Proceedings of the 2014 International Oil Spill Conference. Savannah, GA, USA. (accepted February, 2014).

Bejarano, A.C and M. Barron. 2014. Development and Practical Application of Oil and Dispersant Interspecies Correlation Models for Aquatic Species (in prep).

Bejarano, A.C, A. Mearns, V. Chu, J. Farr. 2014. Use and Application of Acute Toxicity Data in Spill Response with Focus on the Use of Dispersants (in prep).

7.5 Other Forms of Dissemination

Computer Software: Bejarano, A. C. and J. Dahlin. 2013. DTox: a Quantitative Database of the Toxicity of Dispersants and Chemically Dispersed Oil, Version 1.1 [Computer Software]. A project for the National Oceanic and Atmospheric Administration, and the University of New Hampshire's Coastal Response Research Center (Contract No. 13-034). Research Planning, Inc. Columbia SC.

Internet information dissemination http://www.researchplanning.com/projects/dtox-worldwide-quantitative-database-toxicity-dispersants-chemically-dispersed-oil/, which includes a link to a training video.

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Appendix A- Quality Assurance Quality Control Plan (Revised)

DTox: a Worldwide Quantitative Database of the Toxicity of Dispersants and Chemically Dispersed Oil

A-1 Project Description

The ability to rapidly assess the toxicity of physically and chemically dispersed oils is a goal shared by government, industry, consultants, and academic groups involved in oil spill response. One common need of the oil spill community is the unrestricted and rapid access to available toxicity data on dispersants and chemically dispersed oils. However, there are no centralized data repositories gathering decades of existing toxicity data. The end-result of this project, the Dispersant and Chemically Dispersed Oil Toxicity Database (DTox), addresses that shared need of the oil spill community, and contributes to a better understanding of the biological effects of dispersants and dispersed oil. This quantitative data compilation provides the basis for a more thorough assessment of levels of concern for dispersants and chemically dispersed oil, and helps improve risk estimates during oil spills or drills by allowing the selection of data that most closely match the needs of the end-user. The ultimate goal of this effort is the synthesis of information in a meaningful way to improve scientific decision-making as well as to provide rapid access to centralized toxicity data. To meet the goals of this project, a Quality Assurance Plan was designed to meet the following objectives:

- Outline the procedures and data management implemented during the development of this project to ensure that data selection and data entry, storage, and management are of high quality;
- Provide a means by which the quality of information produced can be maintained throughout the project;
- Provide a sound basis for documenting, evaluating, and verifying the accuracy of data selection and entry;
- Provide guidelines for the preparation and review of project plans and reports; and
- Provide the means that would allow the end-user assess the quality of data compilation efforts.

A-2 Objectives

The main objectives of this project are to identify, evaluate, compile, and integrate all available worldwide toxicity data on dispersants and chemically dispersed oil generated under laboratory and field conditions, and to generate an interactive tool that can assist the oil spill response community in management decisions regarding the use of dispersants.

The specific objectives of this project are to:

1. Identify documents, peer-review and gray literature (e.g., field, laboratory, mesocosm, accidental oil spills), reporting the toxicological effects (acute and chronic) of dispersants and chemically dispersed oil;
2. Rigorously evaluate each data source for their quality and potential for inclusion in the DTox database;
3. Compile all quantitative information including all relevant fields (e.g., species, exposure conditions, oil type and weathering, etc.);

4. Integrate the above information into a tool that can be used by the end-user to guide management decisions regarding the use of dispersants; and
5. Test the suitability of the compiled quantitative data for use in spill response at two pilot study areas.

This effort focuses on aquatic fauna, primarily invertebrates and fish, including all life stages, and includes all pertinent information regarding experimental methods and settings including, oil and dispersant type, oil weathering stage, dispersant to oil ratios, and exposure duration, type (continuous vs. spiked) and concentrations (e.g., oil, PAHs or TPHs). Information from each study also includes analytical chemistry methods and the reported analyte(s). Each paper is carefully evaluated to ensure inclusion of good quality research.

A-3 Quality Assurance

Data included in DTox are evaluated following a strict set of rules aimed at selecting the best available and suitable data. Data entered into the database went through Quality Assurance and Quality Control (QA/QC) procedures including periodic reviews of the database to ensure accurate data entry. Specific QA/QC procedures are described below for each of the main objectives of this project.

Papers initially considered for inclusion in the database met the following minimum criteria:

- Articles published in English; except when information in another language could be accurately translated;
- Full scientific articles, numbered government reports, and independent consultant and industry reports (abstracts are not considered);
- Data should be from original scientific publications and peer review literature (primary source) rather than from reviews or unverifiable sources; a few exceptions are made, but data source penalized via applicability (see below)
- Species' common and/or scientific name, oil source, and dispersant type should be clearly stated;
- Biological test methods should be described, or reference made to an appropriate published method;
- Effects endpoints of treatment tests should be acceptable relative to control tests; studies that do not discuss or mention the use of controls where included on a case by case basis; and
- Methods for the chemical analysis used to quantify exposure concentrations associated with toxicological effects should be described or referenced.

The implementation of these selection criteria led to the exclusion of large amounts of information. Additional data are reconsidered for inclusion by relaxing the selection criterion, but potential data inaccuracies are noted within the database (see below for details). All papers and documents evaluated for potential inclusion in DTox are classified as follows:

- A1: Meets the selection criteria. A1 papers and documents are evaluated and included in the database;

- A2: One or more of the selection criteria are questionable. A2 papers are be kept aside for further consideration and, if included in the database, potential data inaccuracies are be clearly noted;
- Rejected: Does not meet the selection criteria or does not contain data valuable to the goals of this project.

A-3.1 Data Compilation

Data entry followed a systematic, consistent, and accurate review process of the available literature. A carefully designed database template was developed, which included all the relevant database fields (data elements) and as many standardized data entries as possible (Table A-1). Data element definitions and descriptions are summarized in Table A-2. One of the fields within this template was created to enter the applicability of each paper (e.g., high, moderate, low). Applicability is judged based on source-specific considerations including. A brief summary of the criteria used in the assessment of applicability is as follows:

High:

- Papers reporting effects concentrations based on measured analytes (particularly those involving oil exposures)
- Dispersant to oil ratios consistent with typical recommended formulations
- Exposure conditions following existing recommendations for oil spill research

Moderate:

- Papers reporting effects concentrations based on measured analytes (particularly those involving oil exposures)
- Papers reporting effects concentrations for dispersant only exposures as nominal
- Dispersant to oil ratios consistent with typical recommended formulations
- Exposure conditions following standard toxicity testing laboratory practices

Low:

- Papers only reporting effects concentrations as nominal (particularly those involving oil exposures)
- Papers not clearly stating if the reported effects concentration are nominal or measured
- Papers with missing critical information (e.g., exposure conditions, analytical methods)
- Papers reporting only No Observed Effects Concentration (NOEC) or Lowest Observed Effects Concentration (LOEC)
- Papers with toxicity data from unverifiable sources

Note: Source applicability is assigned to individual papers and not to individual records. A paper reporting toxicity data based on oil loading rates (nominal exposures) also reporting effects concentrations based on measured analytes would have the same applicability assigned to each record entered in DTox. Also it is important to note that paper applicability is based on the relevance of its data to spill response, and not on the overall scientific merit of individual papers.

When entering data into the database template, the following rules are implemented:

- To ensure completeness and accuracy, information is entered as not reported (NR) when information is not available, or not applicable (NA) when the field does not apply (e.g., toxicity testing with dispersant only has a NA dispersant to oil ratio);
- To ensure accuracy in data entry, all numbers between zero and one are reported with a preceding zero (e.g., 0.5 not .5);
- Periods are only used to represent a decimal points;
- Effects concentrations are entered as they appear in the original document (no rounding up or down is allowed);
- Drop down menus and standardized terminology are used for unique information (e.g., COREXIT 9500);
- Non-standardized data entry fields are entered exactly as they appear in the original source. Examples include: common name, scientific name, effects concentration, water temperature and complete citation; however, current scientific names are checked and replaced are needed, noting changes in reported versus final scientific names (see below);
- Units of numeric data are entered based on a standardized values (e.g., mg/L for effects concentrations, hours for exposure duration);
- Data sources with detailed data chemistry are noted within the database, and chemistry data entered into a separate form;
- Unique citations are assigned a numeric code that matches the citation's code of the bibliographic database (EndNote®); this unique numeric code provides the link between the data entered and the bibliographic citation; and
- A "Notes" field should include only relevant data not captured within other database fields.

Upon completion of data entry, global changes are applied to "new" data fields in the database. Examples include species (global) distribution, habitat, and water depth. Consideration was given to potential changes in habitat and water depth by species-specific life stages. Species distribution databases were consulted to accurately enter this information by species. Additionally, common and species names are checked, and global changes made including standardization of common names and assignment of official species names (e.g., *Mysidopsis bahia* changed throughout to *Americamysis bahia*). Any changes made to the original data source are clearly documented.

As part of the QA/QC components of this project, periodic reviews of the database are made to ensure accurate data entry. A minimum of 15% of all data sources are reviewed for accuracy and completeness. Critical steps of the QA/QC process includes the review of currently accepted scientific species names, standardization of column content and applicability criteria, and identification of duplicate data (e.g., several papers by the same author(s) reported in several report/manuscripts).

Table A-1. List of standardized data entry fields. In all cases, not applicable (NA), not reported (NR) can be entered in the field cell. Non-standardized data entry fields include: effects concentration and complete citation. In brackets [], descriptive information related to a particular entry field. See Table A-2 for details.

Field Type	Field Name	Examples
		Effects Database
Species	Common name	Inland silverside
	Scientific name	*Menidia beryllina*
	Taxonomic group	Crustacean, fish, coral, mollusk, other[1]
	Life stage	Adult, juvenile, larvae, egg
	Species distribution	Tropical, subtropical, temperate, frigid, pandemic
	Species habitat[2]	Benthic, water column, epibenthic
	US standard test species	Yes, No
Experimental conditions and settings	Study type	Laboratory, field, mesocosm, wave tank
	Water type	Freshwater, seawater
	Dispersant/Oil Treatment	Dispersant only, Dispersant and Oil, Oil only
	Oil name	Alaska North Slope crude oil, South Louisiana crude oil
	API gravity	[Oil specific. Most data from NOAA's ADIOS (Automated Data Inquiry for Oil Spills)]
	Oil class (based on API gravity)	Light, Medium, Heavy, Extra-heavy
	Oil stage	Fresh, weathered, biodegraded
	Dispersant name	COREXIT9500, DISPERSIT, [including mechanical dispersion]
	Dispersant to oil ratio	1:10, 1:20
	Exposure conditions	Continuous, spiked, flow through, field
	Exposure duration (h)	24 hour, 96 hour
	Temperature (°C)	6 °C, 25 °C
Endpoints	Endpoint	Mortality, growth/development, behavior [grouped by endpoint type]
	Endpoint metric- Acute[3]	Acute: LC50, EC50, LOEC; Chronic: EC50, LOEC
	Qualifier	>, <, NA [these are qualifiers associated with the reported effects concentration]
	Effects concentration (mg/L)	200
	Effects concentration range	[Minimum|Maximum or Lower|Upper confidence interval of the reported effects concentration]
	Effects concentration analyte[4]	Total PAHs, TPHs, THCs
	Reported effects concentration	Measured, nominal
	Analyte endpoint	Initial, Final
	Analytical methods	Fluorometry, GC-MS
Data Source	Complete citation	Author, Year, Title, Journal/Agency
	Endnote Reference Locator	[value assigned to each citation entry in Endnote]
Other	Paper selection criteria	A1: Meets the selection criteria A2: One or more of the selection criteria are questionable Rejected
	Paper applicability	Low, Moderate, High, Rejected

Field Type	Field Name	Examples
	Detailed analytical chemistry	Yes, No [if yes, data extracted and entered into chemical database]
	Duplicates	[It includes individual records identified as duplicates. Duplicates are not included in SSD calculations]
	Notes	[It includes any important information not captures in preceding fields]
Chemistry Database		
Analyte	General compounds	Total Petroleum Hydrocarbons, Polycyclic Aromatic Hydrocarbons
	Analyte name	n-Pentadecane (C15), Benzo(a)anthracene
	CAS#	50-32-8
Experimental conditions and settings	Dispersant/Oil Treatment	Dispersant only, Dispersant and Oil, Oil only
	Dispersant name	COREXIT9500, DISPERSIT, [including mechanical dispersion]
	Oil name	Alaska North Slope crude oil, South Louisiana crude oil
	Oil stage	Fresh, weathered, biodegraded
	Source type	Source oil, exposure media
	Concentration qualifier	>, <, NA
Analytical endpoint	Concentration (mg/L)	200
	Analytical methods	Fluorometry, GC-MS
Data Source	Complete citation	Author, Year, Title, Journal/Agency
	Endnote Reference Locator	[value assigned to each citation entry in Endnote]
Other	Notes	[It includes any important information not captured in preceding fields]

[1] Other include: bacteria (e.g., *Vibrio*), aquatic plants (e.g., giant kelp), phytoplankton, and echinoderms.
[2] Specific to the life stage of the tested species. For example, adult oysters would be categorized as inhabiting the epibenthos, while their larvae would be more likely found in the water column; [3] LC50: median lethal concentration, EC50: median effects concentration, NOEC: No Observed Effect Concentration, LOEC: Lowest Observed Effect Concentration;
[4] PAH: polycyclic aromatic hydrocarbons; TPH: total petroleum hydrocarbons; THC: total hydrocarbons content.

Table A-2. Key data element definitions.

Element Definition	Definition
Species common and scientific name	Refers to the species used in toxicity testing within each data source. Typically reported as common name and/or scientific name. Scientific names are checked against currently accepted names. Other information associated with species includes their taxonomic group, and the life stage used in toxicity testing. Both the global distribution of the tested species, and the habitat of the tested life stage are entered manually (typically not reported within data sources) based on information reported on global databases. Species are also assigned to whether these correspond to U.S. standard test species.
Water type	Refers to the nature of the water used in toxicity testing (freshwater or seawater).
Study type	Refers to the physical location where toxicity tests were conducted. It includes exposures under laboratory, field (e.g., outdoor uncontrolled conditions), mesocosm or wave tank conditions.
Dispersant/Oil Treatment	Refers to the type of aqueous exposure media used in toxicity

Element Definition	Definition
	testing. It includes oil only (e.g., physically dispersed oil, or water accommodated fraction), dispersant and oil (e.g., chemically dispersed oil, or chemically enhanced water accommodated fraction), dispersant (e.g., dispersant in aqueous solution).
Oil name	Refers to the oil type (typically reported) used in toxicity testing within each data source. Other information associated with each oil entered into the database includes oil class categories (light, medium, heavy, extra-heavy) assigned based on API gravity (most information from NOAA/ADIOS).
Oil condition	Refers to the nature of the oil used to derive the exposure media. It includes fresh, weathered (naturally or artificially) or biodegraded oil.
Dispersant name	Refers to the dispersant product (typically reported) used in toxicity testing within each data source. Entered as reported, typically commercial name. Other information associated with each dispersant, if used in combination with oil, includes the dispersant to oil ratio (DOR) used to prepare the aqueous exposure media.
Exposure conditions and other related exposure information	Refers to the type of experimental design used to conduct toxicity testing. Examples include: Constant static (with or without open vessels) – Refers to toxicity tests performed in the absence of low. Aqueous exposure media typically remains unchanged throughout the duration of the test. Static or semi-static renewal– Refers to the a test without continuous flow of solution, but with renewal of aqueous exposure media Flow through test– Refers to the continuous or very frequent passage of aqueous exposure media through a test chamber with no recycling. Spiked, pulsed, and spiked, flow-through (with or without open vessels) – Refers to initial spike in concentrations in the exposure media, which is allowed to decline over the duration of the exposure period. Other information associated with the exposure conditions include exposure duration and water temperature (not always reported).
Endpoints and other related endpoint information	Endpoint refers to the biological metric used to characterize toxicity. For the purpose of this database, endpoints are grouped by– Mortality (primarily LC50 data); Growth and Development (e.g., blue sac disease, embryo abnormalities) (primarily EC50 data); Reproduction (e.g., fecundity, fertilization inhibition, percent Hatch) (primarily EC50 data); Biochemical (e.g., CYP1A induction, EROD activity) (primarily EC50 data); Physiology (e.g., Heart rate, Impaired byssal activity, Impaired shell-closure) (primarily EC50 data); and Behavior (e.g., feeding rate, impaired swimming) (primarily EC50 data). Endpoints include: LC50 – Median lethal concentration that kills 50% of the exposed organisms at a specific time interval; EC50 – Median effects concentration that causes an response in 50% of the exposed organisms at a specific time interval;

Element Definition	Definition
	LOEC (Lowest Observed Effect Concentration)– The lowest concentration that causes a response statistically different from the control; and NOEC (No Observed Effect Concentration)– The highest concentration that causes a response statistically different from the control. Whenever available information is also included on control Endpoints– How test treatments compared to controls.
Effects Concentration and other related information	Effects Concentrations (mg/L) refer to the mean reported value. Note: All concentration information is standardized to a single consistent concentration unit (mg/L). Whenever reported, the database also includes: Minimum or lower confidence interval of the effects concentrations (mg/L)– Either the minimum or the lower confidence interval of the reported value; and Maximum or upper confidence interval of the effects Concentrations (mg/L) – Either the maximum or the upper confidence interval of the reported value. Information is also included on whether or not the effects concentrations were derived from measured or nominal concentrations of the exposure media. Analytes include: total polycyclic aromatic hydrocarbons (PAHs), total hydrocarbon content (THC), among other analyte types. If available, information is also entered on the analytical method used to characterize the exposure media: Fluorometry, GC-MS
Data Source	Refers to the source from which toxicity data are obtained. It includes a complete citation (author, year, title, journal/agency)

A-3.2 Tool Development

Data were initially entered into a spreadsheet and later migrated into a database program (FileMaker® Pro 12) with expanded capabilities. The database contains multiple data formats, including graphs and relational tables that reflect the nature of the data, and is flexible enough to allow incorporation of ongoing and future studies. The format and structure of this interactive database has the characteristics of a sister database CAFÉ (Chemical Aquatic Fate and Effects Database, NOAA/ERD), allowing current CAFÉ users to query data in DTox without additional training. A similar data structure also allows for potential integration of DTox with CAFÉ.

Integration of the data template into FileMaker® Pro 12 required the following, in operational order:

- Set field requirements to identify data errors during and after data import into FileMaker® Pro 12;
- Establish data check routines to identify legitimate and illegal field combinations (e.g., oil exposures only should not have a dispersant name), check for blank cells that should have either numeric or text entries, ensure that tables (e.g., DTox and chemistry table) are properly linked based on a common numeric code link (e.g., unique EndNote® citation number);
- Verify that 100% of the data fields have converged into FileMaker® Pro 12

- Design tools and reports that address the needs of end-users with disabilities (e.g., color blind) (Section 508 29 U.S.C. ‘749d) by selecting colors suggestions for color blind, as well as font size and style options;
- Run tests and other assessment procedures on the user interface tool, data queries and database products (reports, graphs) to make sure these meet the goals of the database. These test involved the selection of a variety of likely end-user scenarios (e.g., queries with few to several end-user requirement specifications);
- Additional tests aimed at improving system performance, response time, and vulnerability;
- Perform an internal review of an alpha version of the database within project team, including potential RPI end-users and members of CAFÉ’s development team;
- This phase of the QA/QC plan also included detailed documentation of decisions and procedures (e.g., data entry, tracking and manipulation), as well documentation of assumptions, theory, and parameterization used in developing Species Sensitivity Distribution curves (SSDs) (see below); and
- As part of the QA plan, computer file back-up procedures were regularly undertaken.

A beta version of the interactive database was designed and tested internally and externally for input and suggestions on improvement, prior to its dissemination among selected end-users. This process allowed the project team to address and improve the tool prior to its public release.

Key attributes of this database include:

- Easy to follow layout;
- Query screens to allow for user-specific data inclusion/exclusion;
- Interactive standard navigation buttons containing the most common search attributes;
- Search results displayed in tables and graphics;
- Appearance and functionality;
- A “How To” document detailing how to perform data queries, and a copy of the most recent QA/QC Plan; and
- A copy of the EndNote® library containing the complete list of citations of all papers reviewed as part of this project.

A-3.2.1 Data Queries and Species Sensitivity Distributions

The first version of DTox contains several navigation windows allowing data selection by the end-user. Following data selection, the remaining data are plotted in separate windows in the form of Species Sensitivity Distributions (SSDs). SSDs are constructed by calculating the geometric mean of reported toxicity for each individual species (by scientific name). Data included in geometric mean calculations are:

- Data with effects concentrations qualifiers equal to NA
- Effects concentrations with qualifiers ≥, ≤, > or < are not included in calculations
- Data identified as duplicates are not included in calculations
- Data from Rejected papers are not included in calculations

- SSDs are only generated for datasets with a minimum of 5 species

Additional details on SSDs include:

- SSDs are generated by fitting the empirical toxicity data to a logistic function defined by $F(\mathrm{x}) = \frac{e^{(\frac{\mathrm{x}-\mu}{\sigma})}}{\sigma\,(1+e^{(\frac{\mathrm{x}-\mu}{\sigma})})^2}$, x∈ R, with parameters μ(location) and σ (scale);
- Fitted SSDs do not include a "Goodness of Fit" test;
- Two Hazard concentrations (HC) (HC1 and HC5 equivalent to the concentrations at which 1% and 5%, respectively, of the species in the SSD may not be protected) are included for plots with a minimum of 5 species;
- Up to two SSDs are plotted per display window (Dispersant Only, Dispersant and Oil, Oil Only);
- 1 SSD per display window includes common names;
- 2 SSDs per display window omits common names;
- Data are displayed based on color coding selections; and
- All SSDs are plotted over a colored background representing a common scale of relative toxicity.

Scale
Very highly toxic (<0.1 mg/L)
Highly toxic (0.1-1 mg/L)
Moderately toxic (1-10 mg/L)
Slightly toxic (10-100 mg/L)
Not acutely toxic (>100 mg/L)

A-3.2.2 Tool Testing and Distribution

A stand-alone executable file (beta version) of the interactive database was further tested internally, and shared with external potential users and volunteers for input and suggestions on improvement, prior to its dissemination among selected end-users. This process allowed the project team to address and improve the tool prior to its public release. A stand-alone executable file of the first version of DTox was made available and shared with a selected number of end-users. End-users were asked to provide feedback and to report issues, which will be considered in future updates of the tool.

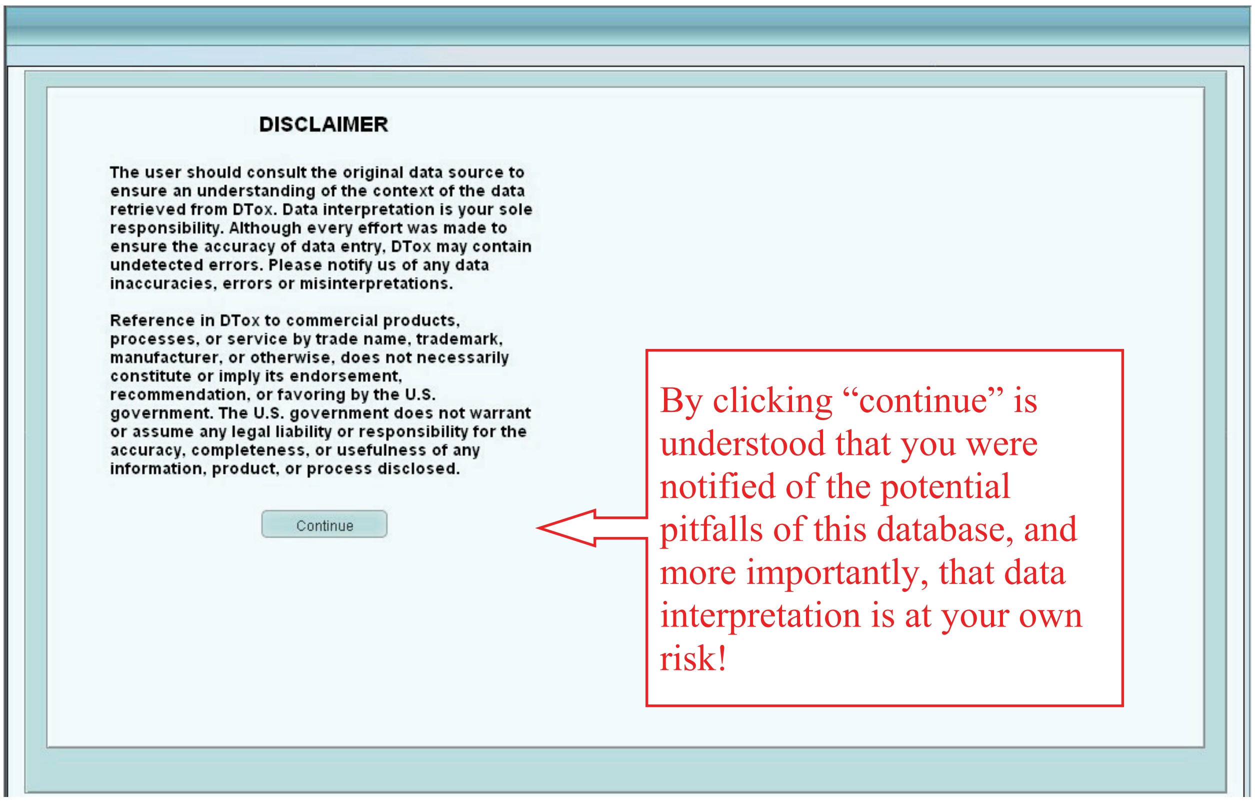
Appendix B- HOW TO "DTox" Version 1.

This document provides a brief overview on how to navigate through DTox. Before you start querying DTox, please read through the information presented here as it is intended to facilitate the use of this tool.

Performing queries in DTox-

Below you will find a series of screens shots through which you would have to navigate to perform the desired queries

1. **Disclaimer**

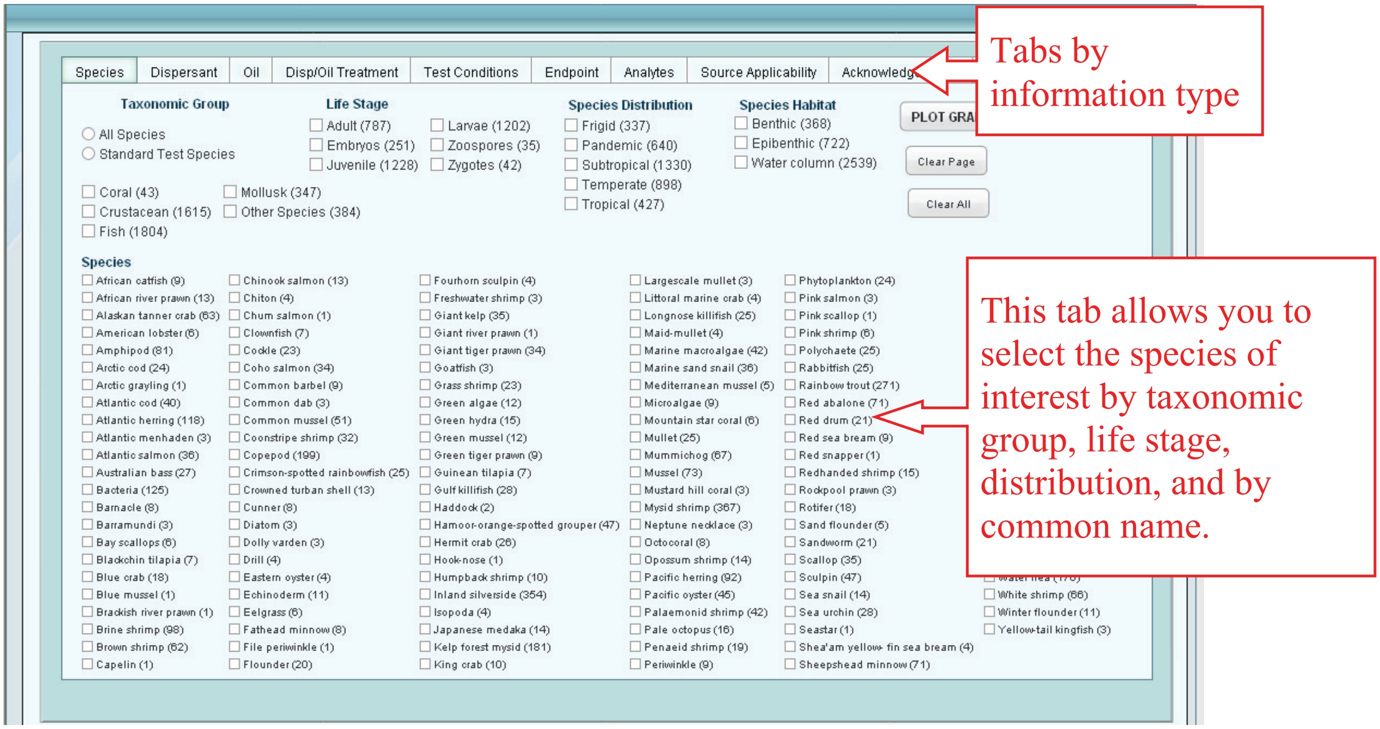


2. **Data selection**

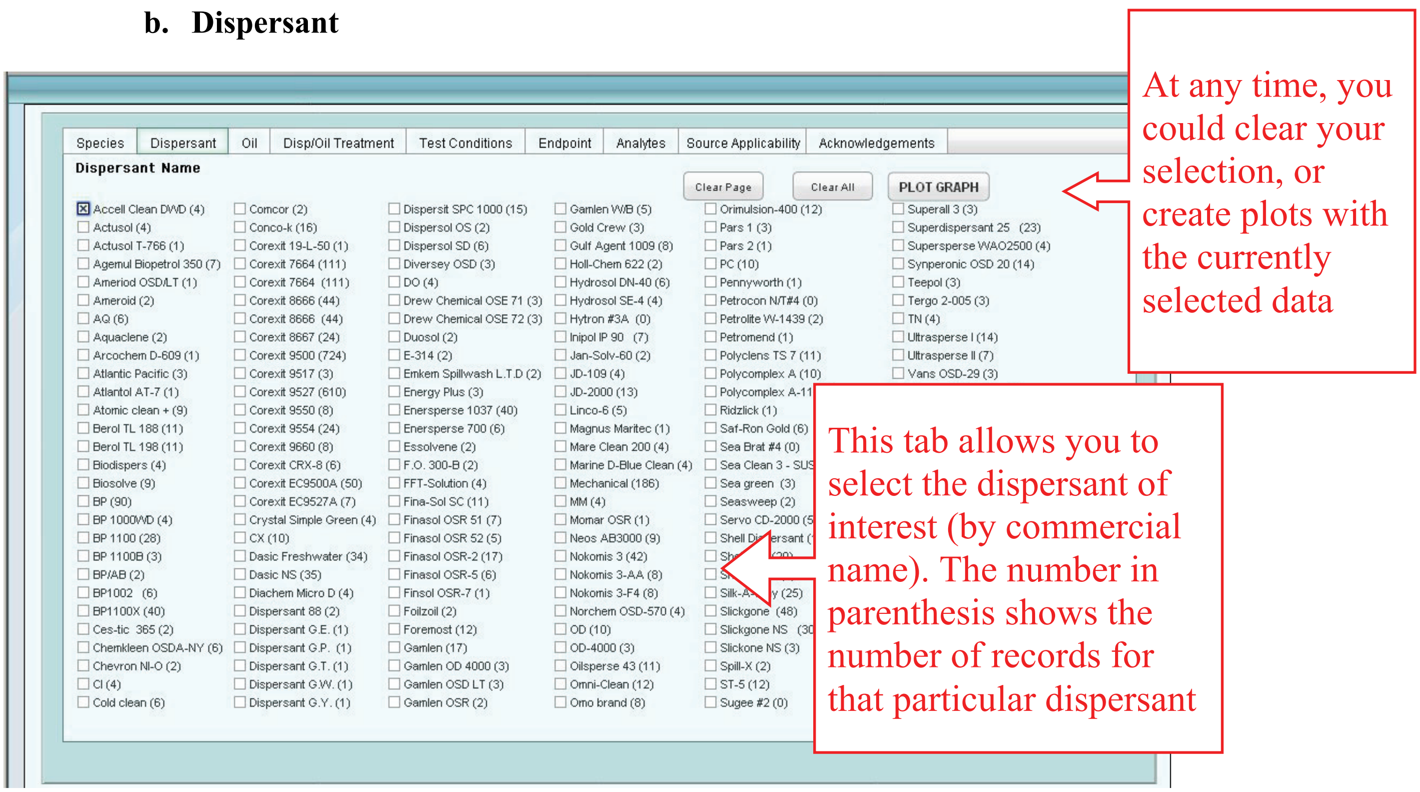
There are several windows allowing the selection of the type of data you want included in your query. **Note** that if selections are not made, by default, the program will select all the available data.

   a. **Species**

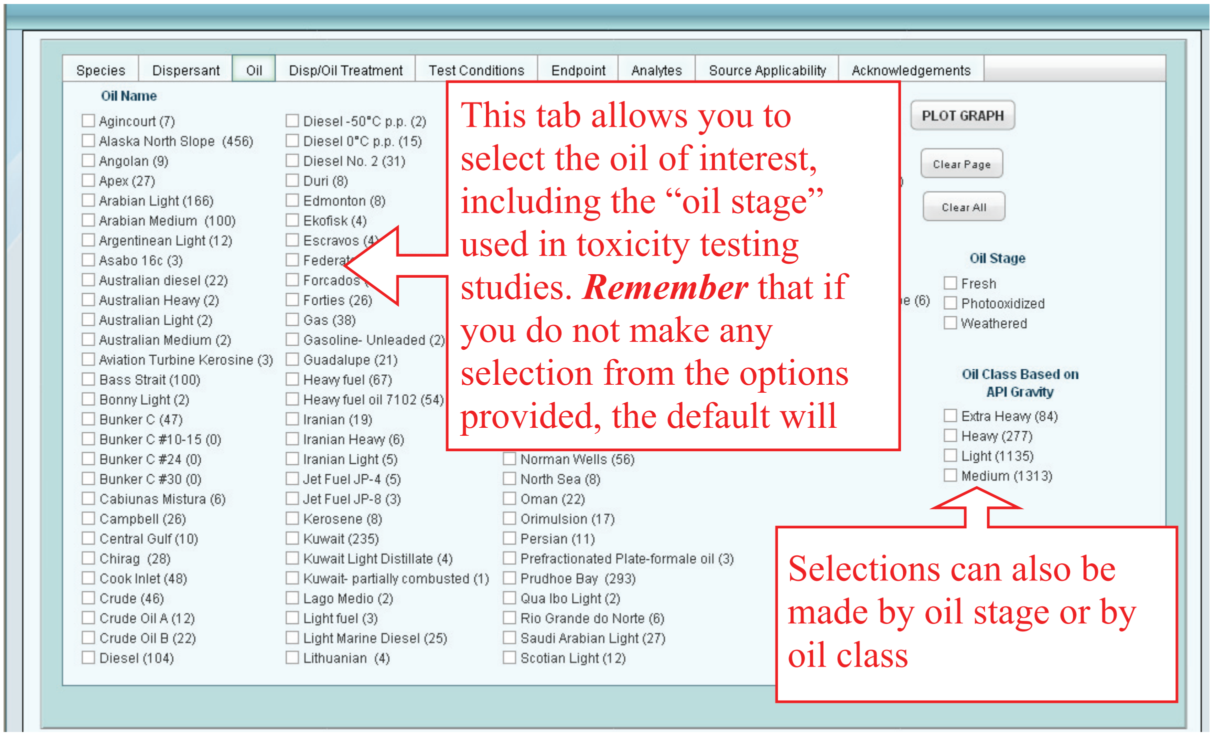
Note that while only common names are listed, these correspond to "unique" scientific names.



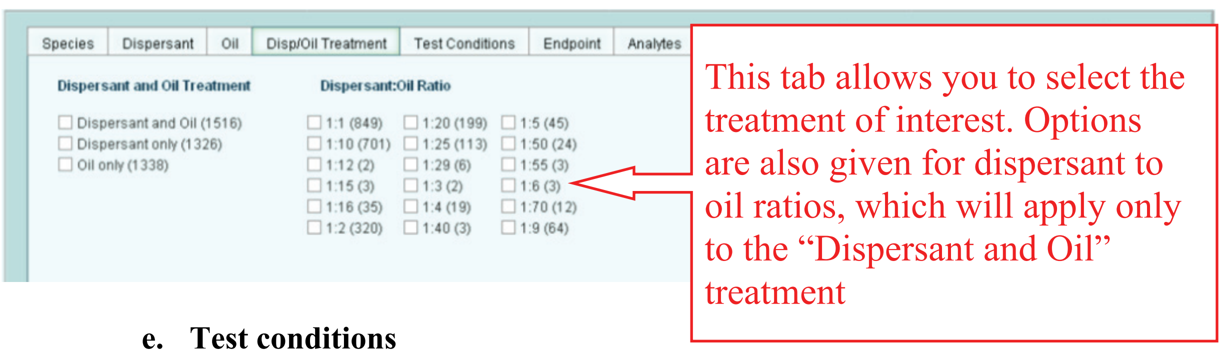
b. Dispersant



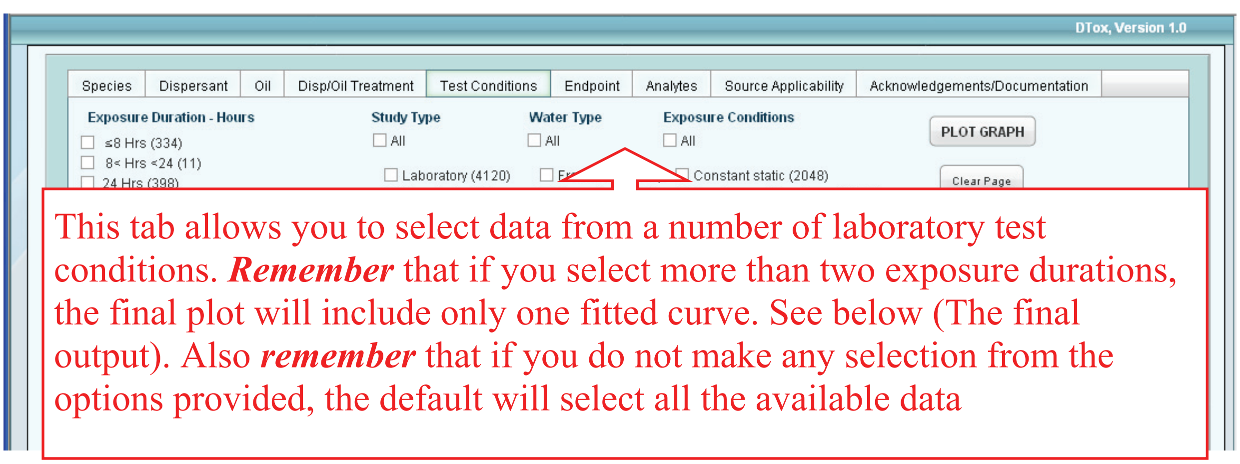
c. Oil



d. Dispersant/oil treatment

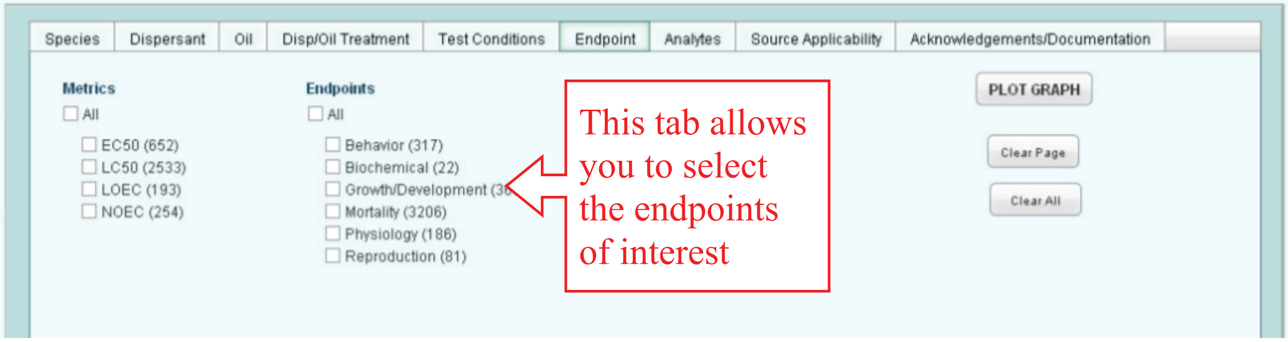


e. Test conditions

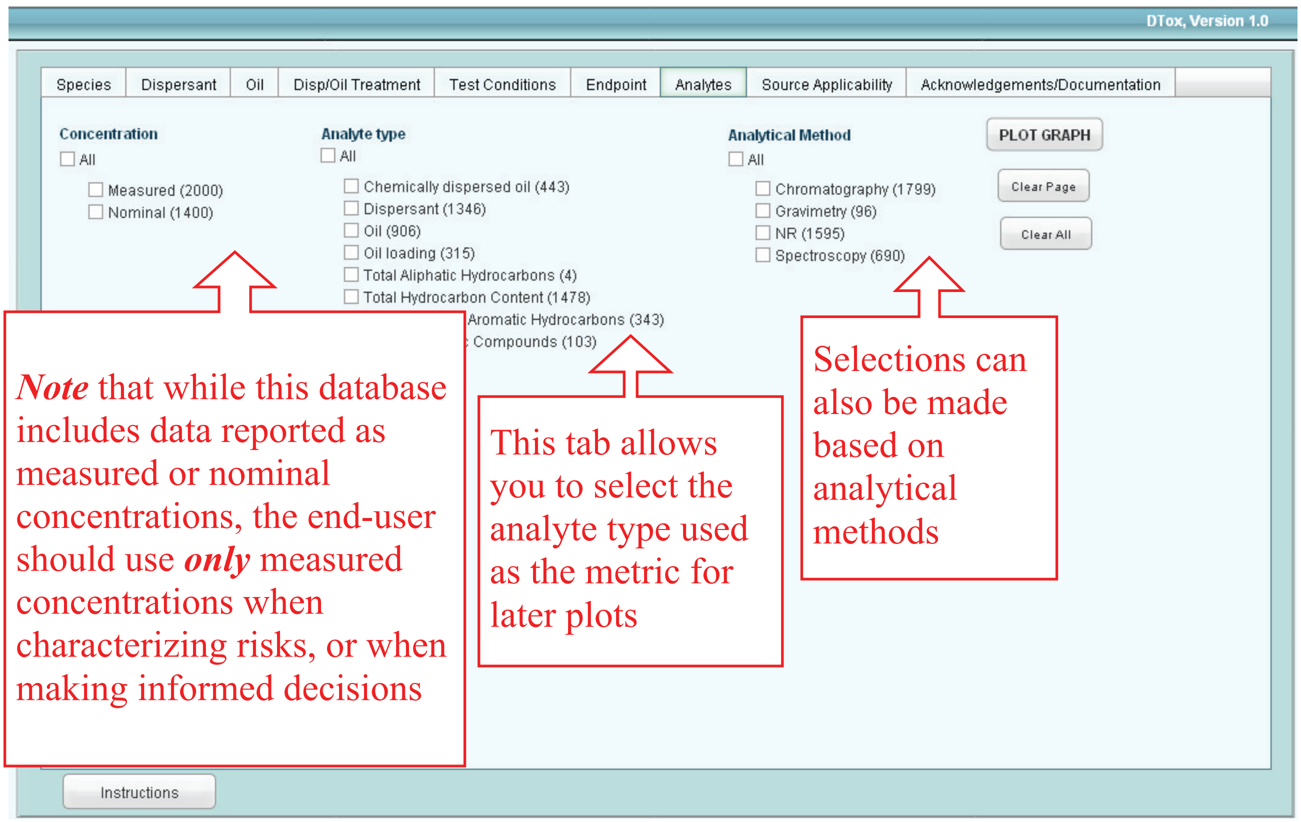


f. Endpoints

Toxicity metrics included in DTox include the most commonly reported types, grouped by lethal and sublethal endpoints.



g. Analytes



h. Source applicability

A detailed Quality Assurance/Quality Control plan was written prior to the development of this tool. A brief summary of the criteria used in the assessment of applicability[2] is shown below:

High:

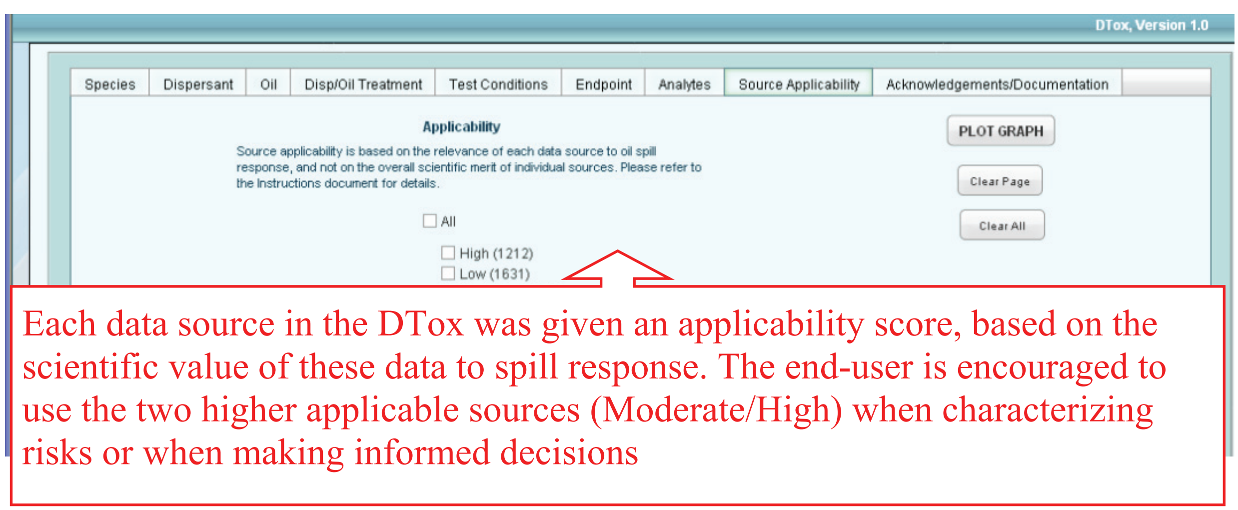
[2] "Applicability" is meant to indicate the applicability or usability of these data to spill response, and to the specific goals of this project. Assigning "applicability" to each data source is not to be interpreted as a judgment of the scientific quality of each data source.

- Papers reporting effects concentrations based on measured analytes (particularly those involving oil exposures)
- Dispersant to oil ratios consistent with typical recommended formulations
- Exposure conditions following existing recommendations for oil spill research

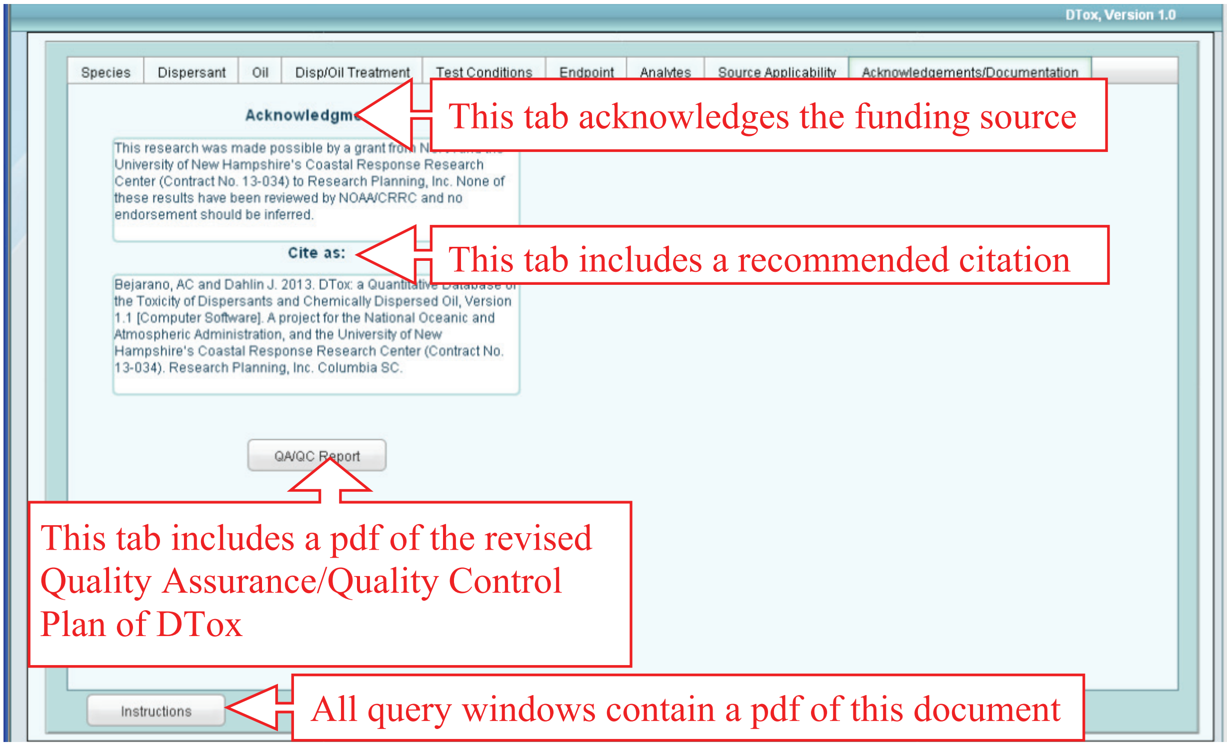
Moderate:
- Papers reporting effects concentrations based on measured analytes (particularly those involving oil exposures)
- Papers reporting effects concentrations for dispersant only exposures as nominal
- Dispersant to oil ratios consistent with typical recommended formulations
- Exposure conditions following standard toxicity testing laboratory practices

Low:
- Papers only reporting effects concentrations as nominal (particularly those involving oil exposures)
- Papers not clearly stating if the reported effects concentration were nominal or measured
- Papers with missing critical information (e.g., exposure conditions, analytical methods)
- Papers reporting only NOEC, LOEC effects concentrations
- Papers with toxicity data from unverifiable sources

Note: Source applicability is assigned to individual papers and not to individual records. A paper reporting toxicity data based on oil loading rates (nominal exposures) also reporting effects concentrations based on measured analytes would have the same reliability assigned to each record entered in DTox.

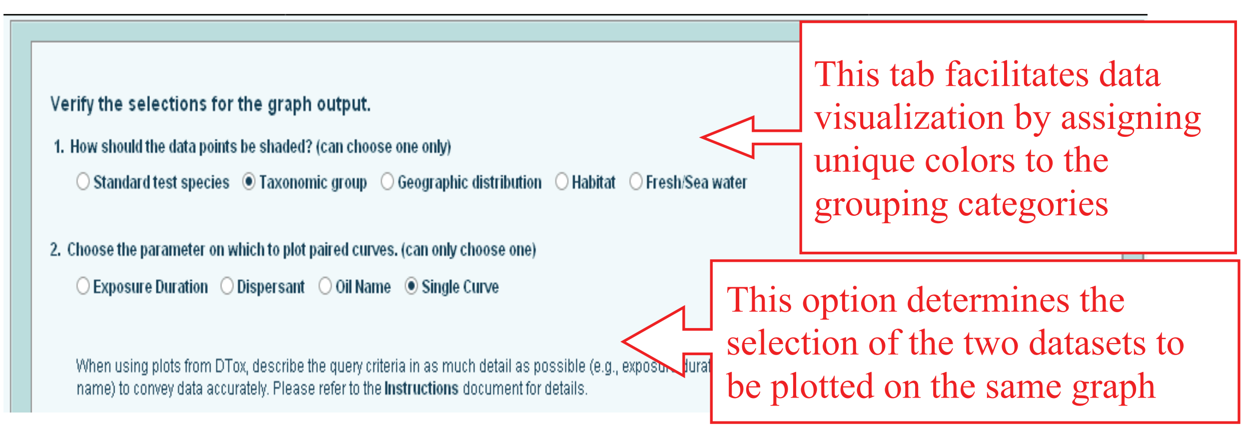


i. Acknowledgements and Documentation



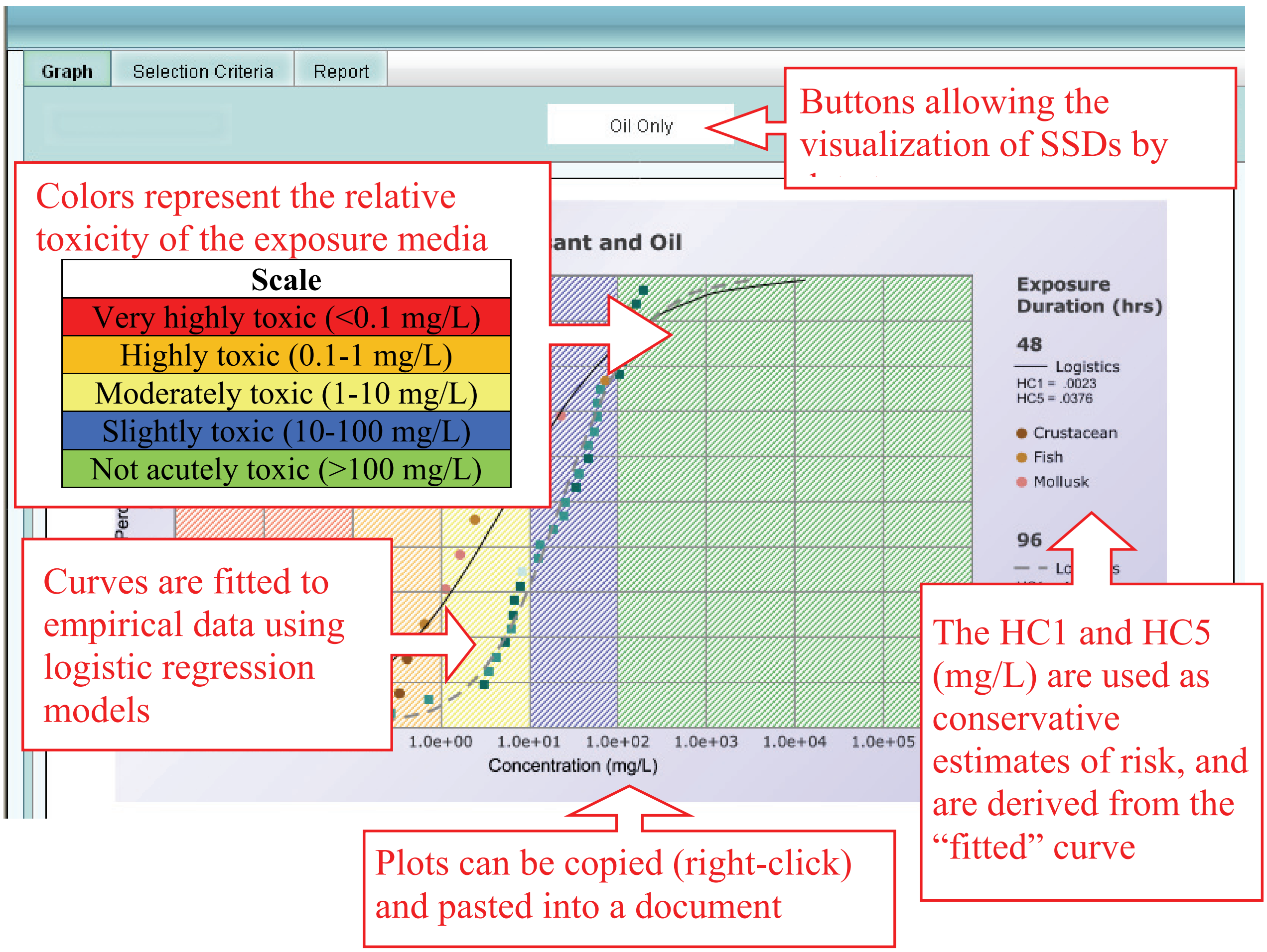
3. Data plotting options

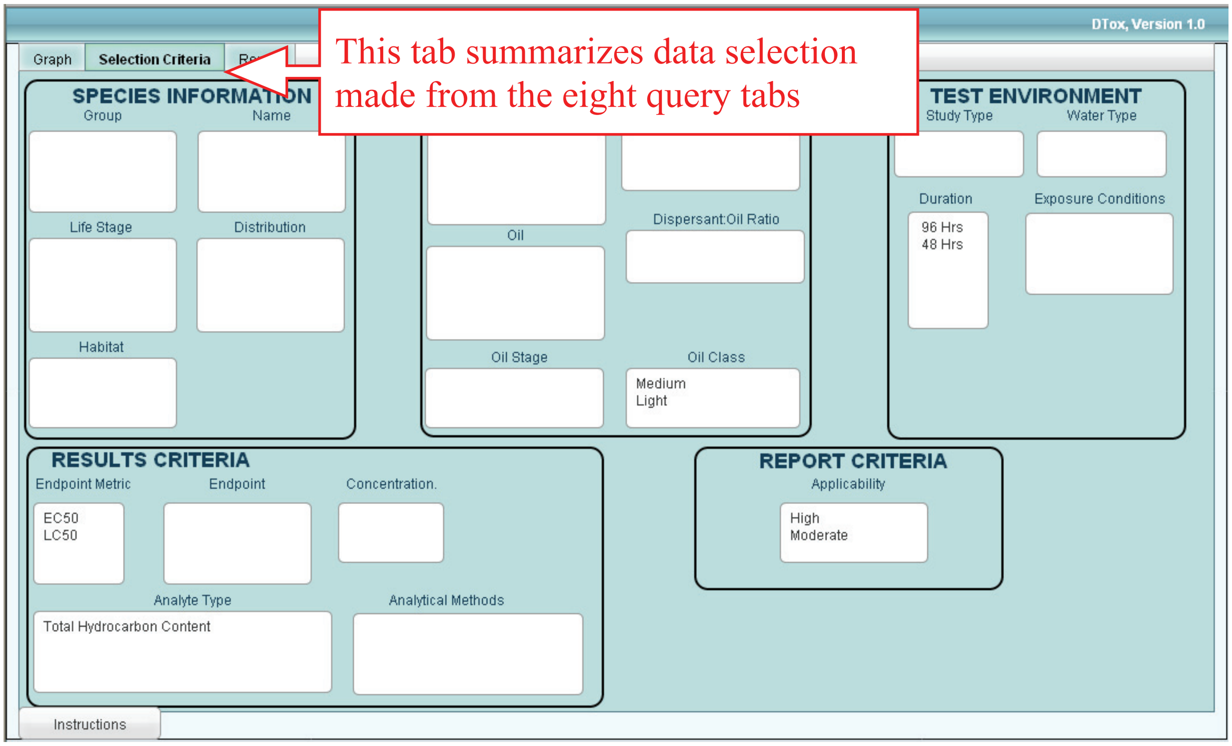
Once you have gone through the data selection tabs, your will get to chose how you want your data plotted. **Note** that only two curves can be plotted simultaneously on the same window. If more than three options are selected, only two will be plotted. For example, under exposure duration select two (e.g., 24 h and 96 h). Press "Plot Graph" to see the plotted output. This may take a few seconds… Following the step above, you will see the internal query being performed. You may need to wait a few seconds while the plots are generated.

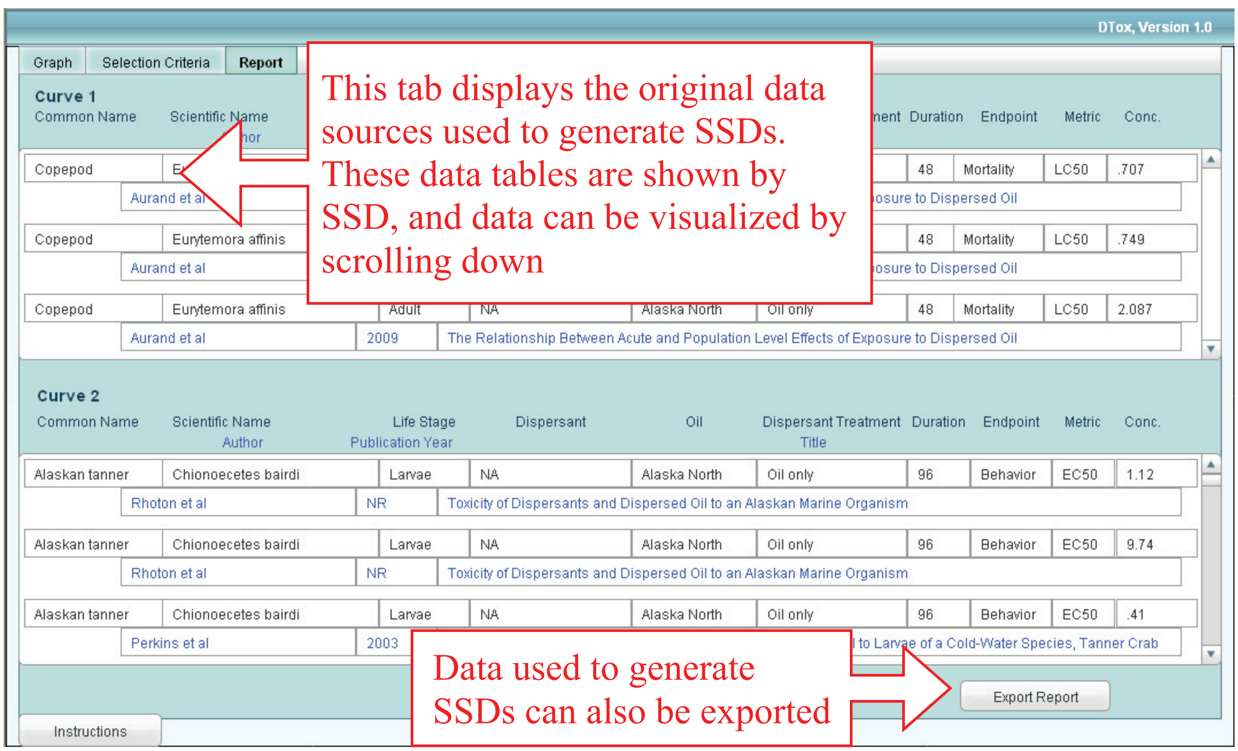


4. The final output

Queried data are combined to generate Species Sensitivity Distributions (SSDs). SSDs describe the sensitivity of aquatic species to the exposure media, where each point on the curve represents the geometric mean of all toxicity data available for a uniquely identified species (e.g., calculated by scientific name). SSDs are generated by ranking the relative sensitivity of individual from the least to the most sensitive, and are useful in that benchmark concentrations (hazardous concentration, HC) can be derived as a measure of risk. Here the 1st and 5th percentiles of the SSD (HC1 and HC5, respectively; in mg/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.

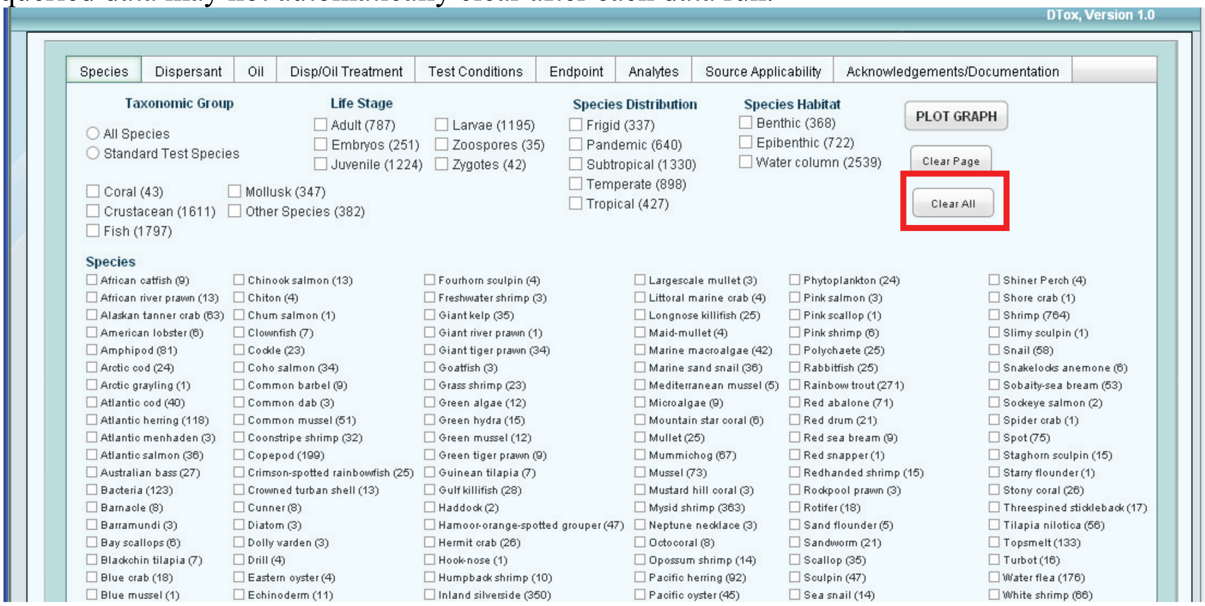



DTox, Version 1.0
Graph
Selection Criteria
This tab summarizes data selection made from the eight query tabs
SPECIES INFORMATION
Group
Name
Life Stage
Distribution
Habitat
Oil
Dispersant:Oil Ratio
Oil Stage
Oil Class
Medium
Light
TEST ENVIRONMENT
Study Type
Water Type
Duration
Exposure Conditions
96 Hrs
48 Hrs
RESULTS CRITERIA
Endpoint Metric
Endpoint
Concentration.
EC50
LC50
Analyte Type
Analytical Methods
Total Hydrocarbon Content
REPORT CRITERIA
Applicability
High
Moderate
Instructions


DTox, Version 1.0
Graph
Selection Criteria
Report
This tab displays the original data sources used to generate SSDs. These data tables are shown by SSD, and data can be visualized by scrolling down
Curve 1
Common Name
Scientific Name
Duration
Endpoint
Metric
Conc.
Copepod
48
Mortality
LC50
.707
Aurand et al
Copepod
Eurytemora affinis
48
Mortality
LC50
.749
Aurand et al
Copepod
Eurytemora affinis
Adult
NA
Alaska North
Oil only
48
Mortality
LC50
2.087
Aurand et al
2009
The Relationship Between Acute and Population Level Effects of Exposure to Dispersed Oil
Curve 2
Common Name
Scientific Name
Life Stage
Dispersant
Oil
Dispersant Treatment
Duration
Endpoint
Metric
Conc.
Author
Publication Year
Title
Alaskan tanner
Chionoecetes bairdi
Larvae
NA
Alaska North
Oil only
96
Behavior
EC50
1.12
Rhoton et al
NR
Toxicity of Dispersants and Dispersed Oil to an Alaskan Marine Organism
Alaskan tanner
Chionoecetes bairdi
Larvae
NA
Alaska North
Oil only
96
Behavior
EC50
9.74
Rhoton et al
NR
Toxicity of Dispersants and Dispersed Oil to an Alaskan Marine Organism
Alaskan tanner
Chionoecetes bairdi
Larvae
NA
Alaska North
Oil only
96
Behavior
EC50
.41
Perkins et al
2003
Data used to generate SSDs can also be exported
Export Report
Instructions

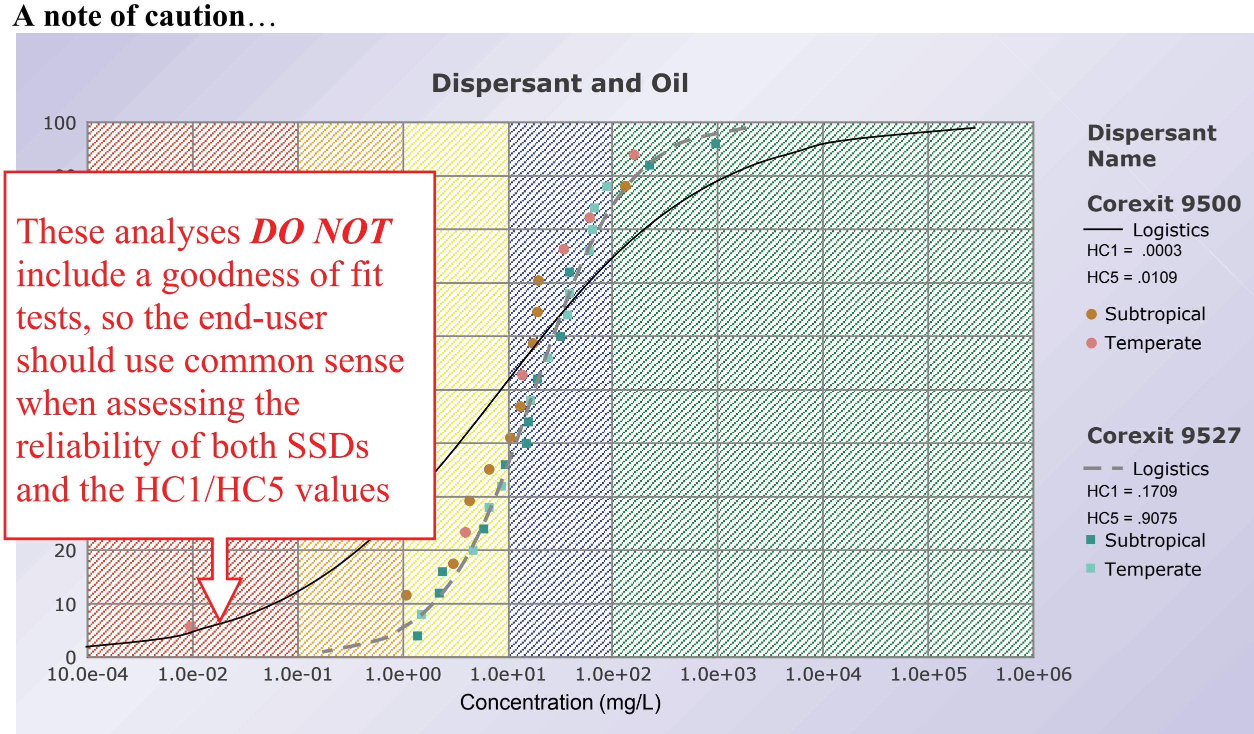
Note 1:

To ensure optimal performance and query replicability, press “clear all” after each query run. This is highly recommended step when performing multiple queries as the table containing the queried data may not automatically clear after each data run.

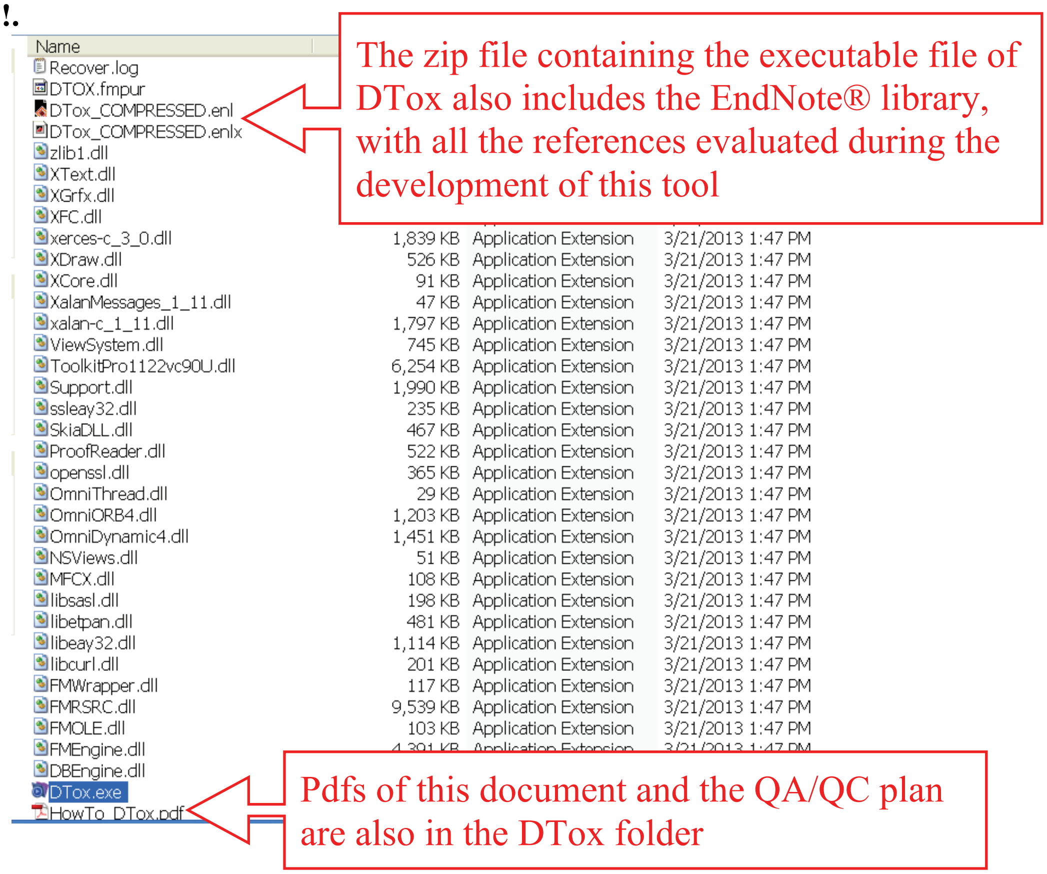


Note 2:

A note of caution…

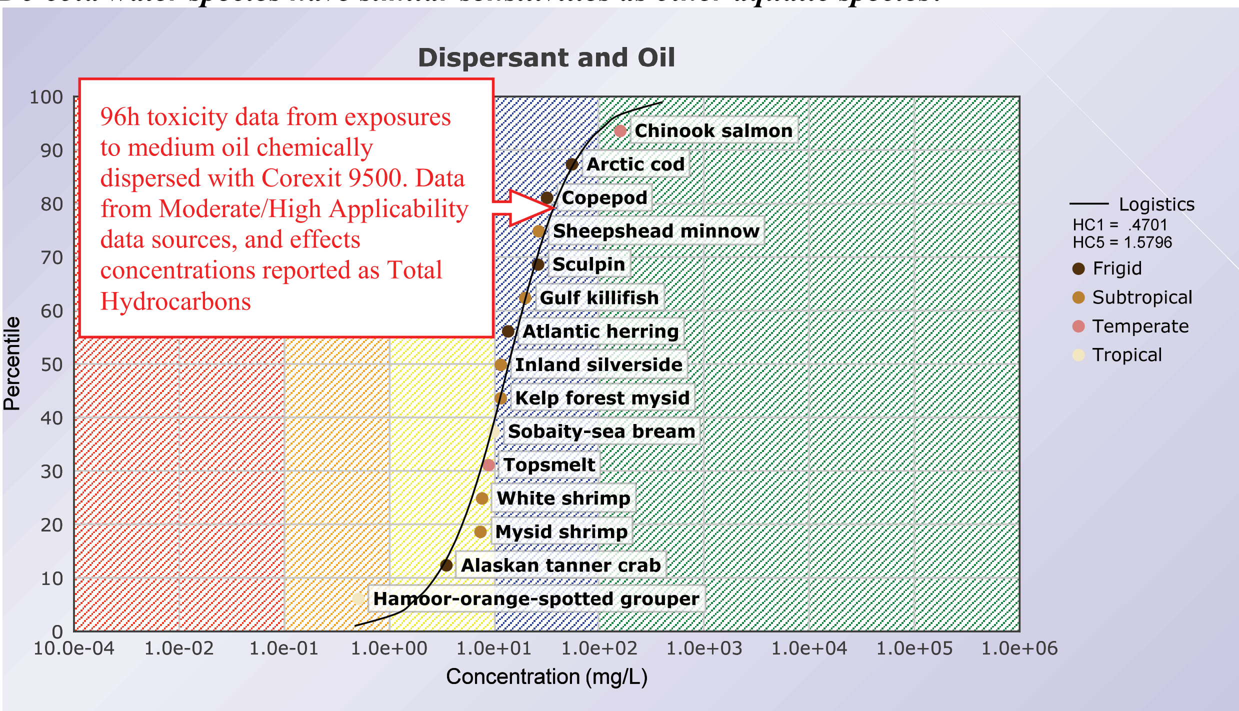


Zip File Bonus!.



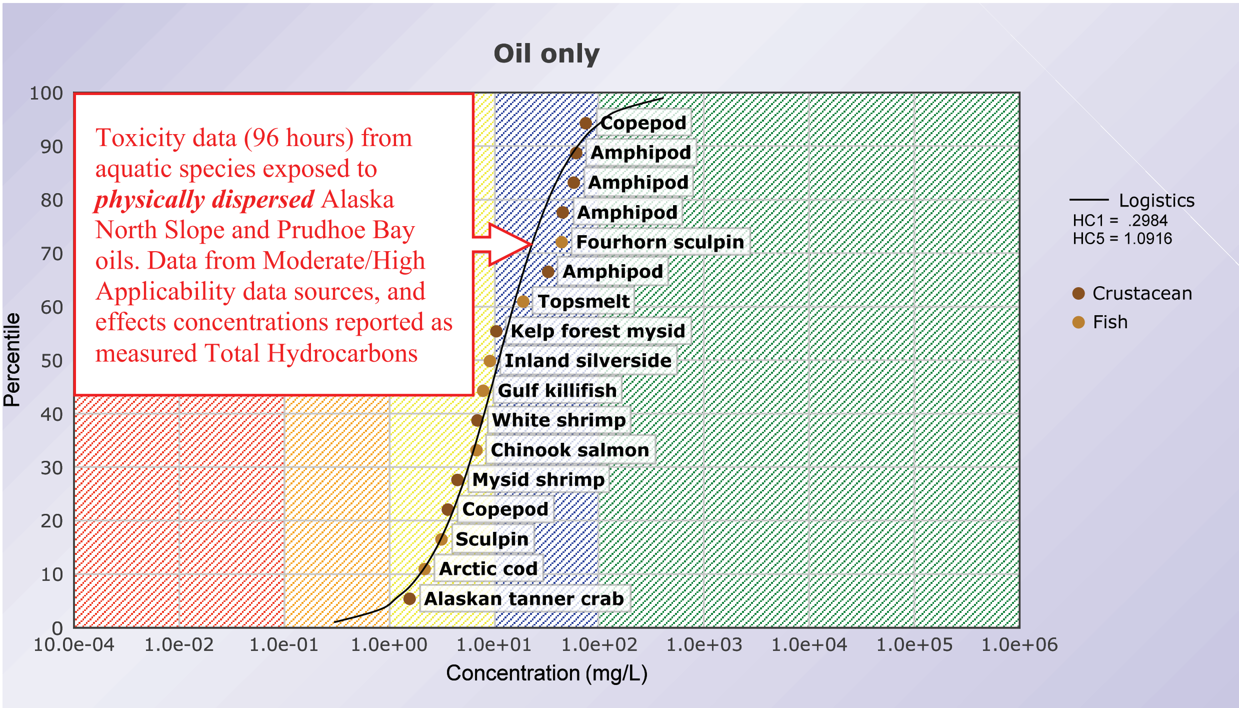
How to use outputs from DTox:
Data in DTox has several practical applications, including their use to address and answer basic questions:

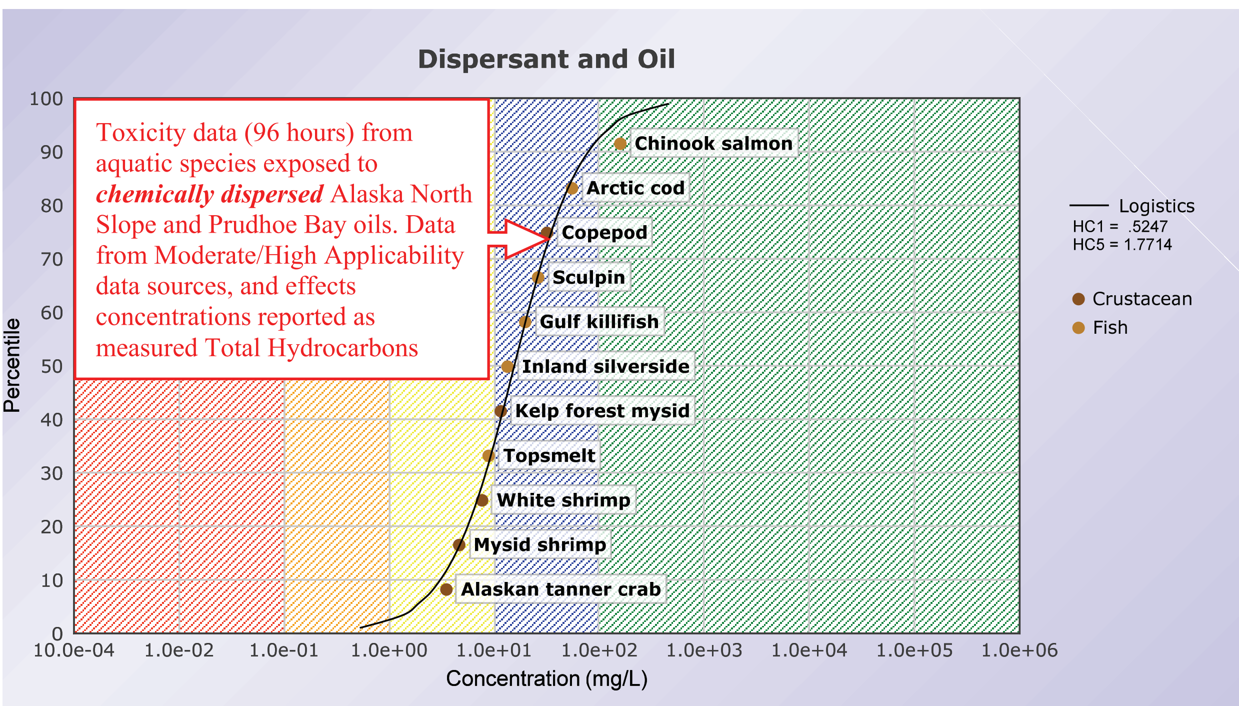
Do cold water species have similar sensitivities as other aquatic species?



Answer: Yes. Cold water species have similar sensitivities to medium oil chemically dispersed with Corexit9500 as temperate species (top plot), as well as one of the U.S. standard test species (topsmelt) (bottom plot). Therefore, both temperate and U.S. standard test species may be suitable surrogate for cold water species in toxicity testing of oil and dispersants.

Does Corexit 9500 increase the toxicity of Alaskan oils?





Answer: No. Based on the best available toxicity data available to date, there is no evidence that Corexit9500 increases the toxicity of Alaskan oils. As shown above, curves from physically and chemically dispersed oil are similar and both have comparable hazard concentrations (HCs).