

CHEMMAP – An Operational Application for the Assessment of Marine Pollution.

An Operational Modeling Tool for Response Support.

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Outline

- Introduction / Presentation of ASA (RPS group)
- Operational Modeling Tools
 - Applications, Components, Quality of results
 - Main processes to be modeled
 - Balance between Accuracy and Operationality
- Chemical spill modeling software – CHEMMAP
 - Graphic Environment
 - Model Output

Applied Sciences Associates Inc. (now RPS ASA)

Environmental, Coastal and Marine Consultancy in Rhode Island, USA

Scientific & Technological Solutions to manage and protect the marine environment.

Now part of the *RPS Group* (UK)

- **Services & Consultancy**

Water quality and hydrodynamic modeling

Support Oil Industry (E&P activities, EIA, drilling, etc.)

Natural Resource Damage Assessment

Operational Metocean Data Provision (winds and currents forecasts)

Training, Drill Exercises

- **Products & Modeling Tools**

In Support of Decision Making (Emergency, Pollution, Search & Rescue)

In Support of Environmental Evaluation (Impact, Risk, Mapping)

Water quality, hydrodynamic modeling, Biological Impact

GIS Framework, OGC Data distribution

Water, air, land dispersion modeling

Oil, Chemicals, LNG, Drilling materials

ASA activities

Public Sector

- Marine Pollution Research Institutes/Centers, Responders (e.g. Cedre - France, RWS – Dutch Water Institute, EMSA)
- Coast Guards (e.g. Sasemar – Spain, Irish CG)
- National Administrations (e.g. NOAA, BOEMRE – USA)
- Local/regional agencies (e.g. MPA – Singapore)

Private Sector

- Consulting firms (ERM, CH2M Hill, WP, URS)
- Oil companies (TOTAL, Shell, Chevron, ExxonMobil, etc.)
- Responders (OSRL)

Products and Services

- Environmental condition studies
- Pollutant drift modeling
- Oil/HNS spills
- Integrated Data Management System
- Development of webGIS environment



Modeling Tools: Operational & Consulting

Applications

- **Environmental Assessment** <-> **Long term**
 - Impacts of pollutant spills, on the coastline, on the marine environment, ecological consequences, etc.
 - Risk Assessment and Contingency Planning
 - Large dataset and combination of several models to assess interaction between the pollutant, the environment and human activities

→ *Ensemble simulations (Stochastic)*
- **Emergency Support** <-> **Short term**
 - Responders need a simple yet robust tool (system) to assess pollutant behaviour (drift, dispersion) in the first hours/days
 - Integration of all available information (pollutant data, location of available resources, etc.)
 - Real-time Met-Ocean Data (<-> Evolution Data Server **EDS**)
 - For use during exercises and real spills

→ *Forecast simulations*

Operational Tool: Components

- Graphic Environment
 - GIS (Geographic Information System) base map
 - Mapping of area of interest
- Database:
 - Chemicals
 - Geographic - Static (e.g. coastline, bathymetry)
 - Geographic - Dynamic (e.g. winds, currents) >> EDS
- Model(s)
 - Water component (pollution in water)
 - Atmospheric component (dispersion in atmosphere)
- Exportation / Importation:
 - Access to external data, standard file format
 - Exportation of results in other environments (e.g. Google Earth)

Quality/Accuracy of Results – Trends

- **Advanced computational resources:**
Numerical models can better reproduce more sophisticated processes by working with more information (data).
- **Better interfacing between the model and graphic tools:**
 - More robust and rapid technologies
 - More information sources
- **Synergy:**
>> Integrate/combine observations into model predictions

The quality of a model prediction is dependent on:

- Input data.....
- Model performance (physical/chemical processes)
- Model users

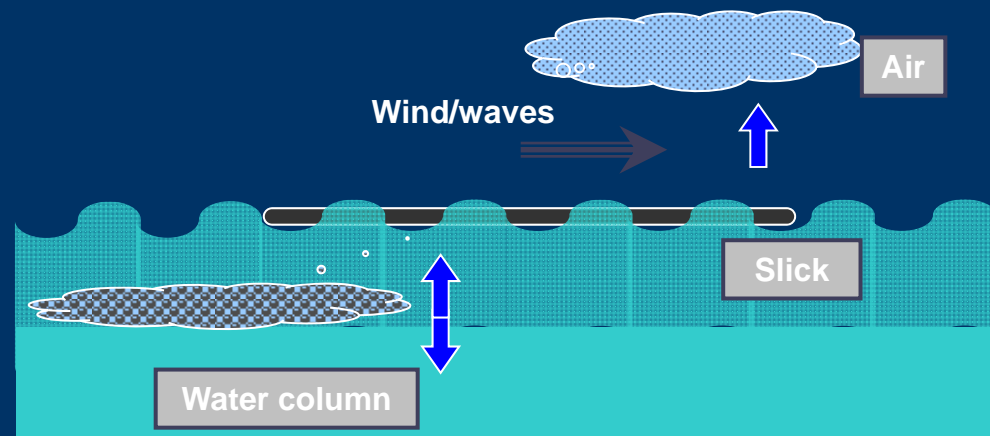
Trend

*

**

Modeling a Chemical Spill

- TRANSPORT and DISPERSION processes
 - Atmosphere (wind)
 - Marine and coastal environment: currents, waves, turbulence, rivers
- CHEMICAL REACTION processes:
 - Transformation of possible components of the chemical
 - Evaporation, dissolution, mixture with sediment, etc.
 - Long term processes
- Components (environment)
 - Volatile (air)
 - Floating (water)
 - Coastal (land)
 - Dispersed (water)
 - Dissolved (water)
 - Sediments (seafloor)

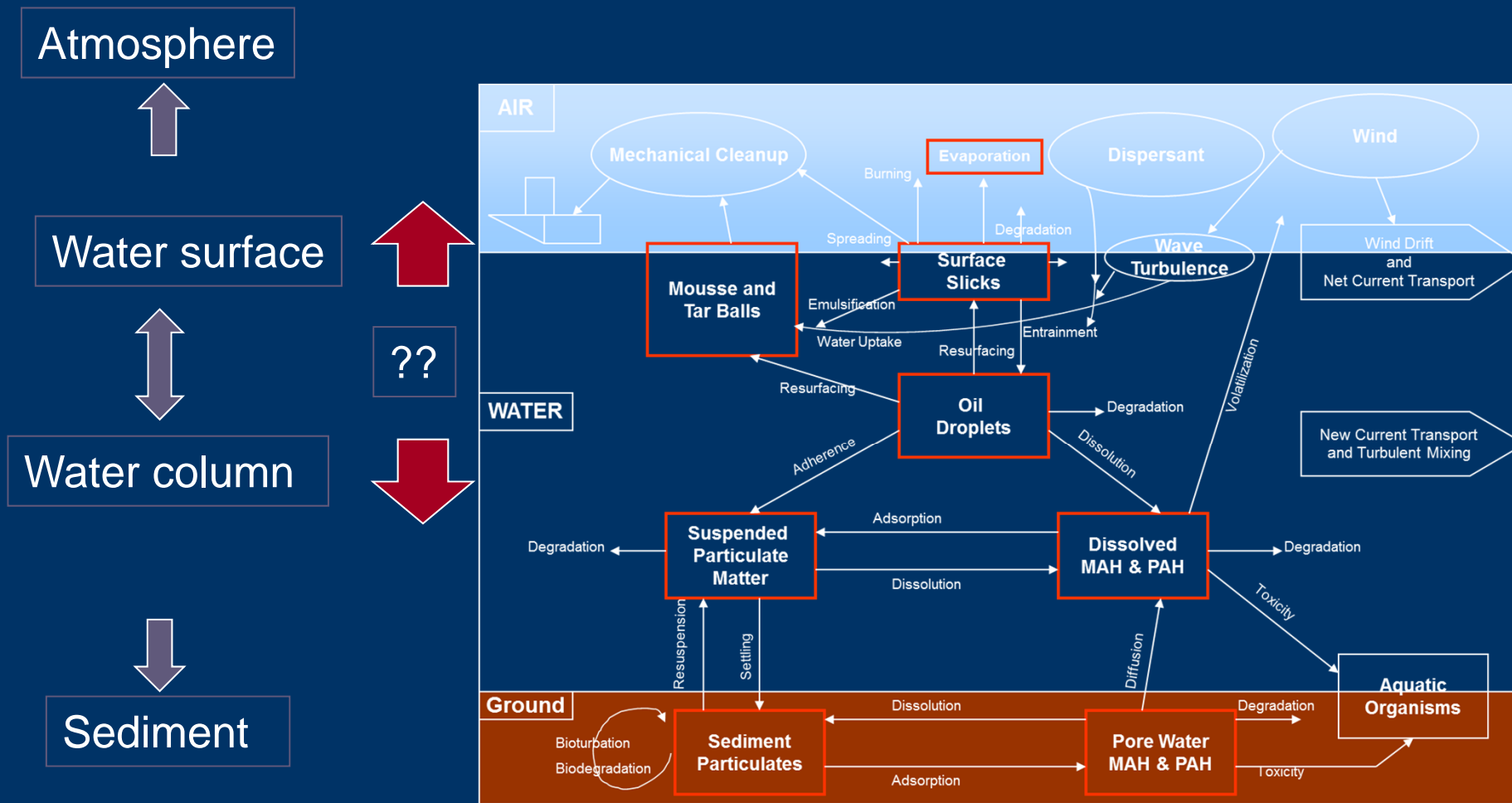


Chemical Classification – Database

- Buoyancy
- Evaporation
- Dissolution

Buoyancy Relative to Water	Solubility Behavior	Volatility
Floaters: density $< 1.0 \text{ g/cm}^3$	Highly soluble: solubility $> 1000 \text{ mg/L}$	Highly volatile: vapor pressure $> 0.1 \text{ kPa}$
Neutral: density $1.01\text{-}1.03 \text{ g/cm}^3$	Soluble: solubility $100 - 1000 \text{ mg/L}$	Semi-volatile: vapor pressure $10^{-5}\text{-}0.1 \text{ kPa}$
Sinkers: density $> 1.03 \text{ g/cm}^3$	Semi-soluble: solubility $1 - 100 \text{ mg/L}$	Low-volatile: vapor pressure $< 10^{-5} \text{ kPa}$
	Insoluble: solubility $< 1 \text{ mg/L}$	

What are the key processes?



Overall distribution?



Response according to our concerns

CHEMMAP:
Chemical spills

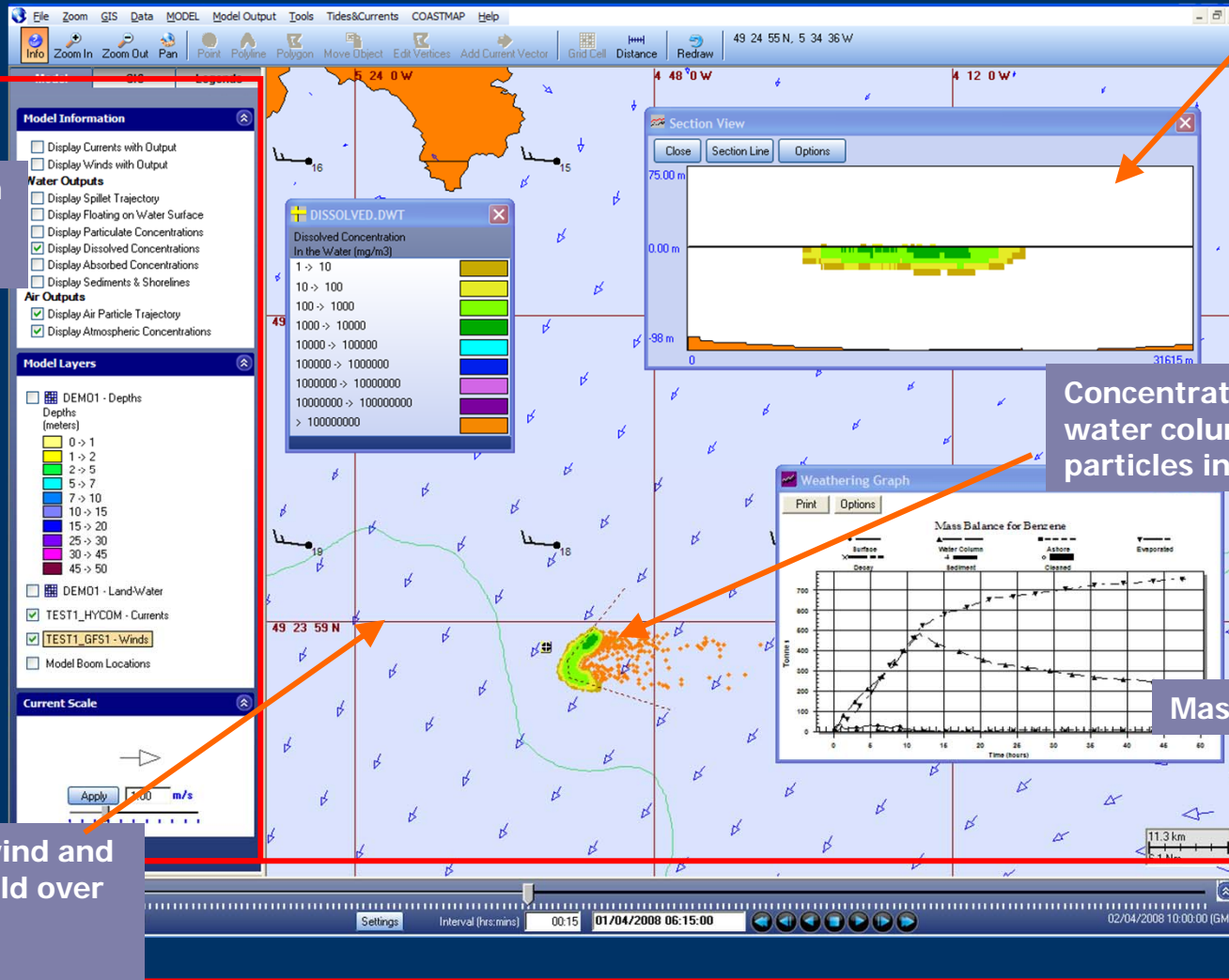
CHEMMAP features

- Mapping tool which includes several models to simulate the drift, evolution and biological effects of a chemical spill in an aquatic and/or terrestrial environment.
- It includes a stochastic component for risk assessment/contingency planning, as well as an exposure model to assess the effect/concentration (toxicity).
- Modules:
 - GIS (Geographic Information System)
 - Digital and online nautical charts (e.g. C-MAP)
 - Chemical database and MSDS (Material Safety Data Sheet)
 - Access to environmental data server (ASA - EDS)
- Limitations:
 - Does not reproduce chemical reactions (e.g. acid/base, pH)
 - Only works with mono-component products (e.g. not oil)

CHEMMAP environment

Vertical cross-section results

GIS/information layer management



Concentration in the water column and particles in air

Mass distribution

Variable wind and current field over time

Animation/time synchronization

Chemical Database

The image displays two overlapping windows from a chemical database software. The background window is for 1,1,1,2-Tetrachloroethane, and the foreground window is for Benzene.

Background Window (1,1,1,2-Tetrachloroethane):

- Buttons: OK, Chemical Summary, Save, Add Chemical, Unknown, Delete.
- Database Selection: ASA Database, Personal Database.
- Chemical Name: 1,1,1,2-Tetrachloroethane
- Author(s):
- Tabbed Interface: Descriptions, MSDS, Information, Physical, Chemical, Initialization, Toxicity.
- General Chemical Behavior (dependent on environmental conditions):
 - 1,1,1,2-Tetrachloroethane:
 - is a sinker
 - is highly volatile
 - is highly soluble
 - moderately adsorbs to particles
- Hazards: >>Hazard Information Unavailable.<< (User may enter Hazard Information under 'User Notes').
- General Description:
 - Clear colorless liquid [NTP, 1992].
 - Water solubility - <1 mg/mL at 68.9°F [NTP, 1992].
 - C₂H₂Cl₄
 - 1,1,1,2-TETRACHLOROETHANE is incompatible with strong oxidizing agents and st...
- User Notes:

Foreground Window (Benzene):

- Buttons: OK, Chemical Summary, Add Chemical to Personal Database.
- Database Selection: ASA Database, Personal Database.
- Chemical Name: Benzene
- Tabbed Interface: Descriptions, MSDS, Information, Physical, Chemical, Initialization, Toxicity.
- Chemical Synonyms: benzol; cyclohexatriene;
- Molecular Formula: C₆H₆
- CAS No.: 71-43-2
- Chemical State:
 - Pure Chemical**
 - Solid, powder
 - Solid, pellets
 - Solid, block
 - Liquid
 - Gas
 - In Bulk Liquid**
 - Dissolved in aqueous solution
 - Particulate suspended in aqueous solution
 - Dissolved in hydrophobic solvent
 - Dissolved in or adsorbed to hydrophobic material suspended in aqueous solution
 - Dissolved in aqueous solution & adsorbed to hydrophobic material emulsion in the aqueous solution
- UN No.: 1114
- Chemical Type Code: Inorganic, Organic, Petroleum Product

Wind and Current via EDS

Online request for wind and current data for the scenario to be simulated (time and space) from the EDS/COASTMAP server

Time step included in current file obtained via EDS

Available data sources for scenario

Scenario Spill Winds Currents Water Air Review

Current File COASTMAP Tides and Currents

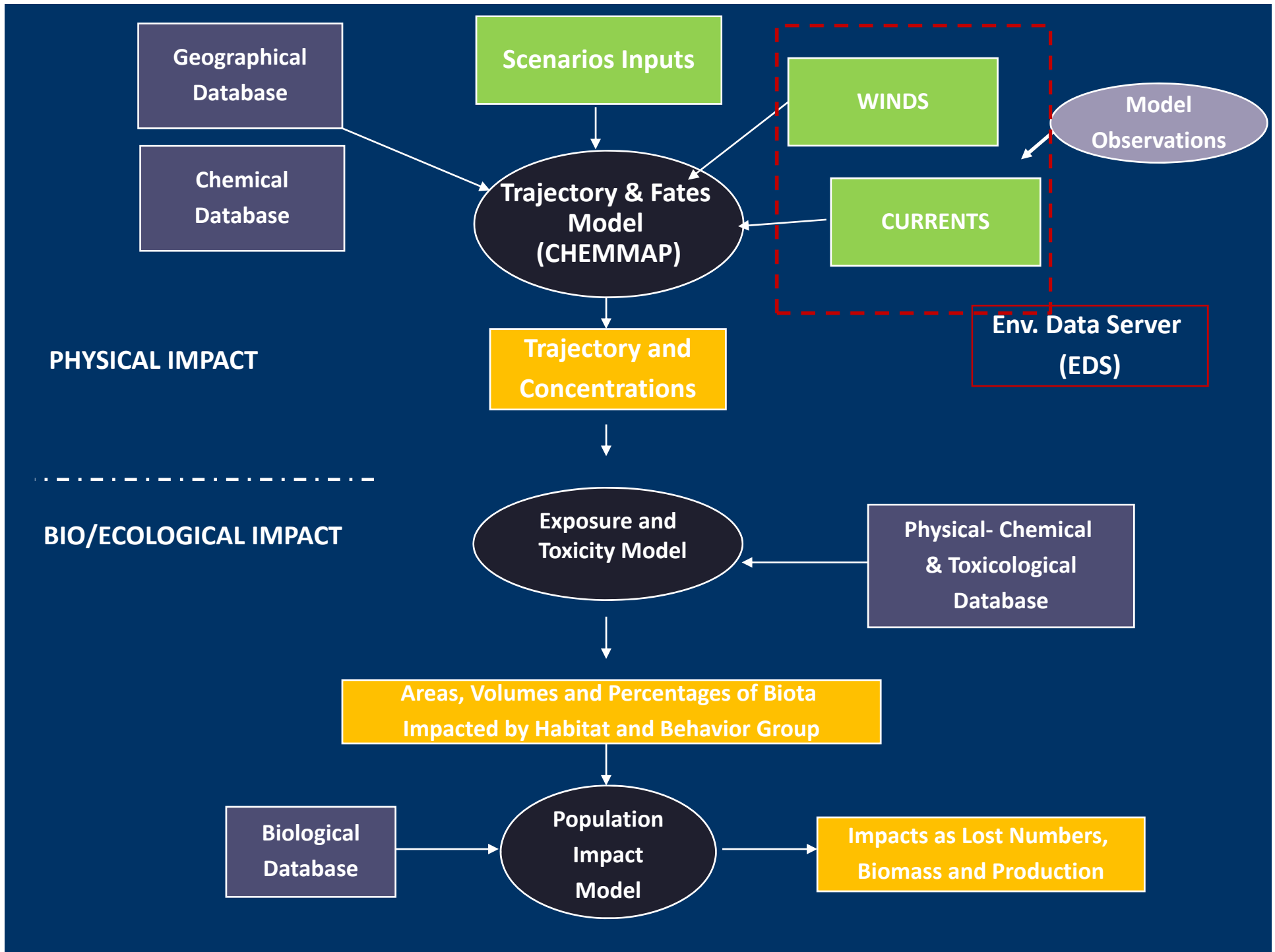
- NOWCASTING
- HYCOM
- NCOM
- MARIANO
- ADCIRC East
- BLUELINK

3/28/2008 3:00:00 PM GMT
3/28/2008 4:00:00 PM GMT
3/28/2008 5:00:00 PM GMT
3/28/2008 6:00:00 PM GMT
3/28/2008 7:00:00 PM GMT
3/28/2008 8:00:00 PM GMT
3/28/2008 9:00:00 PM GMT

Get Data Download Complete Currents File: GULF_OF_MEXICO_CHEM1_HYCOM.NC All times GMT

Close Previous Run Chemical Model Next Save As Default

Extension of current file



CHEMMAP outputs

Types of model outputs

- 'Raw' - Lagrangian particle model
- 'Process' > concentration calculations
- Time series of the concentration at a given point
- Distribution of the concentration in different layers, and/or maximum

Map of Concentrations:

- In air (vapor)
- At surface (liquid/solid - floating)
- Dissolved (in water column)
- Dispersed (liquid – water column)
- Sediment (liquid/solid)

Average maximum values

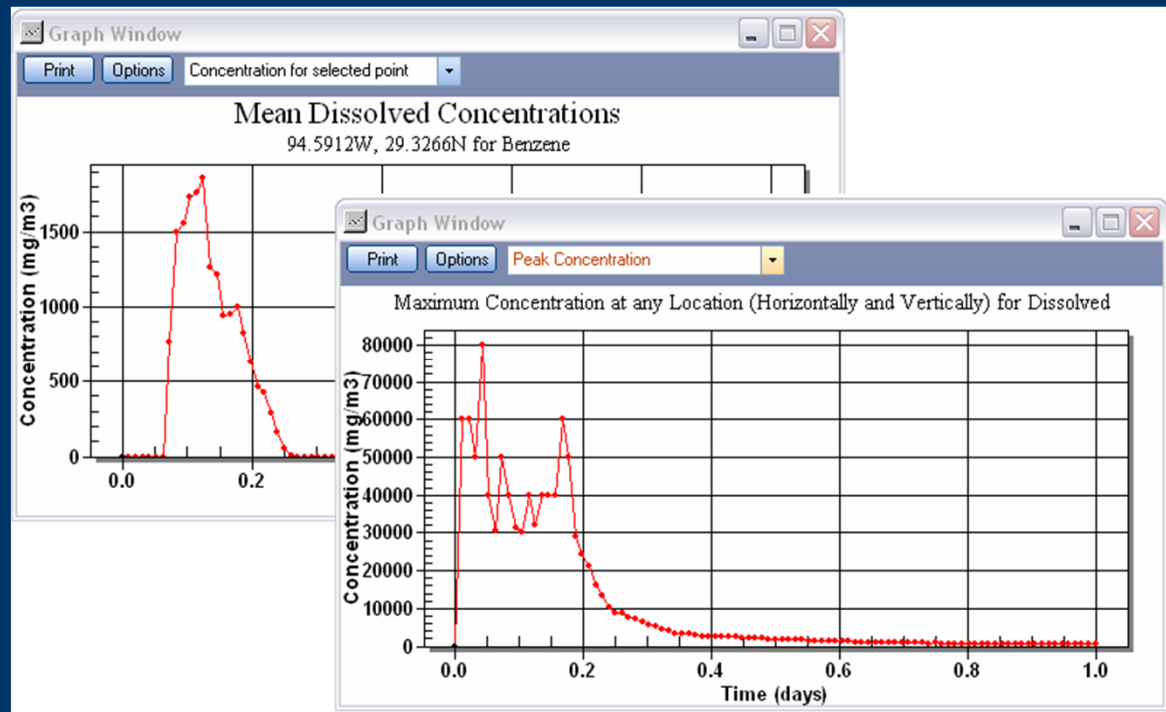
- Time Weighted Average or
- Immediate Dangerous to Life or Health

The screenshot displays the 'Toxicity Parameters' window for Benzene. The window has a title bar with 'OK', 'Chemical Summary', and 'Add Chemical to Personal Database' buttons. Below the title bar, there are radio buttons for 'ASA Database' (selected) and 'Personal Database', and a text field containing 'Benzene'. The main content area is divided into several tabs: 'Descriptions', 'MSDS', 'Information', 'Physical', 'Chemical', 'Initialization', and 'Toxicity'. The 'Toxicity' tab is active, showing a table of toxicity parameters with their values and units. The parameters are:

Parameter	Value	Unit
Predicted No effect Concentration, PNEC (ppb)	Unknown	ppb
No Observable Effects Concentration, NOEC (ppb)	Unknown	ppb
Lowest Observable Effects Concentration, LOEC (ppb)	Unknown	ppb
LC50 for fish (ppb)	Unknown	ppb
LC50 for invertebrates (ppb)	Unknown	ppb
EC50 for plants (ppb)	Unknown	ppb
EC50 for zooplankton (ppb)	Unknown	ppb
EC50 for benthic invertebrates (ppb)	Unknown	ppb
Log10BCF for fish	Unknown	
Log10BCF for invertebrates	Unknown	
Immediately Dangerous to Life or Health, IDLH (ppm)	500.00000	ppm
Time Weighted Average (ppm)		ppm
TLV-TWA	0.50000	ppm
PEL-TWA	1.00000	ppm
REL-TWA	0.10000	ppm
Short Term Exposure Limit, STEL (ppm)	2.50000	ppm
Odor Threshold (ppm)	34.00000	ppm
Human Health threshold in air (ppm)	Unknown	ppm
Human Health threshold in water (ppb)	Unknown	ppb
Human Health threshold in food (ppb)	Unknown	ppb

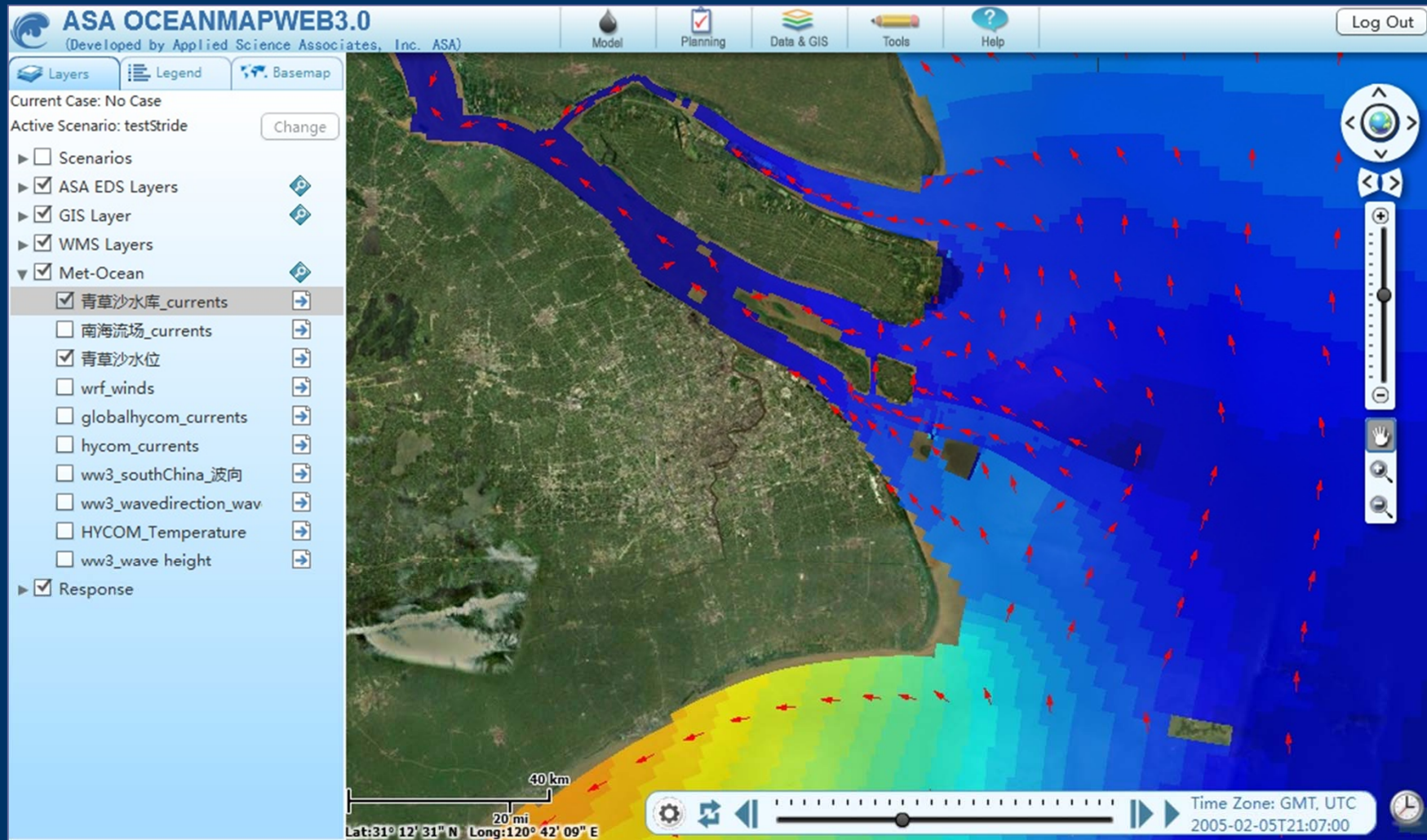
CHEMMAP outputs

Variation in the concentration of the chemical over time



The future: Web environment
Information exchange

Met-Ocean Data



Chemical Modeling

OCEANSMAP Model Data & GIS Tools Help

Layers Legend Basemap

Current Case: No Case
Active Scenario: ChemSpill1

Scenarios
 ChemSpill1
 Trajectory
 Spilllets
 Swept Spilllets
 Surface
 Dissolved
 Particulate
 Absorbed
 Sediment
 Model Currents
 ASA EDS Layers
 GIS Layer
 ASA World Map
 boat_locations
 WMS Layers
 Met-Ocean
 Response

ChemMap Scenario Chemical Winds Currents Review

Chemical Spill Amount: 1000 Tonnes

Release Duration: 0 (minutes) Release Depth: 0 (m)

ID	Chemical Name	cas1	cas2	cas3
17	acetaldehyde	75	7	0
31	Ammonia gas	7664	41	7
33	Ammonia-liquefied gas	7664	41	7
29	Benzene	71	43	2
3	Benzene (gas)	71	43	2
10	carbon tetrachloride	56	23	5

Refresh Chemical List

Number of Particles: 100 Horizontal Dispersion: 3 m²/s
Vertical Dispersion: 0.0001 m²/s

Previous Next

© OpenStreetMap contributors, CC-BY-SA
 Time Zone: GMT, UTC
 2013-01-15T02:00:00

GIS Tools

OCEANSMAP Model Data & GIS Tools Help Account will expire on 4/5/2013!

Current Case: No Case
Active Scenario: OilSpill10

Scenarios

- OilSpill10
 - Trajectory

Edit Layer

Target Layer: areas

Select icon to create feature

ID (serial)	name (text)	description (text)	Shape (Geometry)
1	area1	undefined	POLYGON

Delete feature Save All Merge intersected features

GIS Layer

- Angola_Development
- Angola_Interest
- Angola_ProducingProject
- areas**
- Nigeria_Cameroon_Label
- Nigeria_Cameroon_Oil_
- WMS Layers

Map Labels: OML 133, OML 79, OPL 322, OML 271, OPL 236, OPL 238, OPL 245, OPL 284, OPL 285, OPL 287, OPL 288, OPL 289, OPL 290, OPL 291, OPL 292, OPL 293, OPL 294, OPL 295, OPL 296, OPL 297, OPL 298, OPL 299, OPL 300, OPL 301, OPL 302, OPL 303, OPL 304, OPL 305, OPL 306, OPL 307, OPL 308, OPL 309, OPL 310, OPL 311, OPL 312, OPL 313, OPL 314, OPL 315, OPL 316, OPL 317, OPL 318, OPL 319, OPL 320, OPL 321, OPL 322, OPL 323, OPL 324, OPL 325, OPL 326, OPL 327, OPL 328, OPL 329, OPL 330, OPL 331, OPL 332, OPL 333, OPL 334, OPL 335, OPL 336, OPL 337, OPL 338, OPL 339, OPL 340, OPL 341, OPL 342, OPL 343, OPL 344, OPL 345, OPL 346, OPL 347, OPL 348, OPL 349, OPL 350, OPL 351, OPL 352, OPL 353, OPL 354, OPL 355, OPL 356, OPL 357, OPL 358, OPL 359, OPL 360, OPL 361, OPL 362, OPL 363, OPL 364, OPL 365, OPL 366, OPL 367, OPL 368, OPL 369, OPL 370, OPL 371, OPL 372, OPL 373, OPL 374, OPL 375, OPL 376, OPL 377, OPL 378, OPL 379, OPL 380, OPL 381, OPL 382, OPL 383, OPL 384, OPL 385, OPL 386, OPL 387, 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Map Labels: Benin, Nigeria, EQUATORIAL GUINEA, Mungo Park Seamount, 2166, 2722, 4160, 2833, 312/2013 9:30:00 PM, 3/12/2013 8:00:00 AM, area1

Scale: 200 km, 100 mi

Coordinates: Lat:1° 59' 09" N Long:5° 27' 18" E

Time Zone: GMT, UTC 2013-03-09T19:00:00