A New Framework for Environmental Impact Assessment of HNS: Combining HNS Databases, Population Modelling and Dispersion models

CIIMAR

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Workshop - Using technology towards a better preparedness to HNS Spills

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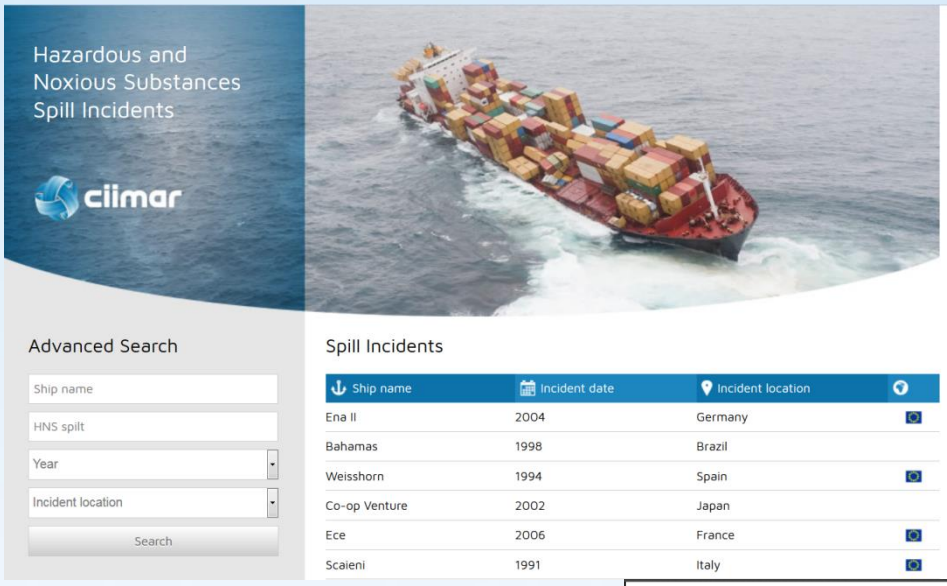

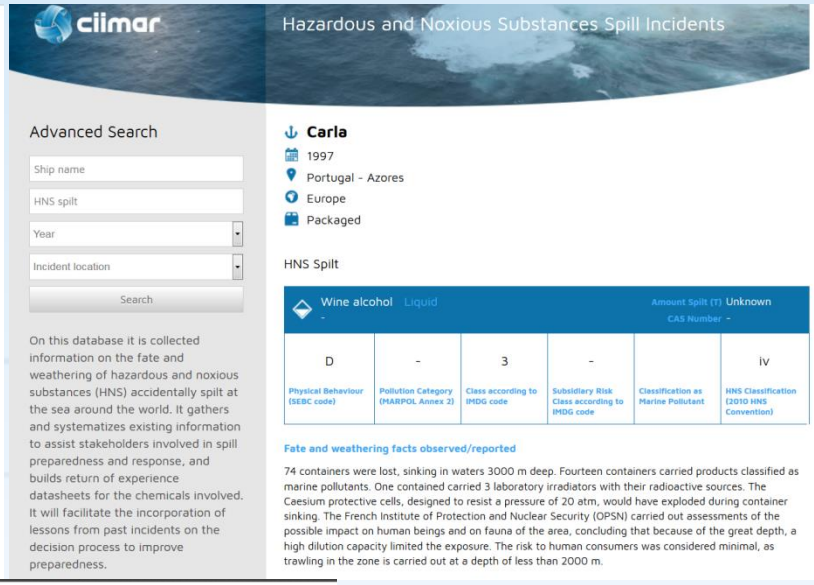

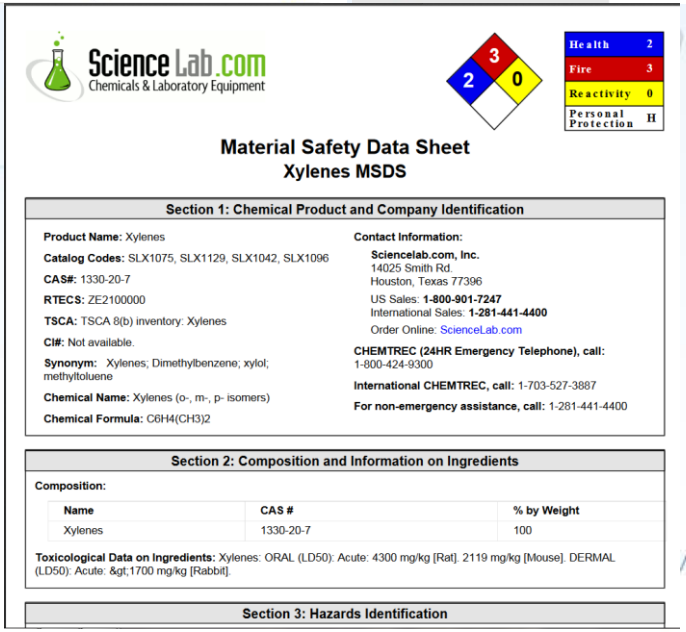

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Actions: Action C.2.3

C.2.3 Tools for modelling impact (toxicology)

Physicochemical properties/Characteristics

E Physical behaviour (GESAMP, 2016) 1, 2	78.114 Molecular Weight (g/mol) 2	0.88 Density (kg/L) 2	12.64 Vapour pressure (KPa; 25°C) 2
5.5 Melting point (°C) 2	80.1 Boiling point (°C) 2	23.3 Volatilization half-life (days) 4	

Substances

Substance name	CAS number	Formulae	Behaviour
1-Dodecanol	112-53-8	C12H26O	Fp
1-Nonanol	143-08-8	C9H20O	Fp
1-Nonene	124-11-8	C9H18	FE
4-Nonylphenol	104-40-5	C15H24O	Fp
Acrylonitrile	107-13-1	C3H3N	DE
Aniline	62-53-3	C6H5NH2	FD
Benzene	71-43-2	C6H6	E
Butyl acrylate	141-32-2	C7H12O2	FED
Cyclohexane	110-82-7	C6H12	E
Cyclohexylbenzene	827-52-1	C12H16	F
Decanoic acid	334-48-5	C10H20O2	Fp
Di-2-ethylhexyl adipate	103-23-1	C22H42O4	Fp
Heptane	142-82-5	C7H16	E
Hexane	110-54-3	C6H14	E
Isononanol	27458-94-2	C9H20O	Fp

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C.2.3 Tools for modelling impact (toxicology)

Algae

Invertebrates

6			
EC50	18	Water flea - *Daphnia magna*	
Parameter	Concentration (mg/L)	Species	
1			
Intoxication, immobilization		Freshwater; Static; 20 24h age	
Endpoint		Observations	

7			
EC50	10	Water flea - *Daphnia magna*	
Parameter	Concentration (mg/L)	Species	
2			
Intoxication, immobilization		Freshwater; Static; 20 exposure; Juvenile(s)	
Endpoint		Observations	

8			
EC50	10.15	Water flea - *Ceriodaphnia dubia*	

13			
LC50	18.4	Water flea - *Ceriodaphnia dubia*	
Parameter	Concentration (mg/L)	Species	
7			
Mortality		Freshwater; Static; 25 °C; 24h-exposure; < 24h age	
Endpoint		Observations	

14			
LC50	20	Bay shrimp - *Crangon franciscorum*	
Parameter	Concentration (mg/L)	Species	
8			
Mortality		Saltwater; Static; 16 °C; 96h-exposure; Mature organism(s)	
Endpoint		Observations	

15			
LC50	27	Daggerblade grass shrimp - *Palaemonetes pugio*	
Parameter	Concentration (mg/L)	Species	
9			
Mortality		Saltwater; Static; 21 °C; 96h-exposure	
Endpoint		Observations	

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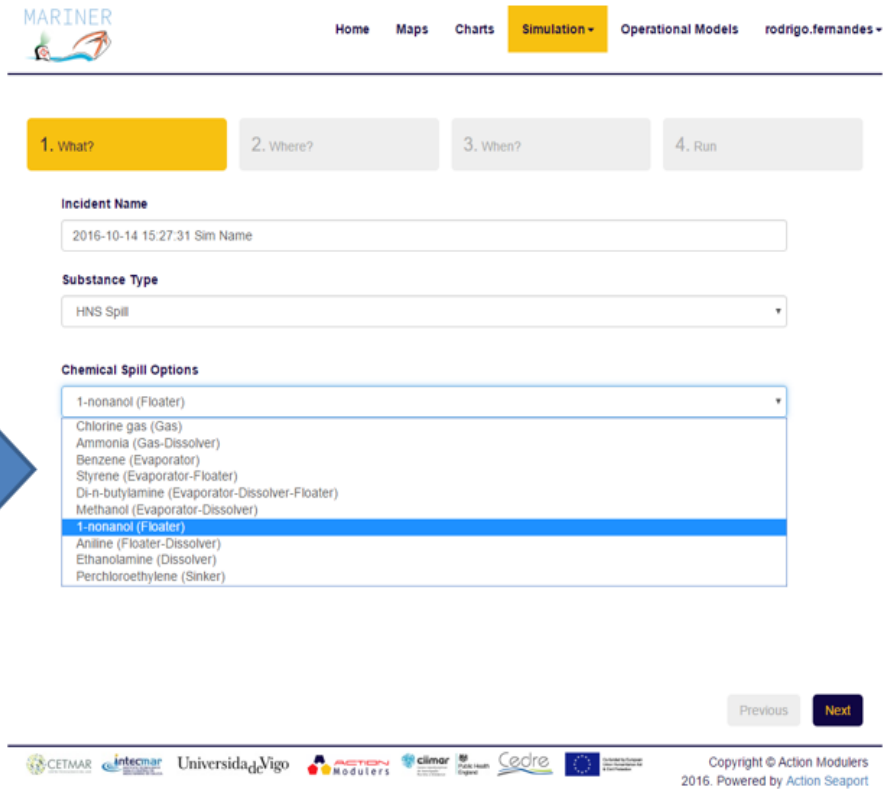
Web Services



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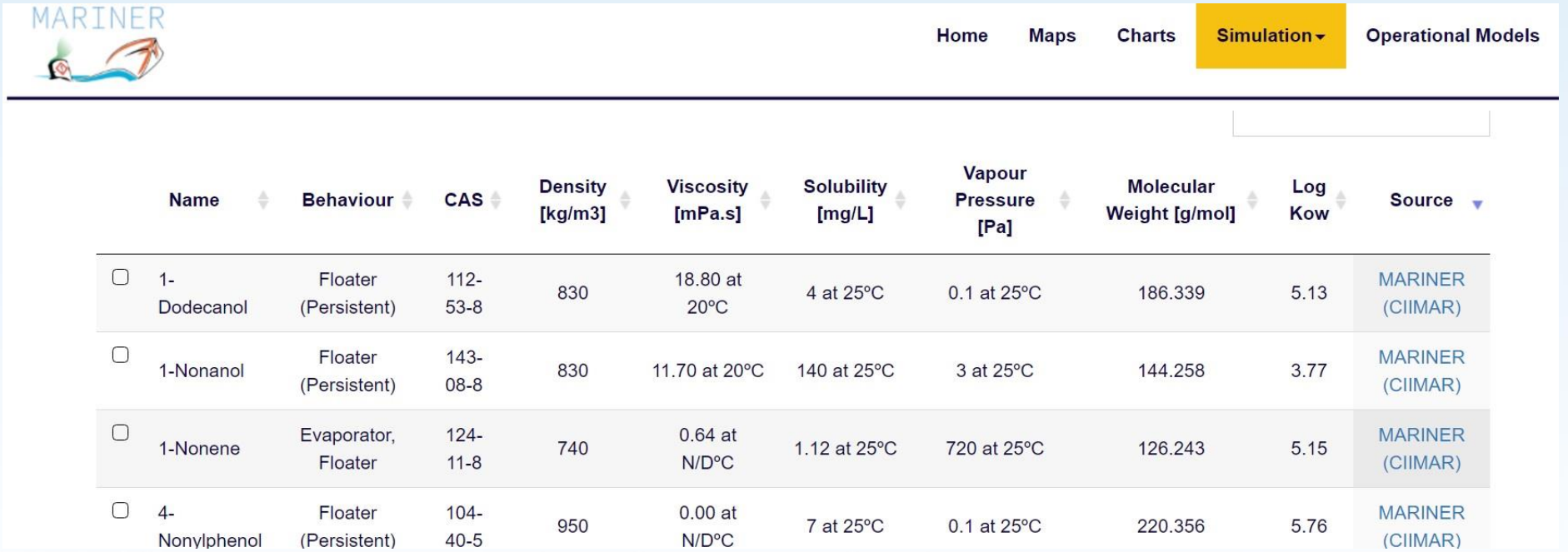
CIIMAR HNS database was integrated in MARINER interface.



	Name	Behaviour	CAS	Density [kg/m3]	Viscosity [mPa.s]	Solubility [mg/L]	Vapour Pressure [Pa]	Molecular Weight [g/mol]	Log Kow	Source
☐	1-Dodecanol	Floater (Persistent)	112-53-8	830	18.80 at 20°C	4 at 25°C	0.1 at 25°C	186.339	5.13	MARINER (CIIMAR)
☐	1-Nonanol	Floater (Persistent)	143-08-8	830	11.70 at 20°C	140 at 25°C	3 at 25°C	144.258	3.77	MARINER (CIIMAR)
☐	1-Nonene	Evaporator, Floater	124-11-8	740	0.64 at N/D°C	1.12 at 25°C	720 at 25°C	126.243	5.15	MARINER (CIIMAR)
☐	4-Nonylphenol	Floater (Persistent)	104-40-5	950	0.00 at N/D°C	7 at 25°C	0.1 at 25°C	220.356	5.76	MARINER (CIIMAR)

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Environmental risk assessment

PNEC

Predicted no-effect concentration

Is the concentration of a substance below which no adverse effects of exposure in an ecosystem are expected to occur, during long-term or short-term exposures.

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Ecotoxicological dose descriptors

Chronic toxicity **NOEC** or equivalent **Ecx**

- ✓ **Algae** (primary producers): **72/96h EC50** (reproduction/growth);
- ✓ **Invertebrates** (primary consumers): 48h **EC50** (immobility) *Daphnia sp*. and **96h LC50** other crustaceans;
- ✓ **Fish** (higher level consumers): **96h LC50** (mortality).

The lowest of the availability toxicity values between and within the different trophic levels is used as a toxicological dose descriptor.

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PNECseawater

Data set	Assessment factor
Lowest short-term L(E)C50 from freshwater or saltwater representatives of three taxonomic groups (algae, crustaceans and fish) of three trophic levels	10,000 [a)]
Lowest short-term L(E)C50 from freshwater or saltwater representatives of three taxonomic groups (algae, crustaceans and fish) of three trophic levels, + two additional marine taxonomic groups (e.g. echinoderms, molluscs)	1000 [b)]
One long-term result (e.g. EC10 or NOEC) (from freshwater or saltwater crustacean reproduction or fish growth studies)	1000 [b)]
Two long-term results (e.g. EC10 or NOEC) from freshwater or saltwater species representing two trophic levels (algae and/or crustaceans and/or fish)	500 [c)]
Lowest long-term results (e.g. EC10 or NOEC) from three freshwater or saltwater species (normally algae and/or crustaceans and/or fish) representing three trophic levels	100 [d)]
Two long-term results (e.g. EC10 or NOEC) from freshwater or saltwater species representing two trophic levels (algae and/or crustaceans and/or fish) + one long-term result from an additional marine taxonomic group (e.g. echinoderms, molluscs)	50
Lowest long-term results (e.g. EC10 or NOEC) from three freshwater or saltwater species (normally algae and/or crustaceans and/or fish) representing three trophic levels + two long-term results from additional marine taxonomic groups (e.g. echinoderms, molluscs)	10

European Chemicals Agency

PNECwater, intermittent: LC(E)50 divided by 100

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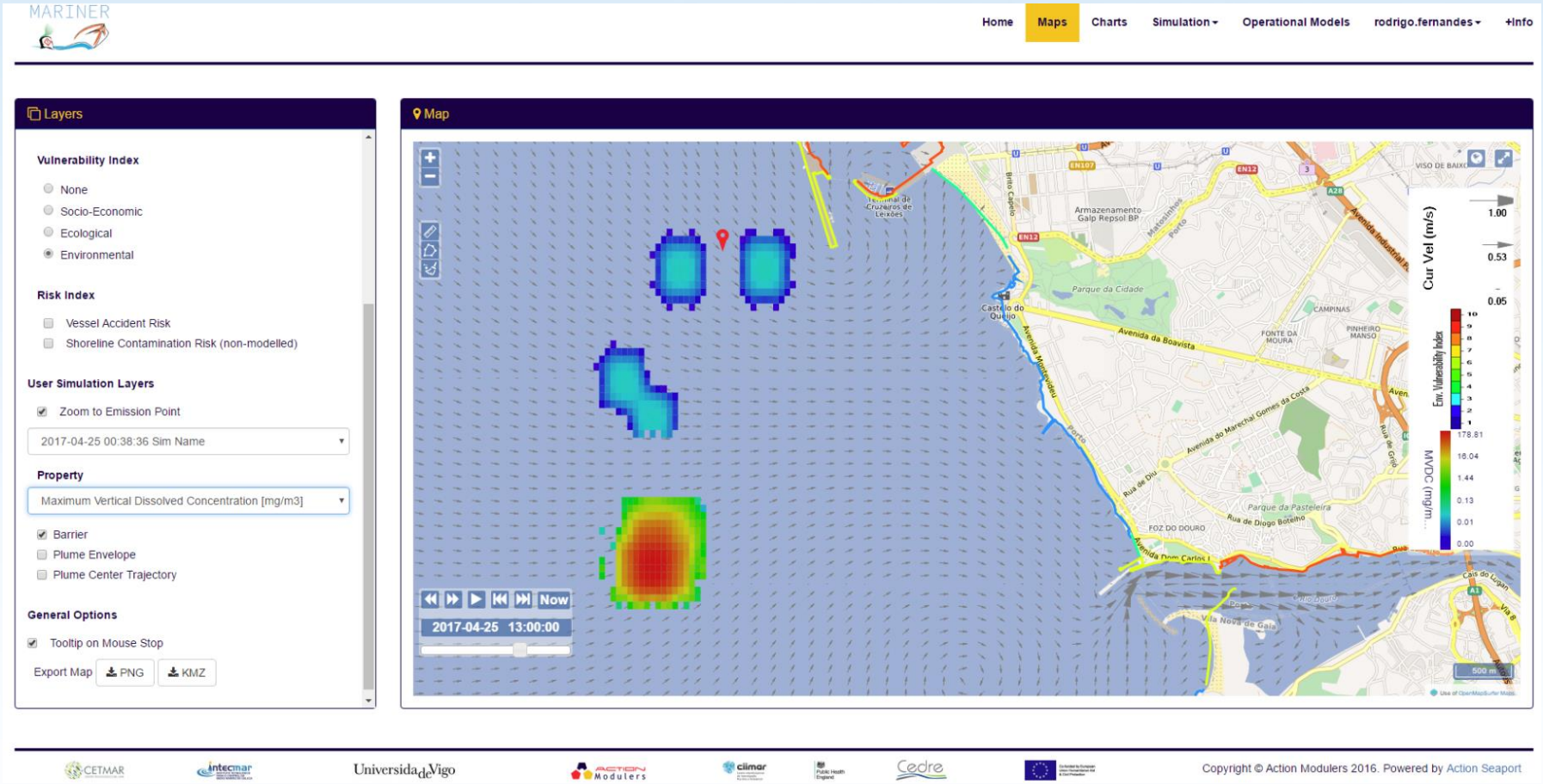

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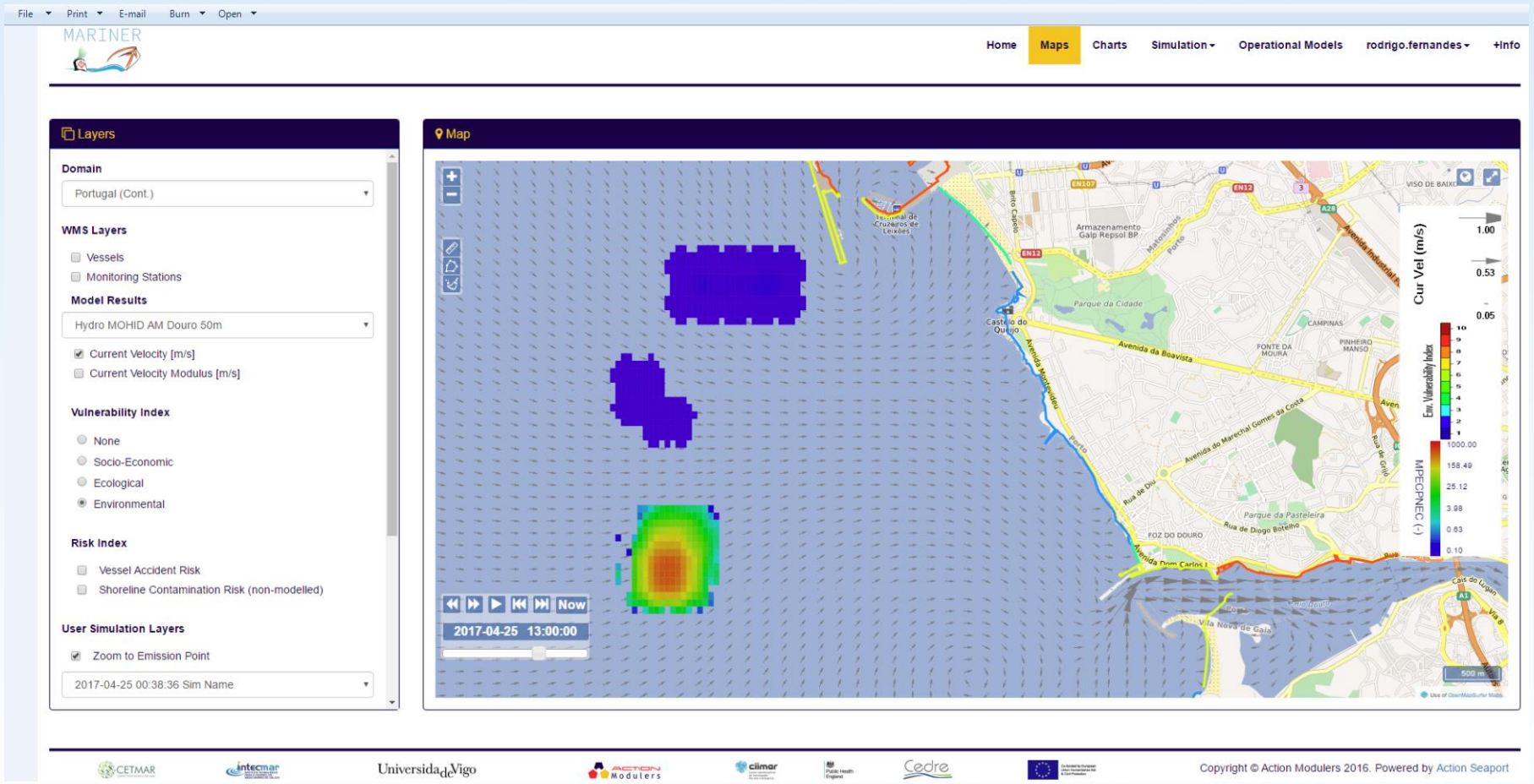

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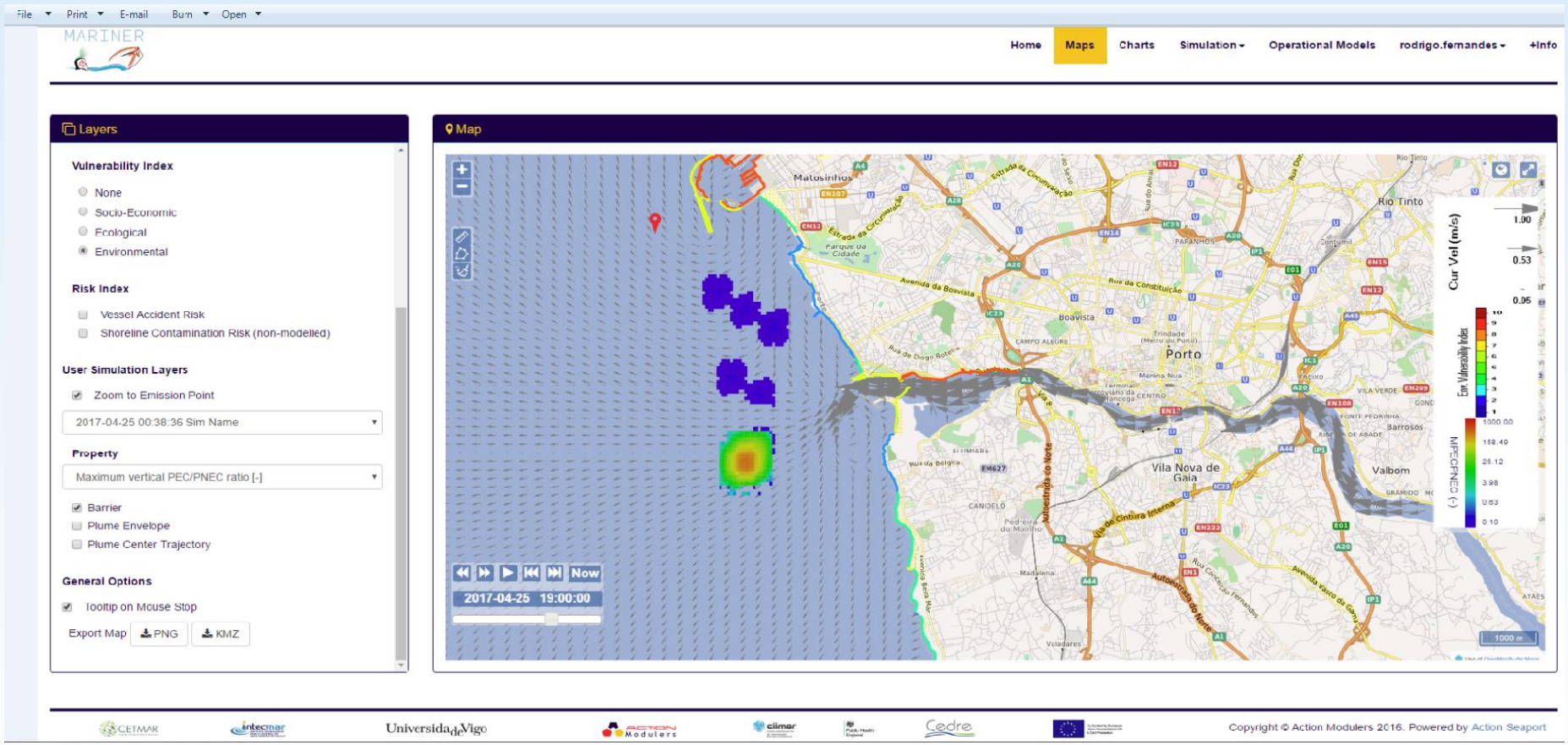

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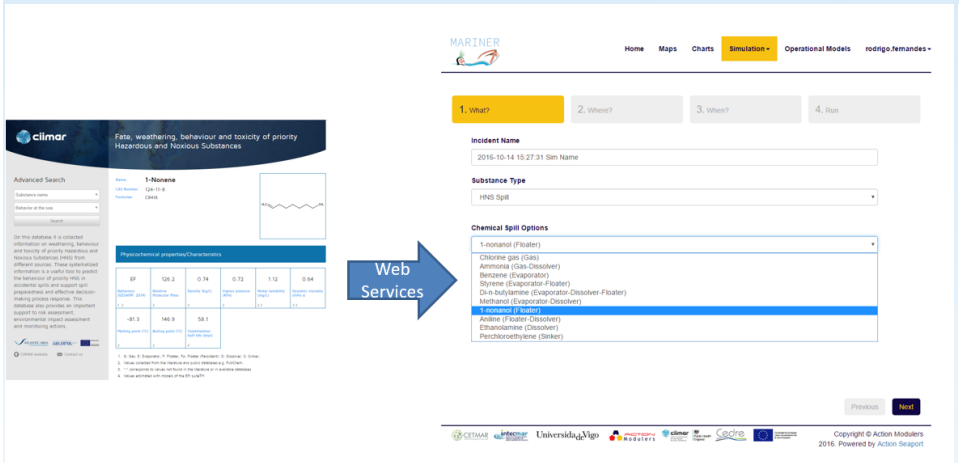

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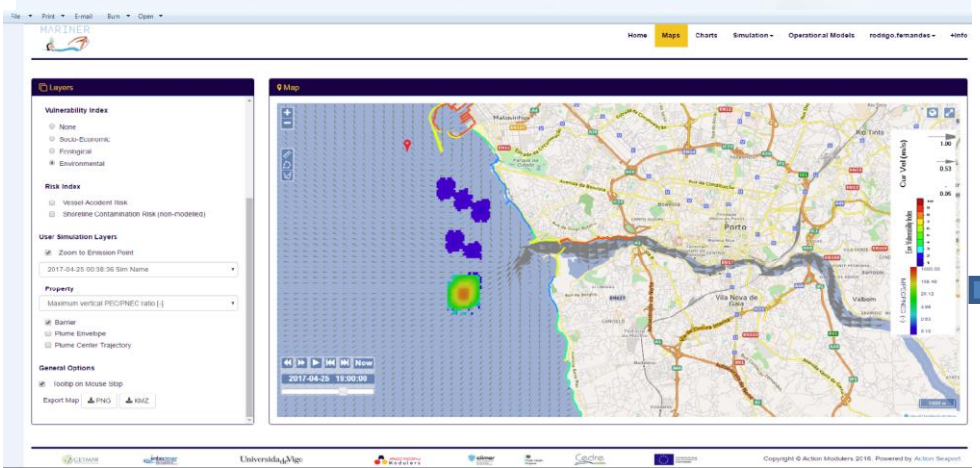

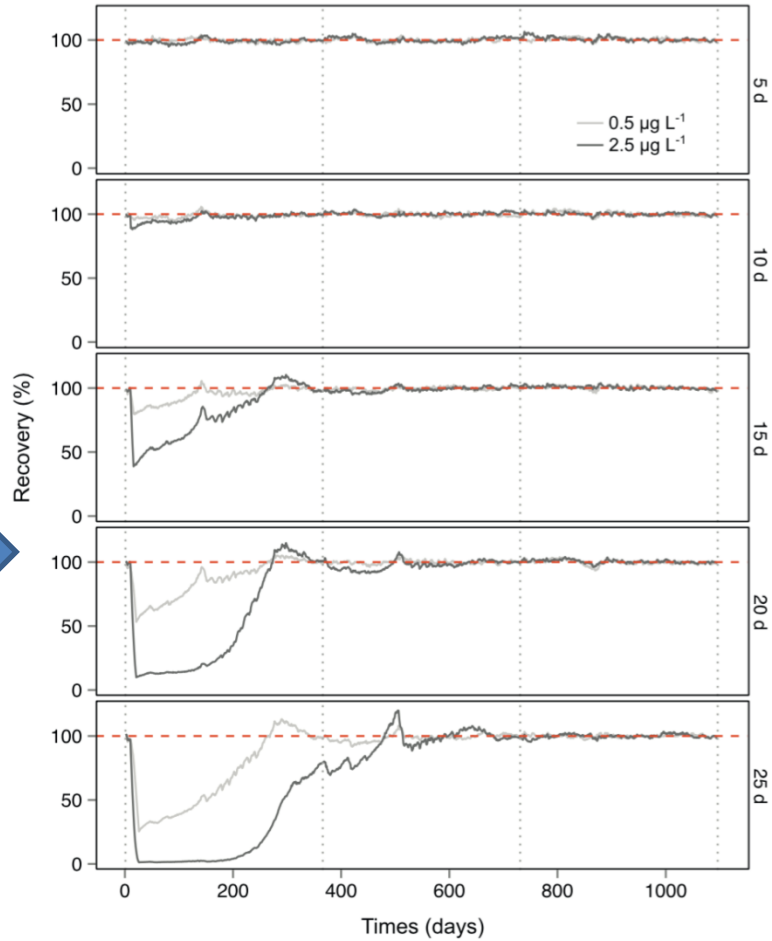

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Thank you
Merci
Gracias
Muito obrigada

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