CHEMMAP

Chemical Spill Transport & Fate Modeling Software

Version 7.7 Release Notes

Leading with Science®

TETRA TECH

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1 GET IN TOUCH

Please use the following contact information to get in touch with RPS Group | a Tetra Tech Company (TT), regarding any questions concerning CHEMMAP.

Note: we have updated our email address; mapsupport@rpsgroup.com is now obsolete.

Email: **MapSupport@tetratech.com**

Phone: +1 401 789 6224

Address: 55 Village Square Drive, South Kingstown RI 02879

2 INTRODUCTION

The first version of CHEMMAP was delivered over 20 years ago and is now used globally by major companies and international governments. It has been used successfully to support spill response, planning, and permitting in over 100 countries. The scientists and researchers at TT have incorporated lessons learned and new technologies into CHEMMAP version 7.7.0.

Version 7.7.0 of CHEMMAP includes enhancements and added features to help improve spill response, drill exercises, impact risk assessments, and contingency planning. Enhancements were mainly made to the user interface. This document describes the various new features and bug fixes included in CHEMMAP v7.7.0.

2.1 Operating System Compatibility

Version 7 (and newer) of the TT MAP Applications, OILMAP, SARMAP, and CHEMMAP, are supported on the following Microsoft Windows platforms: Windows 10 and 11, Windows Server 2016, 2019, 2022 and 2025 as well as cloud computing platforms including Microsoft Azure and Amazon Web Services.

2.2 CHEMMAP v7.7.0 Modules

Surface module	Simulate the behavior of surface chemical spills released on the water surface.
Subsurface module	Simulate chemical releases occurring below the water surface.
Stochastic module	Calculate the probabilistic distribution of chemicals in water and on shore.
Airmap module	Calculate the atmospheric dispersion of the lighter chemical fractions from a spill.
Biological Exposure & Effects module	Calculate area exposed above toxicological threshold and the dose aquatic biota are exposed to.

3 CHEMMAP V7.7.0 USER INTERFACE UPDATES

3.1 General Interface Updates

The following updates and enhancements have been made in the CHEMMAP v7.7.0 interface:

1. In the table of contents to the left of the map window, the “GIS” tab was renamed to “Layers” for maximum clarity.

Figure 1. TOC labels update.

2. Added Time as optional WMS parameter.
3. Added legend font size selection. Under “File” -> “Display Settings”.

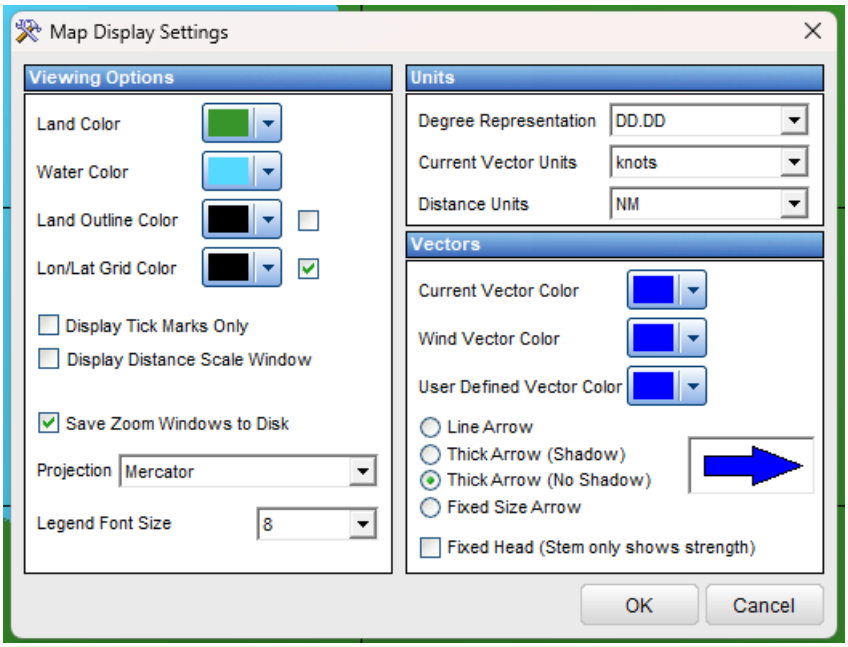

Figure 2. Legend Font Size selection in Map Display Settings.

3.2 Resolved General Interface Bugs

The following bugs have been reported, logged, and **fixed**:

1. Fixed Creation of Loc Data Based on Open Street Map
    a. The user can now create a new Geographic Location (i.e., “Loc Data” – saved in C:\Users\Public\Documents\ASA Software\Loc_Data) from Open Street Map by using the World Database tool:

Figure 3. Loc data creation from Open Street Map.

2. Fixed integration of sevenCs into CHEMMAP. Users with a sevenCs license can now display 7CB files in the interface.

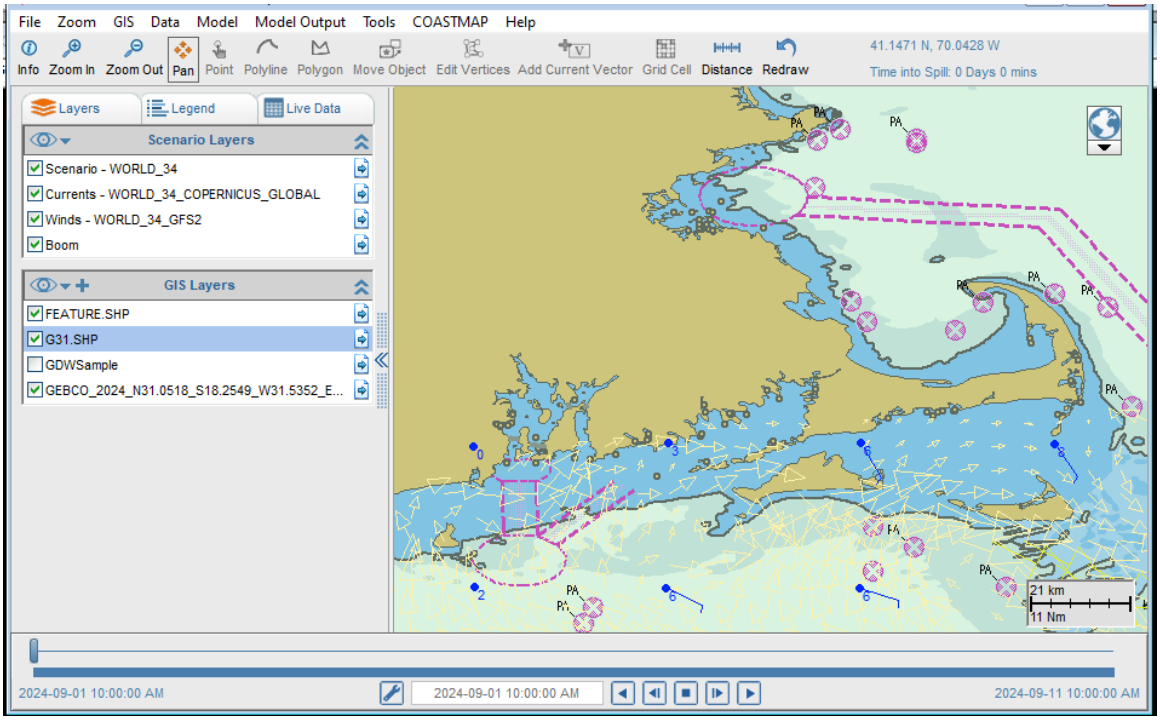

Figure 4. SevenCs files displayed in the interface.

3. Fixed import of NetCDF bathymetry from downloaded from the General Bathymetric Chart of the Oceans database (GEBCO).
    a. A user can select a specific area under the GEBCO data download website and download a 2D netCDF Grid. Once downloaded the user need to create a “Land Water Grid” and import the GEBCO NetCDF bathymetry using the “Import Depth Data” tool.

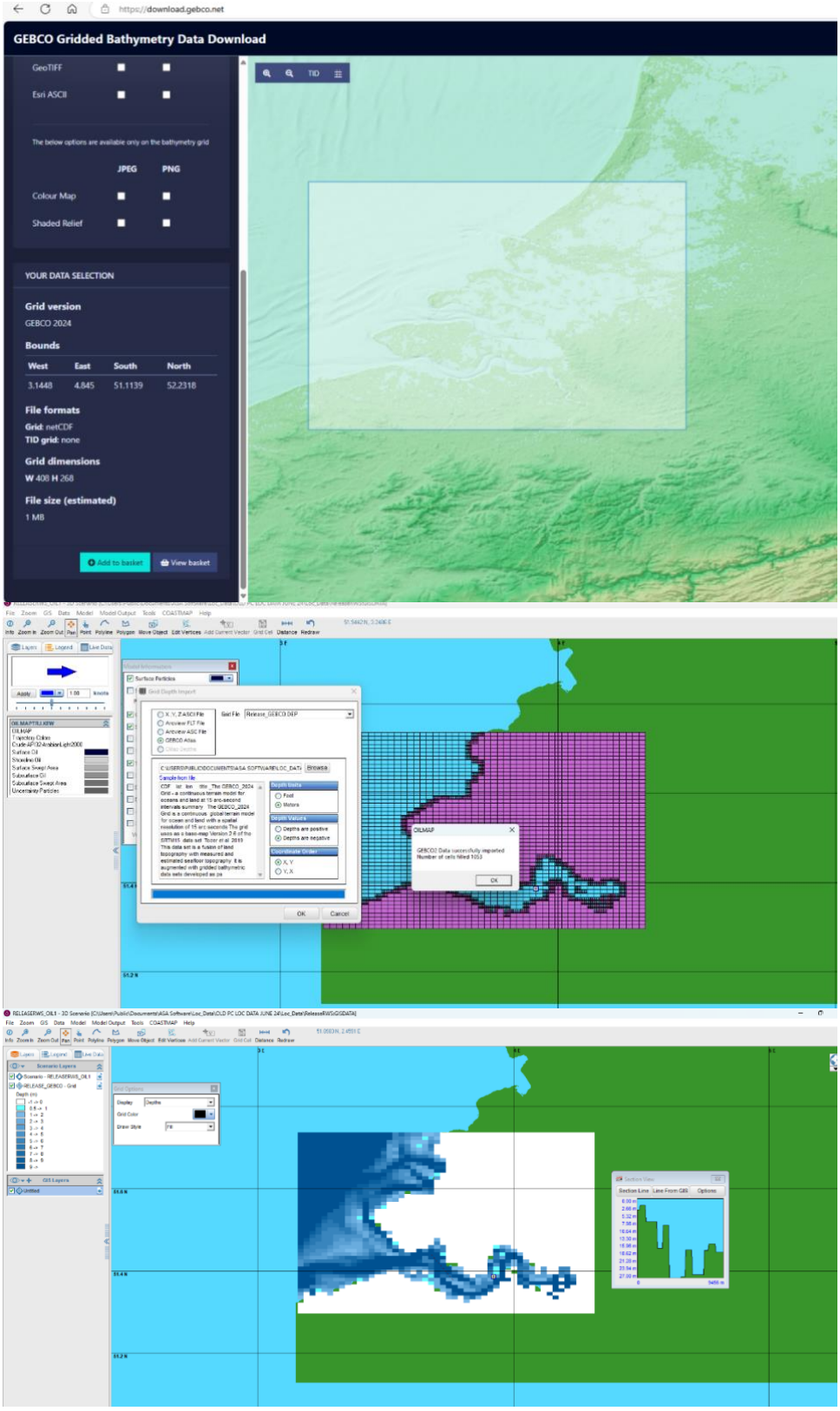

Figure 5. Example NetCDF bathymetry data from GEBCO.

4 CHEMMAP V7.7.0 NEW FEATURE ADDITIONS

4.1 Chemical Database Changes and Improvements

1. Edited/updated the chemical database to include a list of 48 "Standard" chemicals. With the purchase of the "Extended" package, 119 additional chemicals can be added to the chemical database. The development of additional chemicals can be comissioned and can then accessed via CHEMMAP's personal chemicals ("ChemPersonal") database.
    a. Curated a list of commonly bulk-shipped chemicals and their common shipping format (e.g., solid pellet, diluted liquid, etc). See Table 1 for the Standard Chemical Package and Table 2 for Extended Chemical Package. These chemicals are listed in alphabetical order, accompanied by their CAS number (if applicable) and their state (e.g., liquid, solid, etc).
2. Properties of chemical existing in the previous database were verified (or updated, if needed) using more contemporary data.
3. Based on their frequency in bulk shipping, chemicals were added to the Standard or Extended Chemical Packages accordingly. The data for these chemicals were primarily obtained from contemporary sources.
4. Added Standard European Behaviour Classification (SEBC) codes for each chemical entry. These codes are viewable in the database module in the CHEMMAP interface.
5. Updated the corresponding reference list. Much of the updated data was obtained from publicly available sources including the following:
    a. The National Institutes of Health's (NIH) publicly available chemistry database, PubChem (https://pubchem.ncbi.nlm.nih.gov/);
    b. The Royal Society of Chemistry's publicly available chemistry database, ChemSpider (https://www.chemspider.com/); and
    c. The Maritime Integrated Decision Support Information System Transport of Chemical Substances (MIDSIS-TROCS v4.0), which incorporates data from the EU's Harmful Noxious Substances - Marine System (HNS-MS) project.

Table 1. The Standard Chemical Package.

CAS #	Chemical Name	State
71-36-3	1-butanol	Liquid
111-87-5	1-octanol	Liquid
71-41-0	1-pentanol	Liquid
75-07-0	Acetaldehyde	Liquid
7664-41-7	Ammonia (gas)	Gas
7664-41-7	Ammonia (liquefied gas)	Liquid
71-43-2	Benzene	Liquid
56-23-5	Carbon tetrachloride	Liquid
108-90-7	Chlorobenzene	Liquid
67-66-3	Chloroform	Liquid
N/A	Conservative tracer	Dissolved in aqueous solution
110-82-7	Cyclohexane	Liquid
64-17-5	Ethanol	Liquid
100-41-4	Ethylbenzene	Liquid

107-21-1	Ethylene glycol	Liquid
107-15-3	Ethylenediamine	Liquid
142-82-5	Heptane	Liquid
7647-01-0	Hydrochloric acid	Liquid
7647-01-0	Hydrochloric acid (10% solution)	Dissolved in aqueous solution
7647-01-0	Hydrochloric acid (14% solution)	Dissolved in aqueous solution
78-83-1	Isobutanol	Liquid
67-63-0	Isopropanol	Liquid
67-56-1	Methanol	Liquid
78-93-3	Methyl ethyl ketone	Liquid
91-20-3	Naphthalene (pellets)	Solid, pellets
124-18-5	n-decane	Liquid
110-54-3	n-hexane	Liquid
7697-37-2	Nitric acid	Liquid
111-84-2	n-nonane	Liquid
111-65-9	n-octane	Liquid
109-66-0	n-pentane	Liquid
108-95-2	Phenol	Solid, pellets
7664-38-2	Phosphoric acid	Solid, powder
N/A	Polyethylene nurdle	Solid, pellets
71-23-8	Propanol	Liquid
1310-73-2	Sodium hydroxide (10% solution)	Dissolved in aqueous solution
1310-73-2	Sodium hydroxide (25% solution)	Dissolved in aqueous solution
1310-73-2	Sodium hydroxide (pellets)	Solid, pellets
1310-73-2	Sodium hydroxide (powder)	Solid, powder
100-42-5	Styrene	Liquid
7664-93-9	Sulfuric acid	Liquid
7664-93-9	Sulfuric acid (85% solution)	Dissolved in aqueous solution
75-65-0	tert-Butyl alcohol	Solid, pellets
78-00-2	Tetraethyl lead	Liquid
108-88-3	Toluene	Liquid

79-01-6	Trichloroethylene	Liquid
121-44-8	Triethylamine	Liquid
1330-20-7	Xylene mixture	Liquid

Table 2. The Extended Chemical Package.

CAS #	Chemical Name	State
72-20-8	1,1,1-trichloroethane	Liquid
76-44-8	1,1,2,2-tetrachloroethane	Liquid
79-06-1	1,1,2-trichloroethane	Liquid
309-00-2	1,1-dichloroethane	Liquid
7447-40-7	1,1-dichloroethene	Liquid
1305-62-0	1,2,3-trichloropropane	Liquid
1310-58-3	1,2,3-trimethylbenzene	Liquid
7775-09-9	1,2,4-trichlorobenzene	Liquid
25321-14-6	1,2,4-trimethylbenzene	Liquid
16721-80-5	1,2-dibromoethane	Liquid
111-42-2	1,2-dichlorobenzene	Liquid
92-52-4	1,2-dichloroethane	Liquid
120-83-2	1,2-dichloropropane	Liquid
56-38-2	1,2-propylene oxide	Liquid
60-29-7	1,4-dioxane	Liquid
64-18-6	1-heptene	Liquid
64-19-7	1-hexanol	Liquid
71-55-6	1-hexene	Liquid
75-35-4	1-methylnaphthalene	Liquid
78-87-5	1-pentene	Liquid
79-00-5	2,4-dichlorophenol	Solid, pellets
79-10-7	2-Butenal	Liquid
79-34-5	2-heptanone	Liquid
98-01-1	2-nitrotoluene	Liquid
106-89-8	3-methylpyridine	Liquid
106-93-4	4-methylpyridine	Liquid

107-05-1	Acetic acid	Liquid
107-06-2	Acetic anhydride	Liquid
107-10-8	Acetone	Liquid
107-92-6	Acetone cyanohydrin	Liquid
108-05-4	Acetonitrile	Liquid
108-11-2	Acrylamide	Solid, powder
108-20-3	Acrylic acid	Liquid
108-24-7	Acrylonitrile	Liquid
108-84-9	Aldrin	Solid, powder
109-73-9	Allyl alcohol	Liquid
109-86-4	Allyl chloride	Liquid
110-19-0	Aniline	Liquid
110-91-8	Benzyl alcohol	Liquid
111-15-9	Benzyl chloride	Liquid
121-75-5	Biphenyl (solid, pellets)	Solid, pellets
123-38-6	Bis(2-chloroethyl) ether	Liquid
123-62-6	Bromochloromethane	Liquid
123-86-4	Butanal	Liquid
123-91-1	Butyl acetate	Liquid
141-43-5	Butyl benzyl phthalate	Liquid
141-78-6	Butylamine	Liquid
592-41-6	Butyric acid	Liquid
75-00-3	Calcium hydroxide	Solid, powder
127-18-4	Carbon disulfide	Liquid
74-95-3	Chlorine (gas)	Gas
74-97-5	Chlorine (liquefied gas)	Liquid
75-56-9	Chloroethane	Liquid
109-99-9	Chloroethene	Gas
108-94-1	Cyclohexanone	Liquid
107-31-3	Cyclohexylamine	Liquid
80-62-6	Cyclopentane	Liquid

107-12-0	Dibromomethane	Liquid
108-91-8	dichloromethane	Liquid
98-95-3	Diethanolamine	Solid, pellets
108-99-6	Diethyl ether	Liquid
64-67-5	Diethyl phthalate	Liquid
7782-50-5	Diethyl sulfate	Liquid
62-53-3	Diethylamine	Liquid
67-64-1	Diisopropyl ether	Liquid
75-04-7	Dimethyl phthalate	Liquid
75-05-8	Dimethylamine	Liquid
95-47-6	Dinitrotoluene mixture	Solid, powder
75-09-2	Diphenyl ether	Liquid
75-15-0	Endrin	Solid, powder
75-34-3	Epichlorohydrin	Liquid
75-86-5	Ethanolamine	Liquid
76-01-7	Ethyl acetate	Liquid
106-42-3	Ethyl acrylate	Liquid
79-09-4	Ethylamine	Liquid
88-72-2	Ethylene glycol monoethyl ether acetate	Liquid
84-66-2	Ethylene glycol monomethyl ether	Liquid
108-38-3	Formic acid	Liquid
95-50-1	Furfural	Liquid
98-82-8	Heptachlor	Solid, powder
100-51-6	Hexanoic acid	Liquid
95-63-6	Hydrogen peroxide	Liquid
107-13-1	Isobutyl Acetate	Liquid
107-18-6	Isopropylbenzene	Liquid
96-18-4	Malathion	Liquid
109-60-4	Methyl acetate	Liquid
109-89-7	Methyl amyl acetate	Liquid
110-86-1	Methyl amyl alcohol	Liquid

120-82-1	Methyl bromide	Gas
124-40-3	Methyl formate	Liquid
101-84-8	Methyl methacrylate	Liquid
628-63-7	Methyl t-butyl ether	Liquid
110-43-0	Methylcyclohexane	Liquid
4170-30-3	Morpholine	Liquid
111-27-3	m-Xylene	Liquid
131-11-3	n-butylbenzene	Liquid
140-88-5	Nitrobenzene	Liquid
142-62-1	n-Propylbenzene	Liquid
526-73-8	o-Xylene	Liquid
103-65-1	Parathion	Liquid
104-51-8	Pentachloroethane	Liquid
90-12-0	Pentyl acetate	Liquid
287-92-3	Phosphoric acid (85% solution)	Dissolved in aqueous solution
108-87-2	Potassium chloride	Solid, powder
109-67-1	Potassium hydroxide	Solid, powder
592-76-7	Propionaldehyde	Liquid
1634-04-4	Propionic Acid	Liquid
111-44-4	Propionic anhydride	Liquid
123-72-8	Propionitrile	Liquid
7722-84-1	Propyl acetate	Liquid
79-20-9	Propylamine	Liquid
85-68-7	p-Xylene	Liquid
108-89-4	Pyridine	Liquid
100-44-7	Sodium chlorate	Solid, powder
1300-71-6	Sodium hydrosulfide	Solid, powder
74-83-9	Tetrachloroethylene	Liquid
7782-50-5	Tetrahydrofuran	Liquid
75-01-4	Vinyl acetate	Liquid
7664-38-2	Xylenol mixture	Liquid

4.2 Open Sea Map

CHEMMAP users may display the Open Sea Map as their base map in the map window. Users can go to the “GIS” menu to "attach new layer" and then select "map services", then select “Tile Service" and then "Open Sea Map" and click OK. Users then select “Open **Street** Map” from the base map selection in the top right of the map window or the base map of their choice.

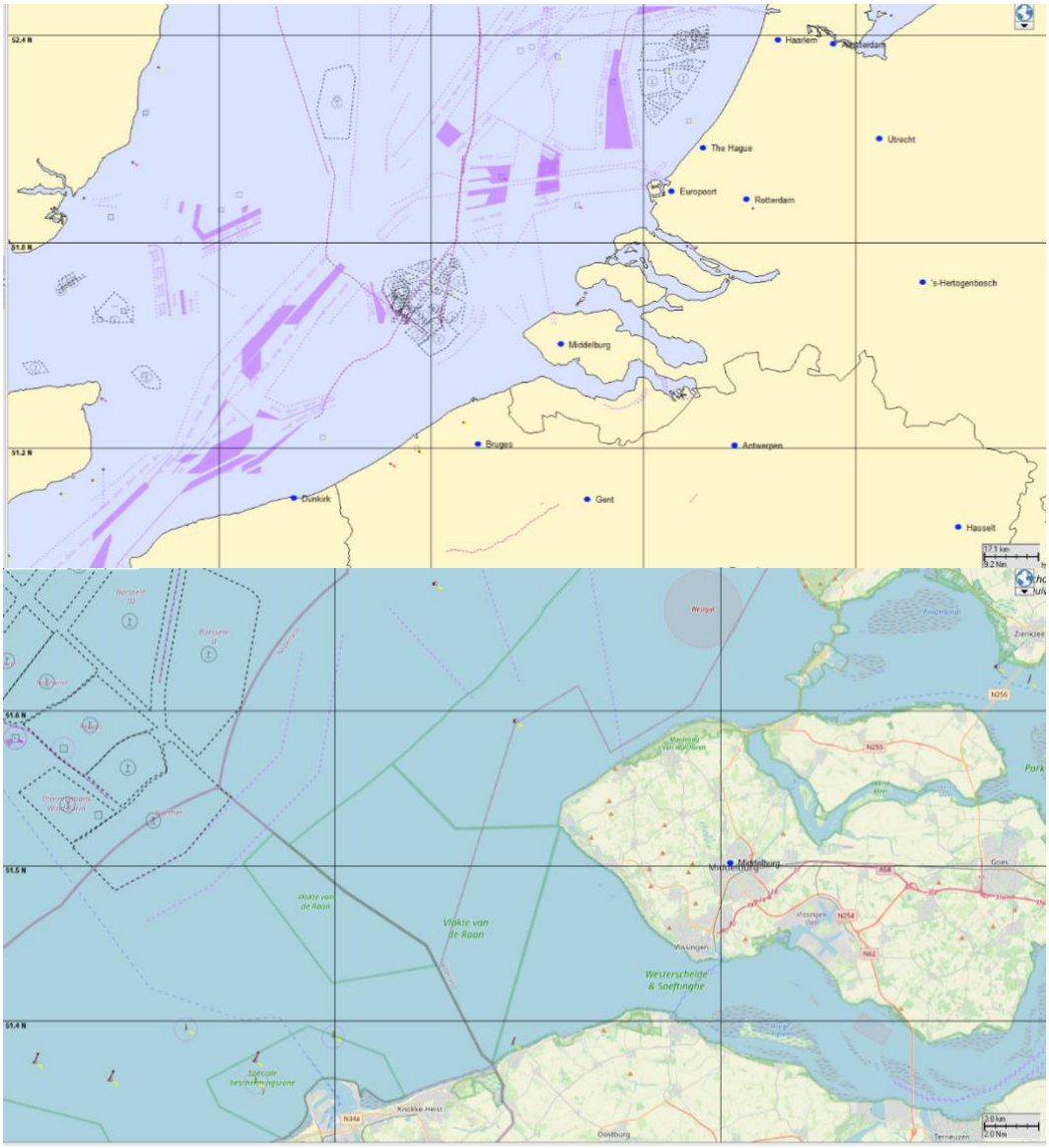

Figure 6. Example Open Sea Map visualization with two base maps: user-set base map (top) and Open Street Map base map (bottom).

4.3 COASTMAP EDS Form Updates

The EDS servers are now labeled as “Primary” and “Secondary”, to clearly indicate which server users should be connecting to.

4.3.1 EDS Metadata Catalog Download Option

The following datasources had a detailed catalogue added:

- GFS
- ECMWF Winds

4.3.2 Full EDS Metadata Catalog

The following datasources contain a detailed catalog:

- AEMET HARMONIE CAN
- AEMET HARMONIE PEN
- ECMWF Open Winds
- GFS
- HFRadar EBRO DELTA
- HFRadar Galicia
- HFRadar Gibraltar
- HFRadar Huelva - Algarve
- HFRadar Ibiza
- NOAA CIOFS
- SAMPA Algeciras
- SAMPA Estrecho de Gibraltar
- SAMPA Gibraltar
- SASEMAR WRF Winds
- WMOP ROMS
- Global HYCOM (NCEP)
- Global HYCOM (Navy) Currents
- Copernicus, GLOBAL
- Bluelink v3
- NAVGEM (Navy)
- NW_ATL
- Copernicus, MED SEA
- ACCESS G3
- CNMI ROMS
- Guam ROMS
- ECMWF Winds
- Copernicus, NW ATL SHELF
- Copernicus, IBI
- Baltic Sea Currents
- Arctic Ocean Currents
- Samoa ROMS
- MOHID Artabro
- MOHID Vigo

5 CHEMMAP V7.7.0 MODEL UPDATES (0.2.25.0)

5.1 Resolved Model Bugs

1. Fixed initialization error with 2D sigma NC files.
2. Fixed uninitialized variables when wind=fill value.
3. Fixed an edge condition in the i,j index computation from the k-d tree index.
4. Fixed an issue in the average stochastic wind code.

5.2 Model Changes and Improvements

1. Updated average k-d tree computation to avoid losing resolution when computing the average of a large number of cells.
2. Added the ability to handle ice data from a regular grid and updated 2D lat/lon ice file processing to improve efficiency.
3. Updated to check for NaN before doing floating point comparison.
4. Added a keyname to make the CLST folder location configurable.
5. Updated current library to new 2D lat/lon interpolation routines.
6. Performance improvements in concentration computation code.
7. Added keyname 'writeLegacyConcOFF' to turn off writing legacy concentration files and increase speed.
8. Added the model version to the CFS file.
9. Write gridded stochastic and concentration data to a netCDF file.
10. Write summary statistics to new output files.
11. Switched runtime libraries to Multithreaded DLL instead of QuickWin.
12. Update to culib to allocate arrays to the heap instead of the stack.