

# “Fate and Transport Modelling of HNS”

MARINER



**Rodrigo Fernandes, David Brito, Frank Braunschweig  
(Action Modulers – Consulting & Technology, Lda.)**

**Mariner Cardiff workshop - Cardiff  
28-6-2017**



Funded by  
European Union  
Humanitarian Aid

- HNS Fate & Behaviour Processes

- Mariner HNS Added Value



- Mariner Platform



Funded by  
European Union  
Humanitarian Aid

MARINER

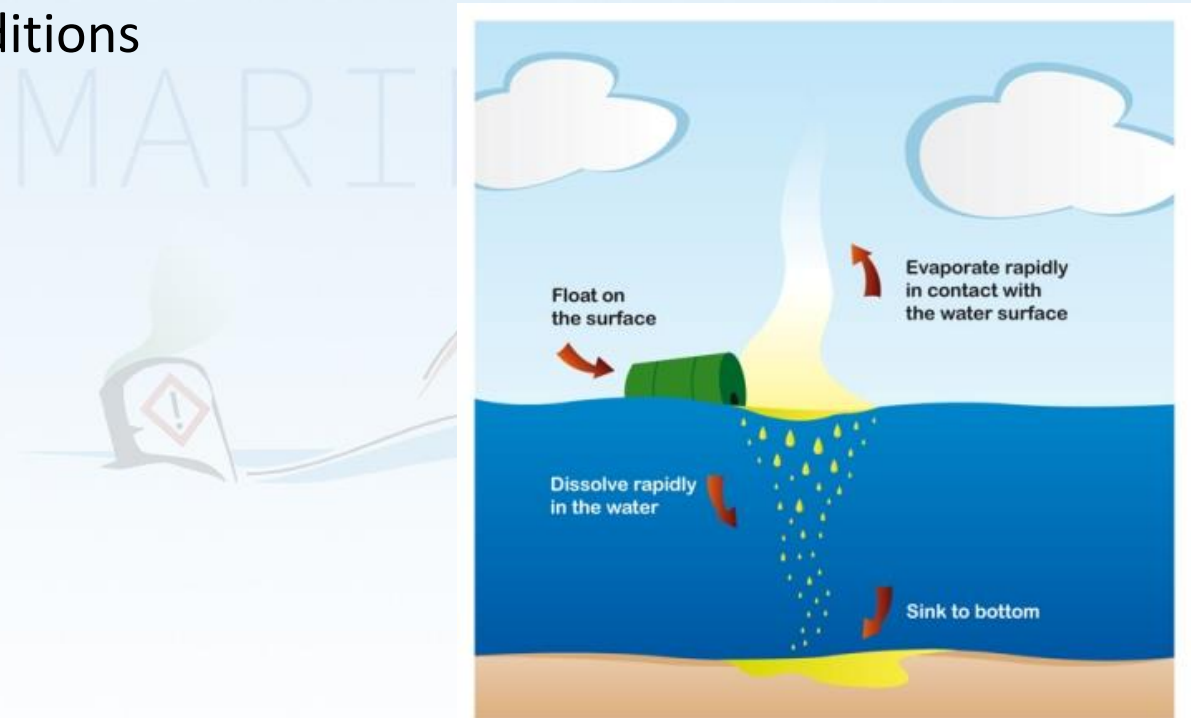
## **“HNS Fate & Behaviour Processes”**



Funded by  
European Union  
Humanitarian Aid

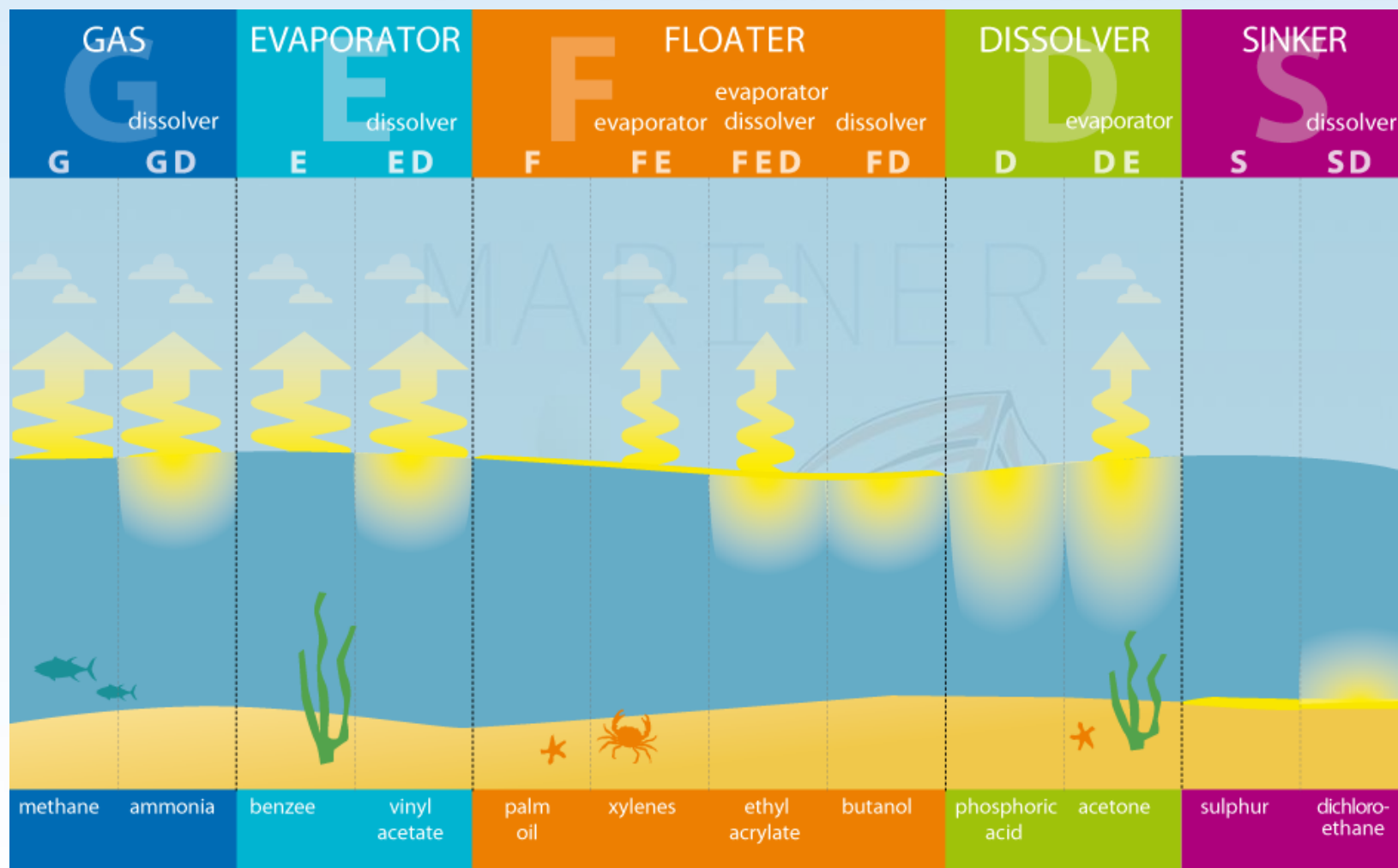
# HNS: fate & behaviour

- Wide variety of chemicals (2000 transported by the sea) => no “standard” behaviour
- Depend on physical-chemical properties and local marine environmental conditions
- Typically, HNS can:
  - Dissolve
  - Evaporate
  - Float
  - Gas
  - Sink



*Processes that can act on a chemical spill into the marine environment*

# HNS: behaviour classes



Funded by  
European Union  
Humanitarian Aid

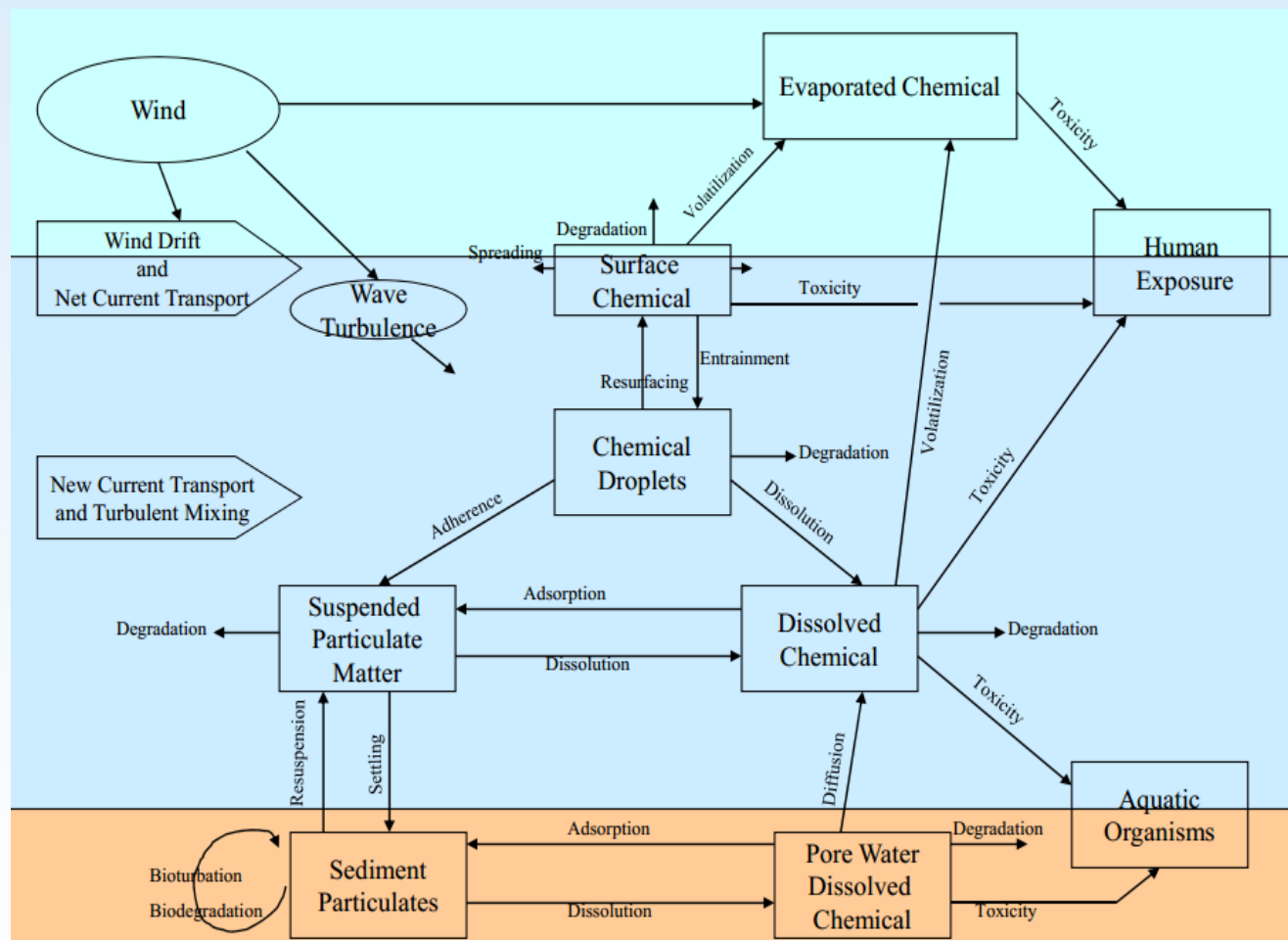
# HNS: behaviour classes

- Classes are far from reality...



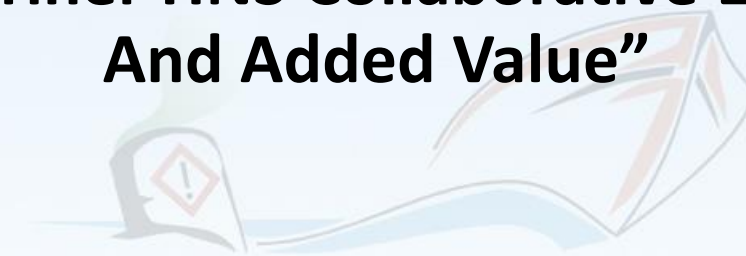
Funded by  
European Union  
Humanitarian Aid

# HNS fate & behaviour



# MARINER

## **“Mariner HNS Collaborative Effort And Added Value”**



Funded by  
European Union  
Humanitarian Aid



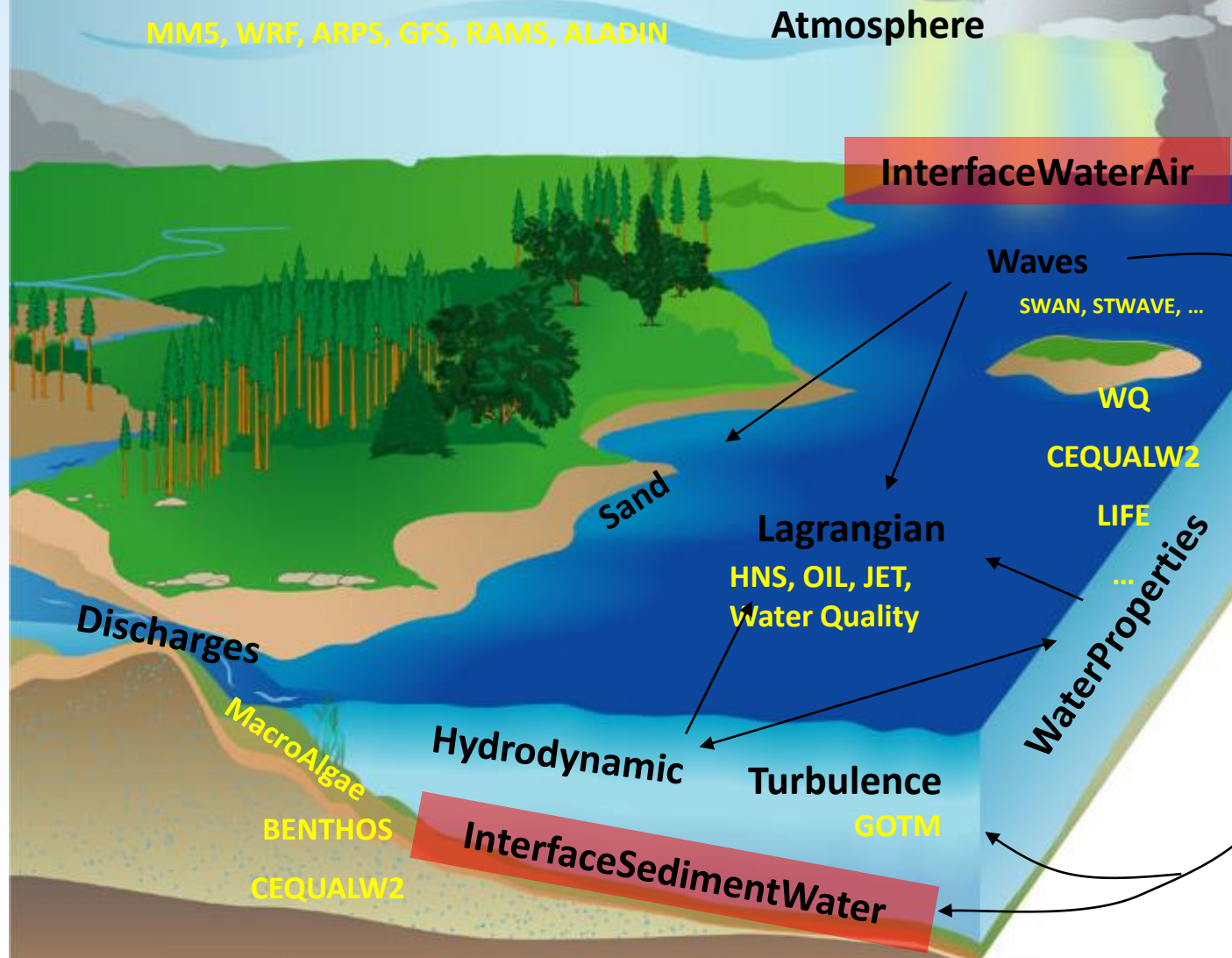
MARINER

## **“HNS Fate & Behaviour Modelling”**



Funded by  
European Union  
Humanitarian Aid

# MOHID Water



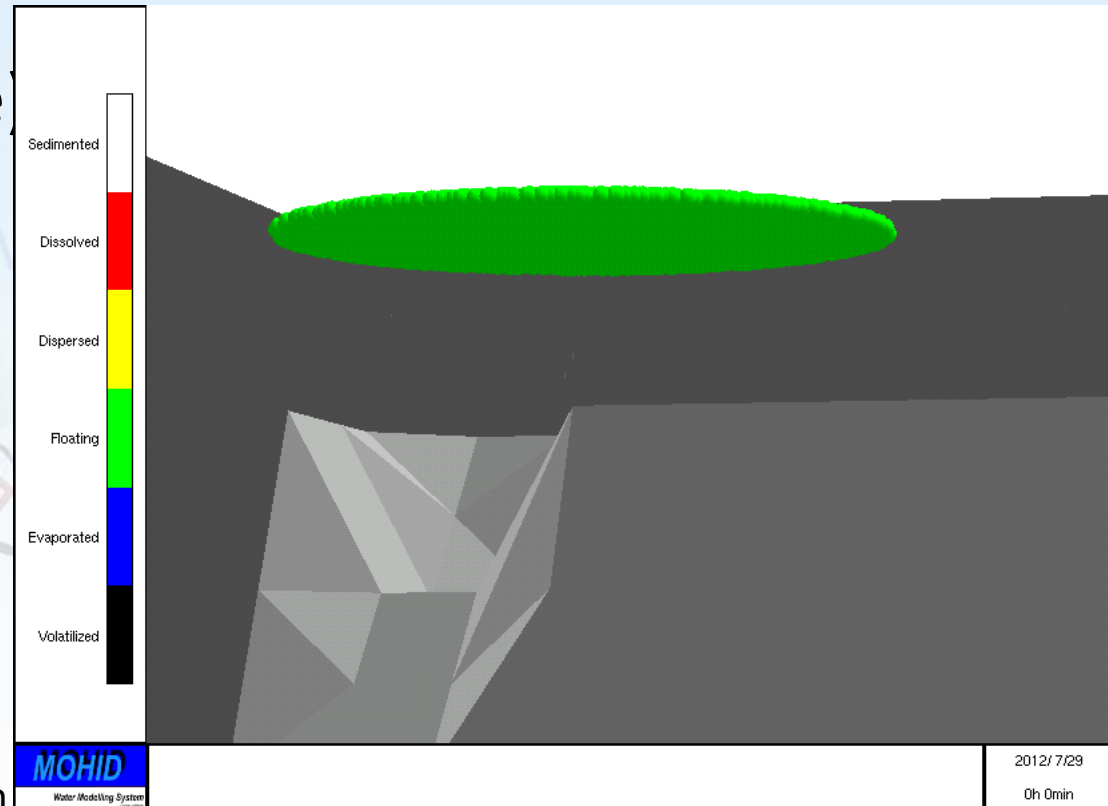
# HNS Modelling Approach

---

- MOHID Water modelling system (open source)
- 3D Lagrangian particle method
- Independent particle phase changes and transport
  - Based on mass balances from different processes (ModuleHNS)
- One chemical per simulation (no chemical mixtures)
- Chemical reactions (with water, oxygen, acids/bases, etc.) not addressed in the model

# HNS Modelling Approach - Phases

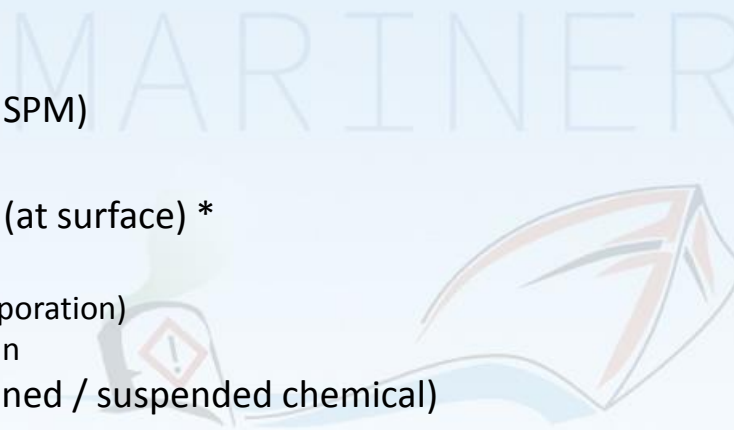
- Air
  - Evaporated (surface)
  - Volatilized (water column)
- Floating at surface
- Entrained / suspended droplets
- Adsorbed to suspended matter (sedimented)
- Dissolved
- Sunk
- Mass lost -> environmental degradation



# HNS Modelling Approach - Processes

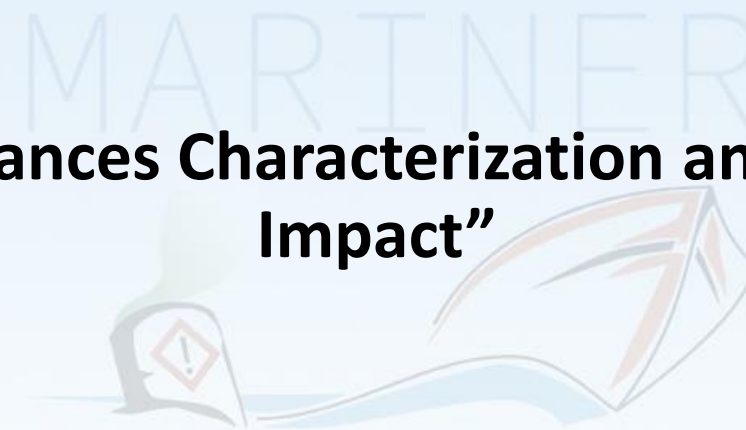
- Movement
  - Currents\*
  - Spreading
  - Turbulence\*
  - Stokes Drift \*
  - Buoyancy \*
  - Sinking (adsorbed to SPM)
- Phase changes
  - Vertical Entrainment (at surface) \*
  - Volatilization
    - From surface (evaporation)
    - From water column
  - Dissolution (of entrained / suspended chemical)
  - Adsorption to Sediments
  - Resuspension (of sunk chemical)
- Degradation
  - From air
  - From water column
  - From sediments

\* Same as used in MOHID oil spill model



Funded by  
European Union  
Humanitarian Aid


# **“HNS Substances Characterization and Biological Impact”**



Funded by  
European Union  
Humanitarian Aid

# HNS Substance characteristics

- Connected to online HNS database from CIIMAR
  - Dynamic link using JSON web service
  - Downloading physical, chemical and **toxicological** parameters
  - PNEC (predicted no effect concentration – several species, exposures, precaution when no data)






## Fate, weathering, behaviour and toxicity of priority Hazardous and Noxious Substances

**Advanced Search**


Substance name

Behavior at the sea

On this database it is collected information on weathering, behaviour and toxicity of priority Hazardous and Noxious Substances (PNOS) from different sources. These systematized information is a useful tool to predict the behaviour of priority PHS in accidental spills and support spill preparedness and effective decision-making process response. This database also provides an important support to risk assessment, environmental impact assessment and monitoring actions.

[Contact us](#)



[Home](#)
[Maps](#)
[Charts](#)
[Simulation -](#)
[Operational Models](#)
[rodrigo.fernandes -](#)

1. What?

2. Where?

3. When?

4. Run

**Incident Name**

2016-10-14 15:27:31 Sim Name

**Substance Type**

HNS Spill

**Chemical Spill Options**

1-nanolol (Floater)

Chlorine gas (Gas)

Ammonia (Gas-Dissolver)

Benzene (Evaporator)

Styrene (Evaporator-Floater)

Di-n-butylamine (Evaporator-Dissolver-Floater)

Methanol (Evaporator-Dissolver)

1-nanolol (Floater)

Aniline (Floater-Dissolver)

Ethanolamine (Dissolver)

Perchloroethylene (Sinkier)

Web Services

**1-Nonene**

CAS Number: 126-10-8

Formula: C<sub>9</sub>H<sub>18</sub>

CCCCCCCCC

Physicochemical properties/Characteristics

EF	126.2	0.74	0.72	1.12	0.64
Behavior (OSLAW) (2016)	Boiling Point (K)	Density (kg/m <sup>3</sup> )	Vapor pressure (kPa)	Wing stability (mg/L)	Dynamic viscosity (cPa.s)
1.2	3	3	2	2.5	2.1
-81.3	146.9	58.1			
Melting point (°C)	Boiling point (°C)	Evaporation half life (days)			
2	2	4			

1. Gao, B.; Espinosa, A.; Paster, P.; Paster-Perichon, D.; Dabonne, S.; Simier, J. *Journal of Hazardous Materials* 2016, 311, 1-10.

2. Values collected from the literature and public databases e.g. PubChem.

3. "1" corresponds to value not found in the literature or in available databases

4. Values estimated with Simion of the EF-Simion



Funded by  
European Union  
Humanitarian Aid

# HNS Substance characteristics

- Connected to online HNS database from HNS-MS
  - Dynamic link using JSON web service (as with CIIMAR)
  - Downloading physical, chemical and toxicological parameters

HNS-MS is funded by DG-ECHO under agreement ECHO/SUB/2014/883708  
hns-ms@naturalsciences.be

Improving Member States preparedness to face an HNS pollution of the Marine System (HNS-MS)

**{HNS-MS}**

Home What are HNS? Background and objectives Actors and beneficiaries Tasks and methods Publications Tools Meeting Contact us

SEARCH RESULT

### Aniline

Description Physico-chemical Behaviour Ecotoxicity Hazards GESAMP profile

Description	
CAS Number	62-53-3
UN Number	1547
Chemical formula	C <sub>6</sub> H <sub>5</sub> N
Accident occurred?	Yes
Standard European Behaviour Classification (SEBC)	Floater that dissolves (FD)

GESAMP profile

A1a	A1b	A1	A2	B1	B2	C1	C2	C3	D1	D2	D3	E1	E2	E3
0	0	0	R	3	2	2	2	3	4	3	CS+T	NT	PD	3

Marine pollution Classification (MARPOL Annex II)

Category	Description
Y	Noxious Liquid Substances which, if discharged into the sea from tank cleaning or deballasting operations, are deemed to present a hazard to either marine resources or human health or cause harm to amenities or other legitimate uses of the sea and therefore justify a limitation on the quality and quantity of the discharge into the marine environment.

Alternate names for this chemical

- Aminobenzene
- Aminophen
- Aniline Oil
- Benzaniline
- Phenylamine
- Aniline

### Physico-chemical properties

Chemical formula	C <sub>6</sub> H <sub>5</sub> N
Molar mass	93.12 g/mol
State at 25 °C and 1 atm	Liquid
Melting point	-6.2 °C
Boiling point	154.4 °C
Density	1020 kg/m <sup>3</sup>
Surface tension at 20 °C	42.9 mN/m
Surface tension at 25 °C	42.12 mN/m
Interfacial tension at 20 °C	5.8 mN/m



MARINER

Home Maps Charts Simulation Operational Models rodrigo.fernandes

1. What? 2. Where? 3. When? 4. Run

Incident Name  
2016-10-14 15:27:31 Sim Name

Substance Type  
HNS Spill

Chemical Spill Options

- 1-nonanol (Floater)
- Chlorine gas (Gas)
- Ammonia (Gas-Dissolver)
- Benzene (Evaporator)
- Styrene (Evaporator-Floater)
- Di-n-butylamine (Evaporator-Dissolver-Floater)
- Methanol (Evaporator-Dissolver)
- 1-nonanol (Floater)
- Aniline (Floater-Dissolver)
- Ethanolamine (Dissolver)
- Perchloroethylene (Sinkers)

Previous Next

CETMAR intecmar Universidade de Vigo ACTION Modellers cimmar Cedre

Copyright © Action Modellers 2016. Powered by Action Seaport

MARINER

Funded by European Union Humanitarian Aid



# **“HNS Substances Characterization and Human Impact”**



Funded by  
European Union  
Humanitarian Aid

# HNS Concern Levels

---

- Protective Action Criteria
- Limits for human in air concentration
- Based on:
  - 1 Acute Exposure Guideline Level,
  - 2 Emergency Response Planning Guideline ,
  - 3 Temporary Emergency Exposure Limit

Existing 3146 HNS substances  
with defined PAC levels (60 min.)  
(from US Department of Energy)

PAC levels:

- PAC-1 : Mild, transient health effects.
- PAC-2 : Irreversible or other serious health effects that could impair the ability to take protective action.
- PAC-3 : Life-threatening health effects



Funded by  
European Union  
Humanitarian Aid

MARINER

**“Mariner Platform”**  
**<http://mariner.actionmodulers.com>**



Funded by  
European Union  
Humanitarian Aid

# HNS modelling and environmental impact

## MARINER PLATFORM: Web responsive design / mobile friendly technology

The image displays three screenshots of the MARINER Platform web application, illustrating its web-responsive design and mobile-friendly technology. Each screenshot shows a browser window with the URL `mariner.actionmodul`.

**Left Screenshot:** The interface shows the 'MARINER' logo and a menu icon. A vertical list of steps is displayed: 1. What? (highlighted in yellow), 2. Where?, 3. When?, and 4. Run. Below this, the 'Incident Name' field contains '2016-10-15 02:14:41 Sim Name'. The 'Substance Type' dropdown is set to 'HNS Spill'. The 'Chemical Spill Options' dropdown is set to '1-nonanol (Floater)'.

**Middle Screenshot:** The interface shows the same steps, but '2. Where?' is highlighted in yellow. Below the steps, the 'Domain' dropdown is set to 'France'. The 'Pick Incident Locations Interactively' section features a map of the Iberian Peninsula and surrounding regions, with labels for France, Monaco, Andorra la Vella, Madrid, and Paris. A red pin is visible on the map.

**Right Screenshot:** The interface shows the same steps, but '3. When?' is highlighted in yellow. Below the steps, the 'Incident Type' section has radio buttons for 'Continuous' and 'Instantaneous', with 'Instantaneous' selected. The 'Incident Instant/Simulation Start' field contains '2016-10-15 00:00'. The 'Simulation End' field contains '2016-10-15 06:00'. The 'Volume (m3)' field contains '100'.

At the bottom of each screenshot, the footer text reads: 'Copyright © Action Modulators 2016. Powered by Action Seaport'.

# HNS modelling and environmental impact

## MARINER PLATFORM: HNS simulations



Home Maps Charts Simulation Operational Models

**Layers**

Monitoring Stations

**Model Results**

MOHID MeteoGalicia Artabro

☒ Current Velocity [m/s]

☐ None

☐ Velocity Modulus [m/s]

☐ Temperature [°C]

☐ Salinity [psu]

**User Simulation Layers**

☒ Zoom to Emission Point

2016-09-29 15:50:49 Sim Name

**Property**

Droplets Concentration [mg/m3]

☒ Barrier

☐ Plume Envelope

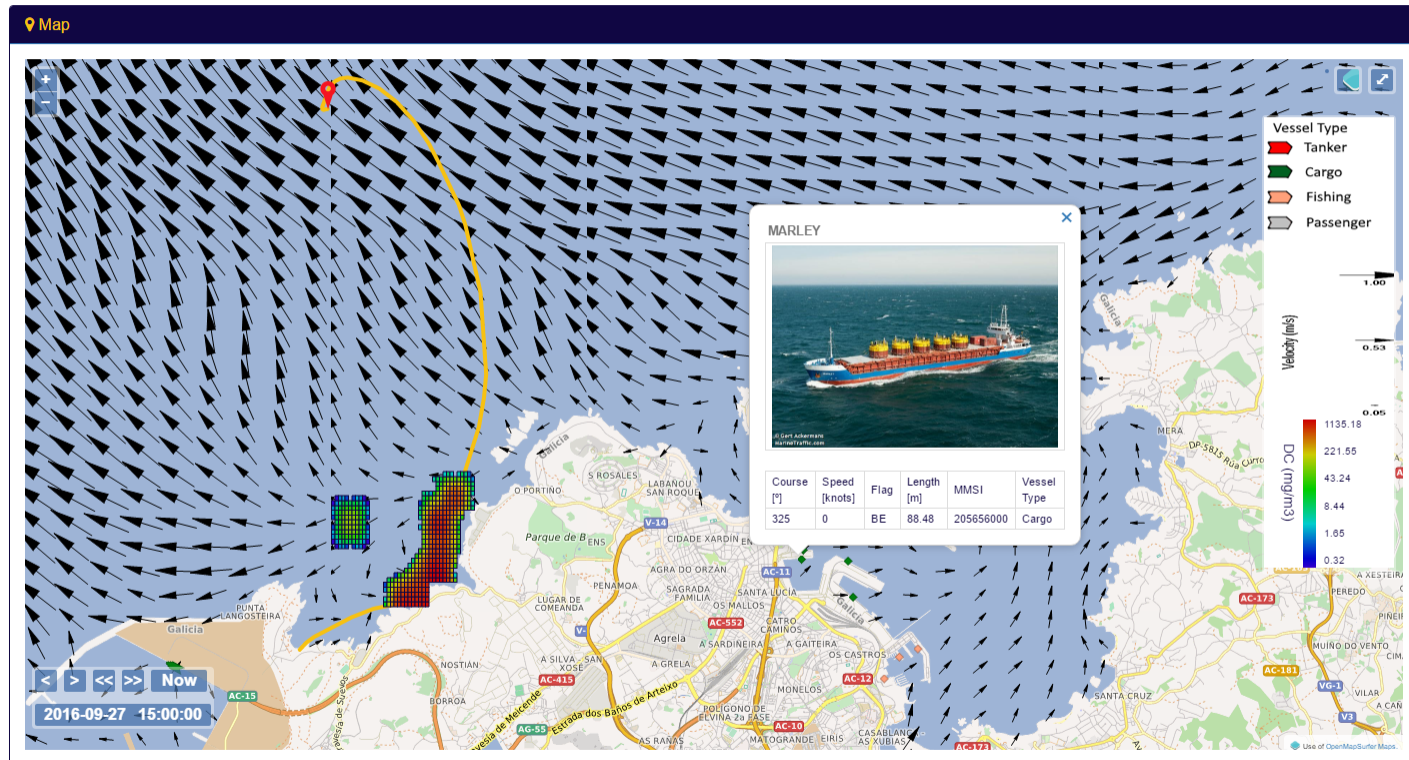
☒ Plume Center

**General Options**

☒ Tooltip on Mouse Stop

Export Map

Export Results



Universidade de Vigo



Copyright © Action Modulers 2016. Powered by Action Seaport



Funded by  
European Union  
Humanitarian Aid

PROJECT CO-FINANCED BY THE EUROPEAN UNION IN THE FRAMEWORK OF THE UNION CIVIL PROTECTION MECHANISM. DG-ECHO.

# HNS modelling and environmental impact

## MARINER PLATFORM: exporting results to 3<sup>rd</sup> party GIS systems



Home Maps Charts Simulation Operational Models rodrigo.fernandes

**Layers**

☒ Vessels  
☐ Monitoring Stations

**Model Results**

MOHID Meteogalicia Artabro

☐ Current Velocity [m/s]  
☒ None  
☐ Velocity Modulus [m/s]  
☐ Temperature [°C]  
☐ Salinity [psu]

**User Simulation Layers**

☒ Zoom to Emission Point

2016-09-29 15:50:49 Sim Name

**Property**

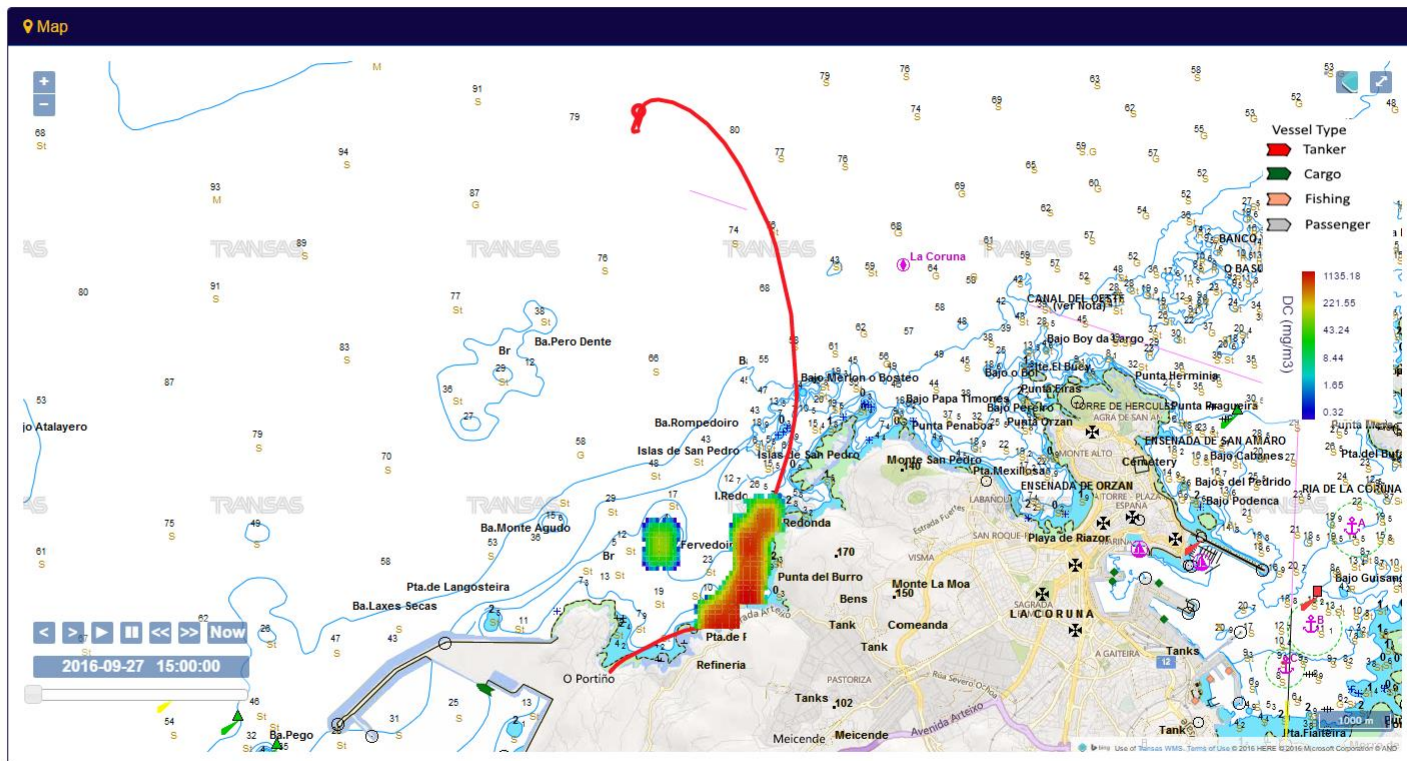
Droplets Concentration [mg/m3]

☐ Barrier  
☐ Plume Envelope  
☒ Plume Center Trajectory

**General Options**

☒ Tooltip on Mouse Stop

Export Map



Universidade de Vigo



Copyright © Action Modulators 2016. Powered by Action Seaport



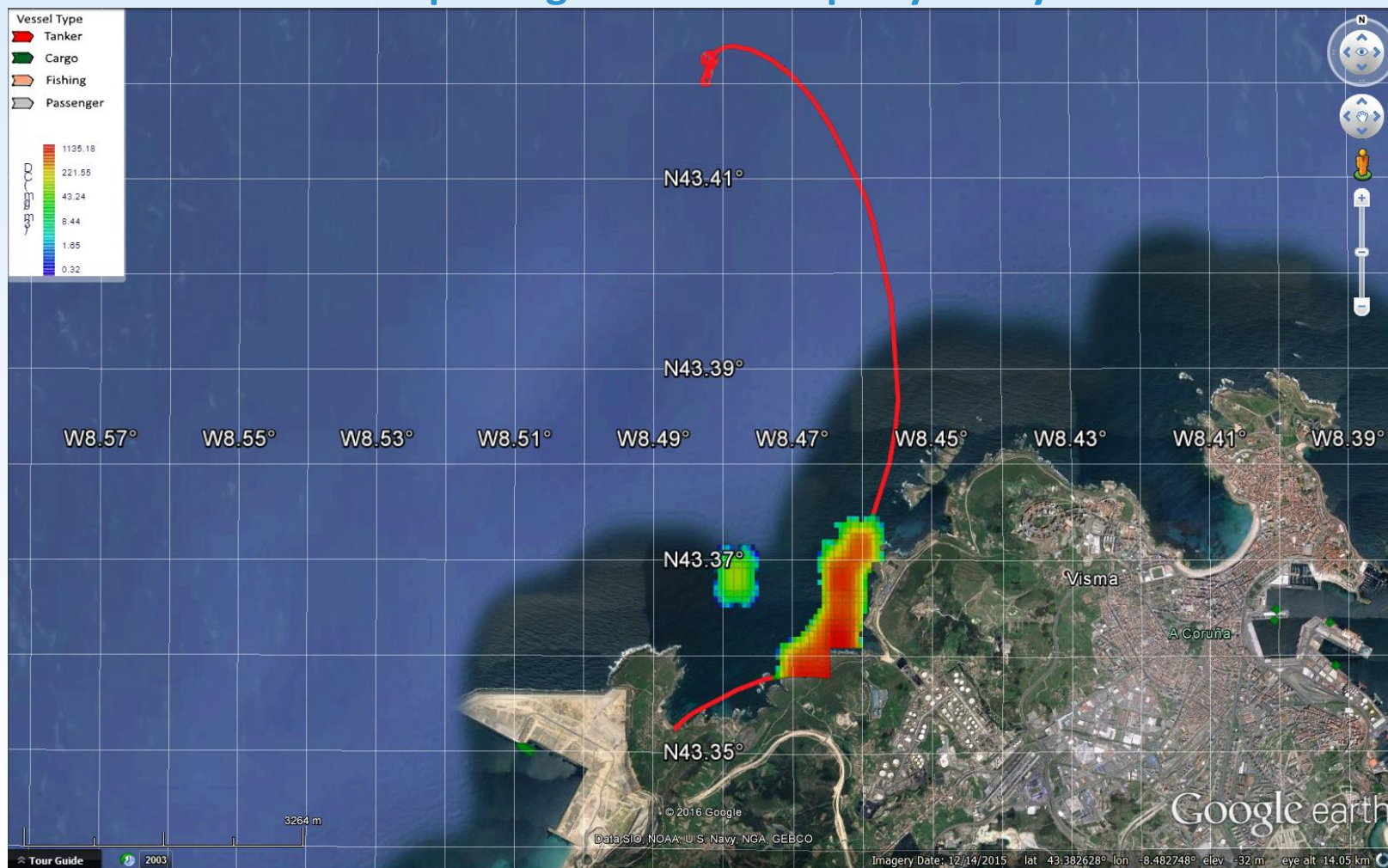
Funded by  
European Union  
Humanitarian Aid

PROJECT CO-FINANCED BY THE EUROPEAN UNION IN THE FRAMEWORK OF THE UNION CIVIL PROTECTION MECHANISM. DG-ECHO.



# HNS modelling and environmental impact

## MARINER PLATFORM: exporting results to 3<sup>rd</sup> party GIS systems



Funded by  
European Union  
Humanitarian Aid

# HNS Impact on Sea Biology

## MARINER PLATFORM: Water Substance Concentration



Home Maps Charts Simulation Operational Models rodrigo.fernandes +Info

**Layers**

**Vulnerability Index**

- ☐ None
- ☐ Socio-Economic
- ☐ Ecological
- ☒ Environmental

**Risk Index**

- ☐ Vessel Accident Risk
- ☐ Shoreline Contamination Risk (non-modelled)

**User Simulation Layers**

☒ Zoom to Emission Point

2017-04-25 00:38:36 Sim Name

**Property**

Maximum Vertical Dissolved Concentration [mg/m3]

☒ Barrier

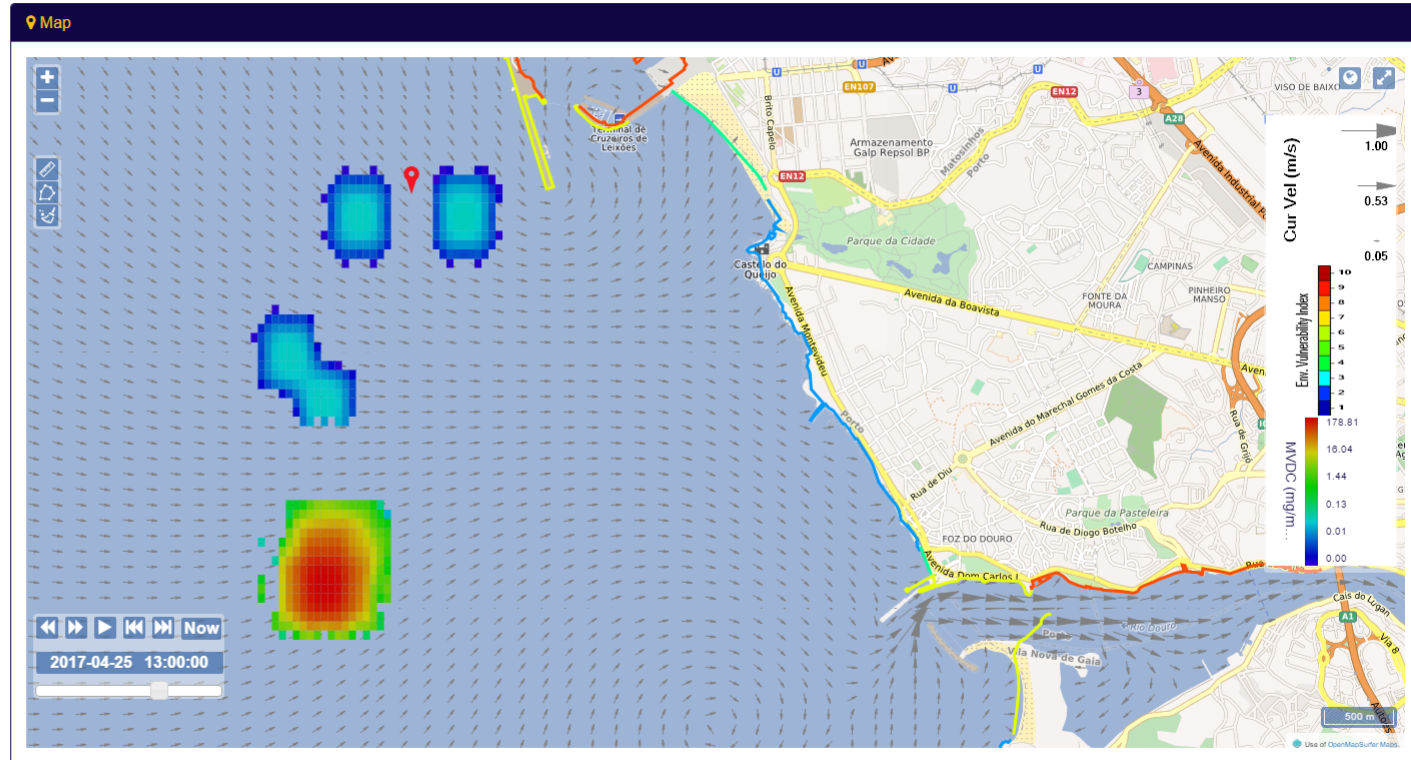
☐ Plume Envelope

☐ Plume Center Trajectory

**General Options**

☒ Tooltip on Mouse Stop

Export Map



Universidade de Vigo



Copyright © Action Modulers 2016. Powered by Action Seaport



Funded by  
European Union  
Humanitarian Aid

PROJECT CO-FINANCED BY THE EUROPEAN UNION IN THE FRAMEWORK OF THE UNION CIVIL PROTECTION MECHANISM. DG-ECHO.



# HNS Impact on Sea Biology

## MARINER PLATFORM: Water Species Impact (PEC/PNEC ratio)



Home Maps Charts Simulation Operational Models rodrigo.fernandes Info

**Layers**

**Domain**

Portugal (Cont.)

**WMS Layers**

☐ Vessels

☐ Monitoring Stations

**Model Results**

Hydro MOHID AM Douro 50m

☒ Current Velocity [m/s]

☐ Current Velocity Modulus [m/s]

**Vulnerability Index**

☐ None

☐ Socio-Economic

☐ Ecological

☒ Environmental

**Risk Index**

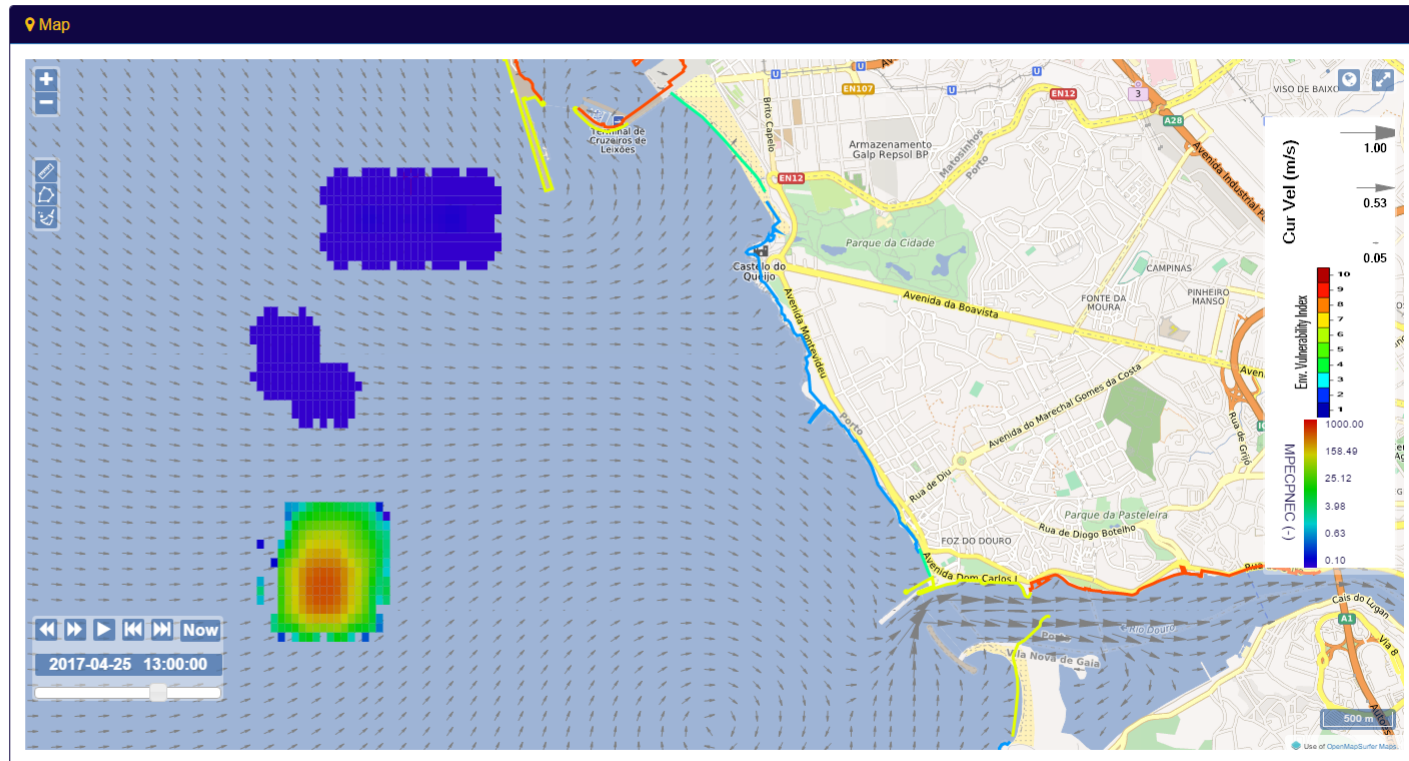
☐ Vessel Accident Risk

☐ Shoreline Contamination Risk (non-modelled)

**User Simulation Layers**

☒ Zoom to Emission Point

2017-04-25 00:38:36 Sim Name



Universidade de Vigo



Copyright © Action Modulers 2016. Powered by Action Seaport

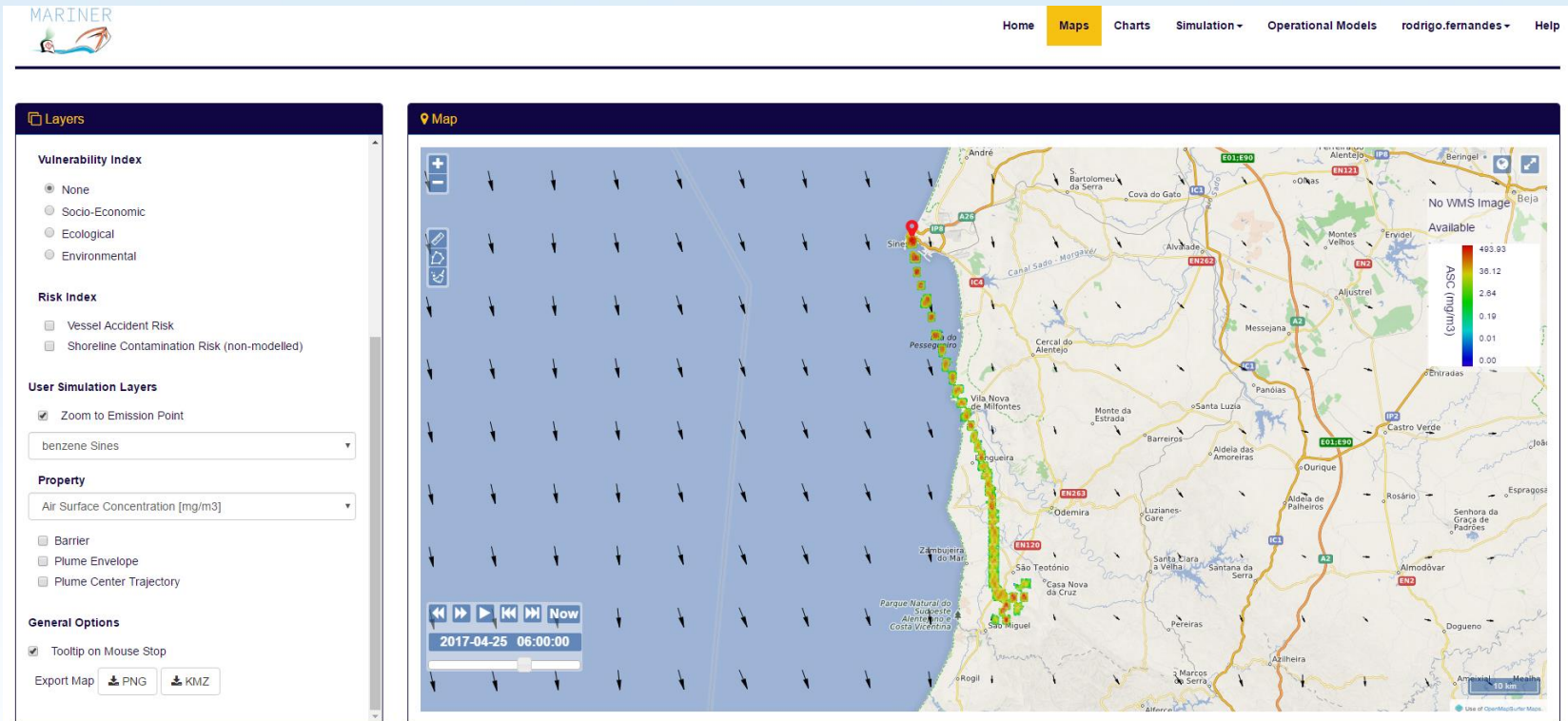


Funded by  
European Union  
Humanitarian Aid

PROJECT CO-FINANCED BY THE EUROPEAN UNION IN THE FRAMEWORK OF THE UNION CIVIL PROTECTION MECHANISM. DG-ECHO.

# HNS Impact on Human

## MARINER PLATFORM: Air Substance Concentration



Universidade de Vigo



Copyright © Action Modulers 2016. Powered by Action Seaport

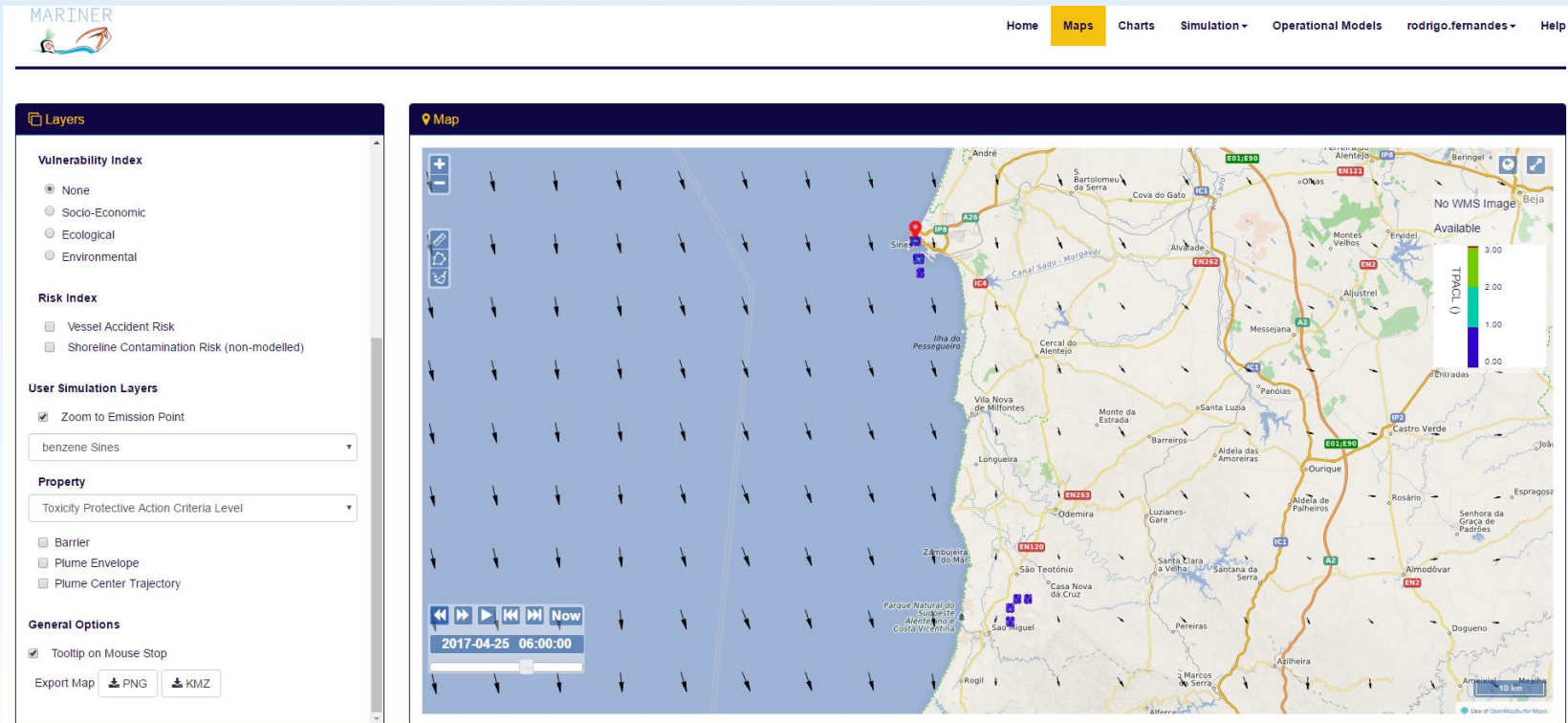


Funded by  
European Union  
Humanitarian Aid

PROJECT CO-FINANCED BY THE EUROPEAN UNION IN THE FRAMEWORK OF THE UNION CIVIL PROTECTION MECHANISM. DG-ECHO.

# HNS Impact on Human

## MARINER PLATFORM: Air Human Impact



# Take Home Message

---

- Mariner mixed different areas of expertise
  - Mathematical modelling
  - Biological Impact
  - Human Health
- Created an inovative tool for HNS spill evaluation in terms of Biological and Human Impact that can be used for training and pollution response scenarios



Funded by  
European Union  
Humanitarian Aid

<http://mariner.actionmodulers.com>

MARINER



*Thank you!*



Funded by  
European Union  
Humanitarian Aid