Oceans
Exploration and Exploitation

Chemical spill simulation with Mohid: implementation and application case

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MOHIDing

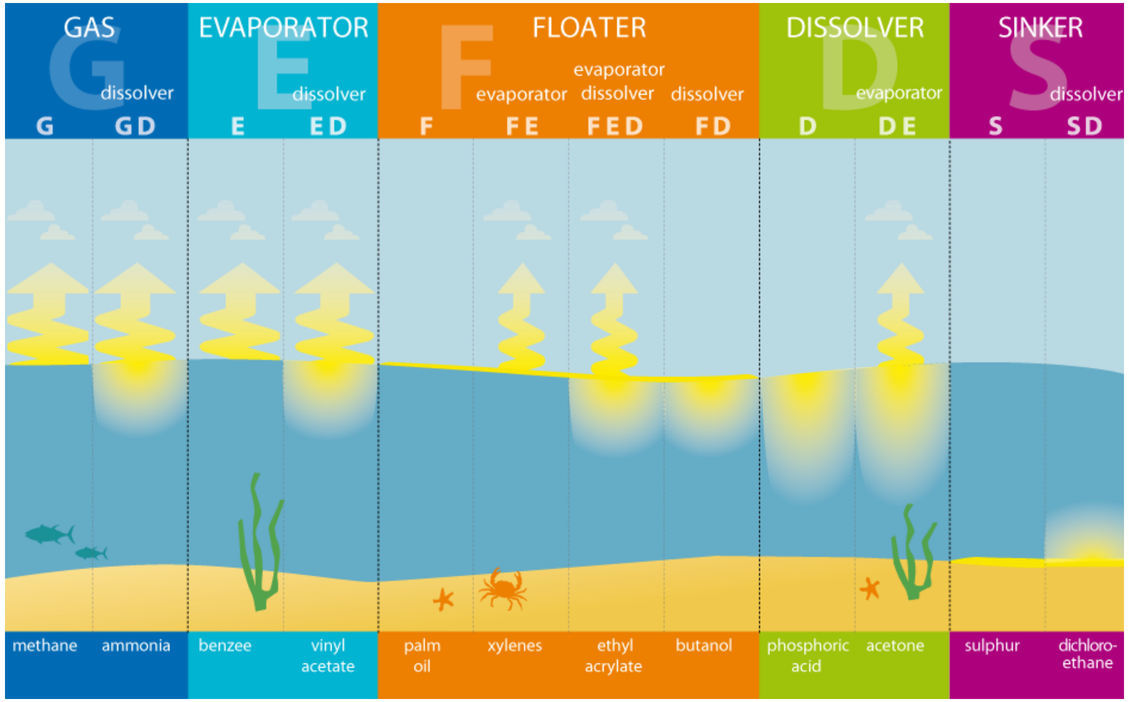
TÉCNICO LISBOA

MARETEC
CENTRO DE CIÊNCIA E TECNOLOGIA DO AMBIENTE E DO MAR
TÉCNICO LISBOA

HNS model

- Chemical fate and behaviour model integrated in lagrangian module of MOHID system (a public-domain / open-source water modelling system – www.mohid.com)
- Comprehensive water & air behaviour chemical spill model:
  - multiple processes and properties evolution at the same time;
  - Based on physical and chemical characteristics (not in classes).

Characterization of spilled loose chemicals as:
gases (G); evaporators (E); floaters (F); dissolvers (D); sinkers (S)
and the various combinations of these, that is:
gases/dissolvers (GD);
evaporators/dissolvers (ED);
floaters/evaporators (FE);
floaters/evaporators/dissolvers (FED);
floaters/dissolvers (FD);
sinkers/dissolvers (SD)



HNS model

- MOHID Lagrangian transport module assumes that the **spilled contaminant** (or water mass) can be **represented as an amount of several different small tracers / spillets**, and tracked as they move in three-dimensional space over time.

- MOHID lagrangian module c**an be run simultaneously with the hydrodynamic model** (currents, water temperature, salinity, etc.), **or in “offline” mode**.
    - In both modes, this model is able to digest currents, water properties, wave parameters and atmosphere properties from different model providers.

HNS model

- Estimates the **distribution of chemical** (as mass and concentrations) on **the water surface, on shorelines, in the water column, in the sediments and at the bottom**.
    - Chemical reactions are not specifically addressed in the model

- Model **tracks separately surface floating chemical, entrained droplets or suspended particles of pure chemical, chemical adsorbed to suspended particulates, and dissolved chemical**.

HNS model

- The **phase changes** are **computed independently for each particle every time step**:
  - The **probabilities of one particle change from one phase to another** (e.g. entrained to dissolved) **is (pseudo-)randomly obtained**, based on the algorithms that quantify the mass balances in the different processes

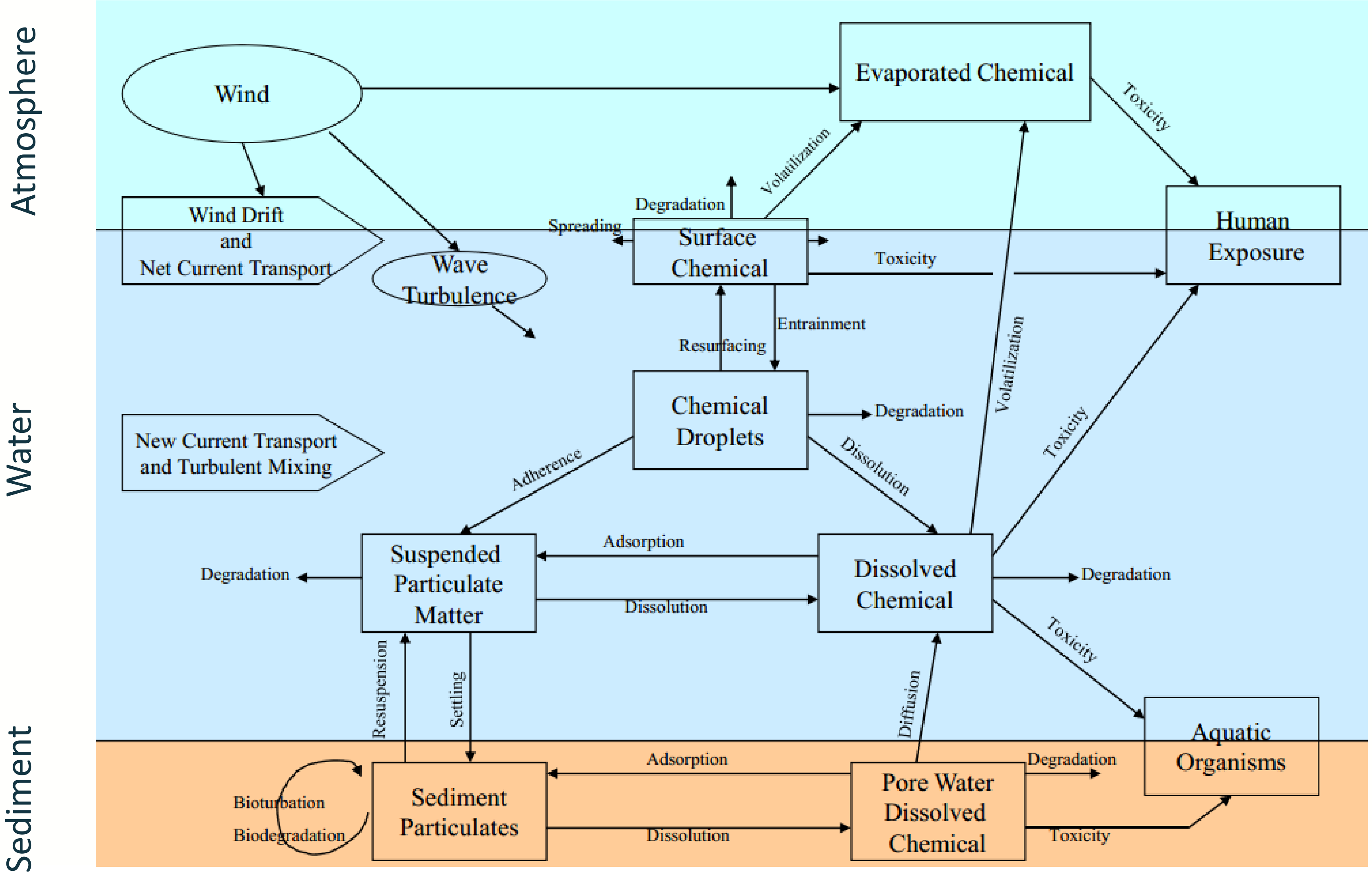
    (correct modelling using this kind of approach require a great number of particles in the simulation, in order to properly reproduce phase changes when slow processes / small mass transfers are involved.)

- The **loss of chemical by reaction to some other form no longer of concern is included in degradation**, which is estimated assuming a constant rate of "decay" specific to the environment where the mass exists (i.e., atmosphere, water columns, or sediment)

HNS model

- Processes simulated include:
  - (three-dimensional) currents advection
  - spreading (on floating liquids)
  - turbulence (vertical and horizontal) dispersion
  - evaporation from water surface
  - volatilization from water column
  - droplets entrainment
  - dissolution
  - partitioning / sedimentation (adsorption to sediments)
  - Sinking
  - resuspension
  - degradation

HNS fate & behaviour



Transport in water

Chemical mass is transported in 3D space and time:

- horizontal movement is controlled by currents, wave-induced velocity (Stokes Drift), wind-drift velocity in the surface layer (for floating substances), spreading, and horizontal turbulence
- vertical movement is estimated in accordance with vertical advection from currents, rising velocity, sinking velocity, and turbulent dispersion.

Currents:

- MOHID can simultaneously simulate currents (in the hydrodynamic module) or use an imposed solution (which is called the “offline” solution) from a previous run, or from a different model (or set of models).

Transport in water

Spreading

- Since MOHID computes the chemical spills using independent lagrangian particles, surface spreading is modelled at three different levels:

a) the initial area of the surface slick (based on Al-Rabeh, et al., 2000), which is randomly populated by MOHID with lagrangian particles;

b) the increasing surface area of individual particle (adapted from Mackay, et al., 1980a);

c) the random movement of individual particles position to reproduce the increasing area of the surface slick (random velocities using diffusion coefficients from Al-Rabeh, et al., 2000).

- If the chemical is released at subsurface, no spreading will happen. Spreading is stopped when all volatiles have evaporated or when a terminal thickness is reached (whichever is sooner)

Transport in water

Wave-induced velocity (Stokes Drift):

- Stokes drift velocity (or mass transport velocity) is the average velocity of a particle due to the orbital motions induced by waves (Stokes, 1847), in the direction of wave propagation. This **velocity is calculated for each particle**, and **velocity components are then added to the horizontal velocities** of the particle.

- For instance, a particle floating at the free surface of water waves, experiences a net Stokes horizontal drift velocity in the direction of wave propagation.

Transport in water

Vertical Entrainment / Droplets size

- For surface floating liquids, the tracers can migrate to the water column due to breaking waves. This entrainment can be estimated by the approach of Delvigne & Sweeney (1988) and Delvigne and Hulsen (1994).

- If the chemical penetrates the water column after a surface spill, this means that chemical substance will be subject to a vertical velocity, depending on the density differences and chemical droplets diameter.

- The **vertical velocity of chemical tracers inside the water column** (entrained droplets due to breaking waves) is a **balance between their intrinsic buoyancy, advection and turbulence**.

Atmospheric transport

If a specific fraction of the chemical is evaporated, it is available for atmospheric transport. The chemical is transported horizontally by the wind velocity and subject to (random) turbulent dispersion velocities in both the horizontal and vertical directions.

Inputs/outputs

- Inputs:
- Model results (Hydrodynamic, Waves, Meteorological); HDF5 format.
- Fixed value for current velocity, wave regime, wind velocity
- Time series for current velocity, wave regime, wind velocity
- HNS property (HNS database)

- Outputs:
- - HDF5 format
- - Particle position (x,y,z), Mass budget, concentration (air, water, sediment), Integrated trajectory of the mass centre

Simulation data files

- **Model. Dat**
- **Lagrangian.dat**

- **Model.dat**
- START : 2024 07 18 07 00 0
- END : 2024 07 18 11 00 0
- DT : 30
- LAGRANGIAN : 1
- WAVES : 1

Simulation data files

- **Lagrangian.dat**

```
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...
<<BeginProperty>>
NAME                    : hns
UNITS                   : m3
CONCENTRATION           : 1
EQUAL_TO_AMBIENT        : 0
AMBIENT_CONC            : 0
<<EndProperty>>
```

Activate/disactivate HNS processes

HNS data
[HNS database]

```
<<BeginHNS>>
NAME                          : Ammonia
DT_HNS_INTPROCESSES           : 60
HNS_SPREADING                 : 1
HNS_EVAPORATION               : 1
HNS_ENTRAINMENT               : 1
HNS_DISSOLUTION               : 1
HNS_VOLATILIZATION            : 1
HNS_SEDIMENTATION             : 0
HNS_DEGRADATION               : 1
HNS_GAS                       : 0
HNS_ATMOSPHERIC_DISPERSION :  1
ORGANIC_COMPOUND              : 1
DENSITY                       : 900
VISCOSITY                     : 0.2186
MOLECULARWEIGHT               : 35.05
VAPORPRESSURE                 : 47400
HNSWINTERFACIALTENSION        : -999
WATERSOLUBILITY               : 305000
OWPARTITIONCOEF               : -0.17
AIR_DEGRADATIONRATE           : 0
WATER_DEGRADATIONRATE         : -999
SEDIMENT_DEGRADATIONRATE  : -999
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<EndOrigin>
```

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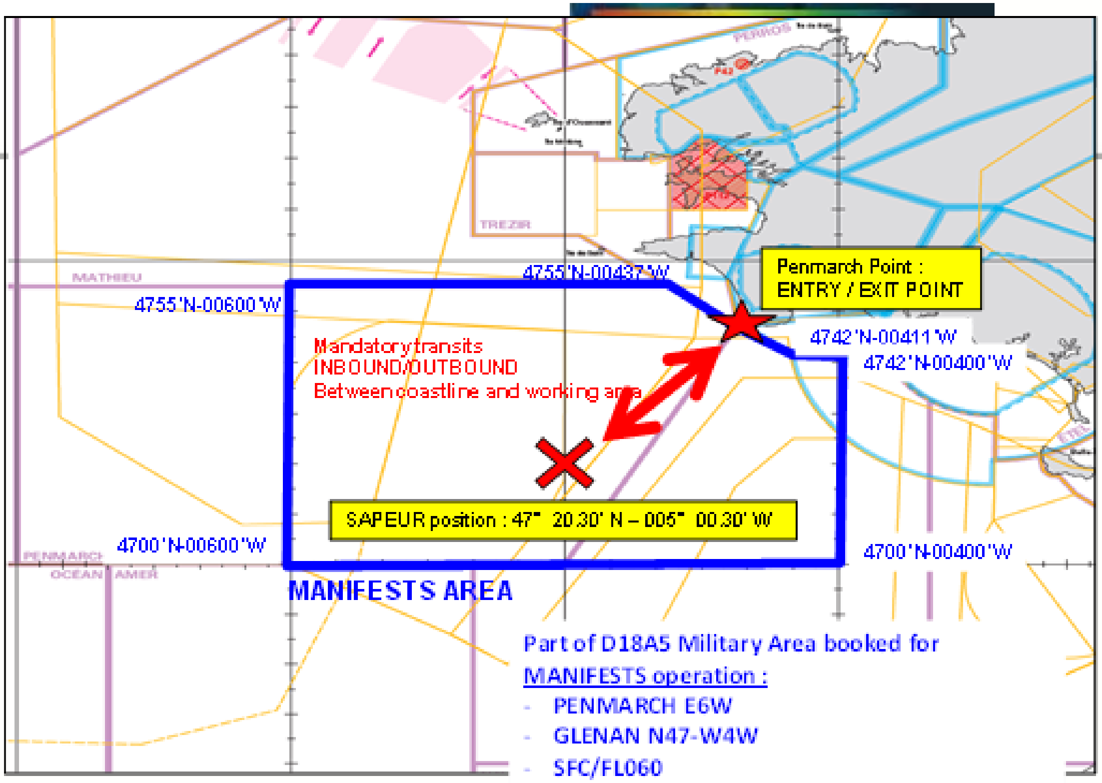
Sea Trial - trajectory



Homemade « buoys»

Commercial buoys (MARGET II)

Co-funded by the European Union Civil Protection

4 models, all similar but all different

museum — OSERIT

Norwegian Meteorological Institute — OpenDrift

TÉCNICO LISBOA — MOHID

Cedre — rps Chemmap

Simulation Forcing:

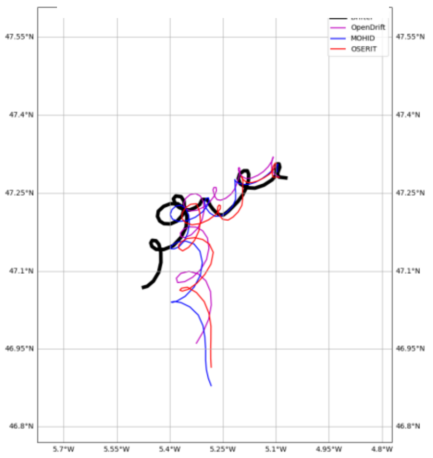
OSERIT: CMEMS NWS + ECMWF

MOHID : CMEMS NWS + ECMWF

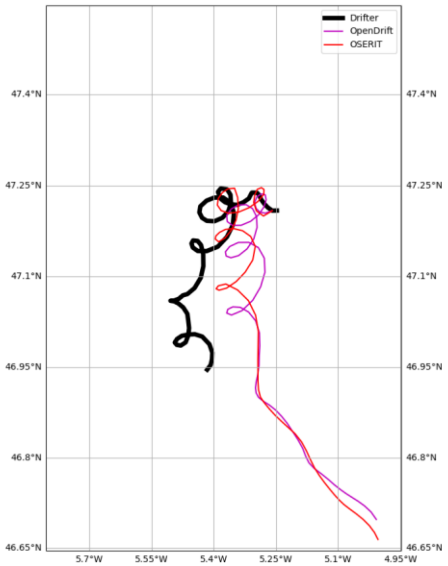
OpenDrift: CMEMS NWS + NCEP

Chemmap: CMEMS NWS + AROME

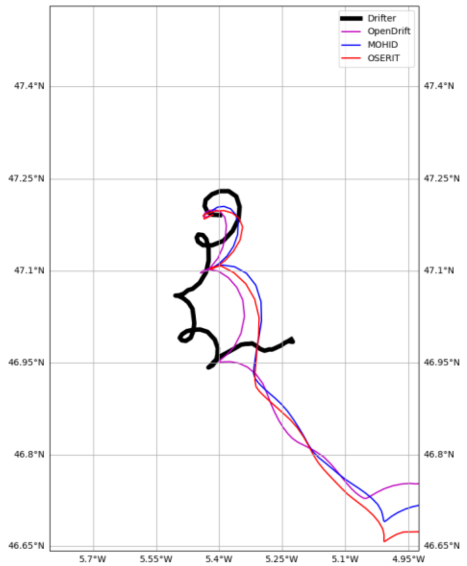
31May -
2 June



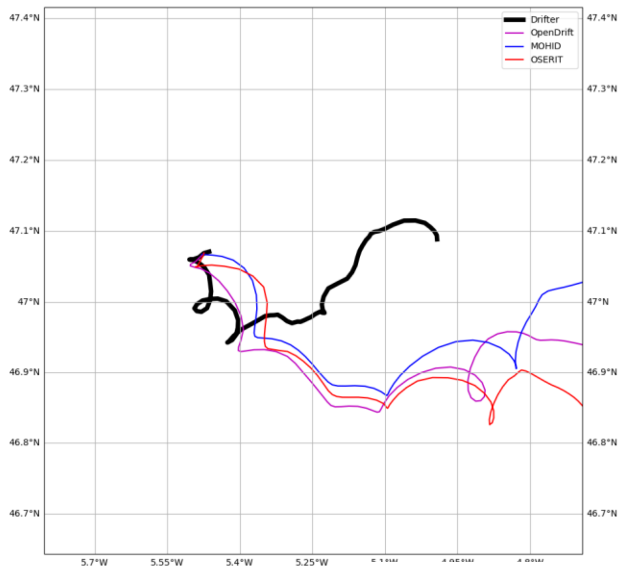
1-3 June



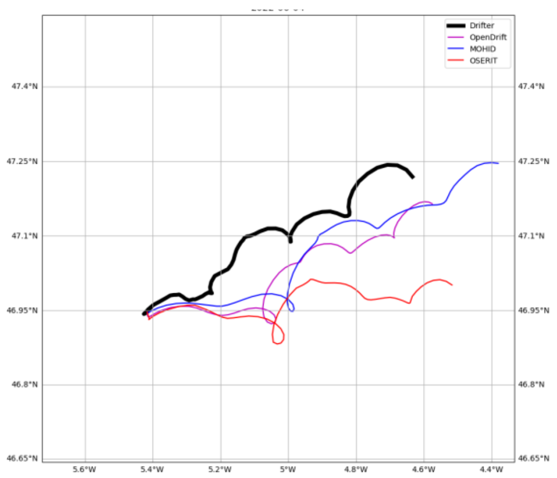
2-4 June



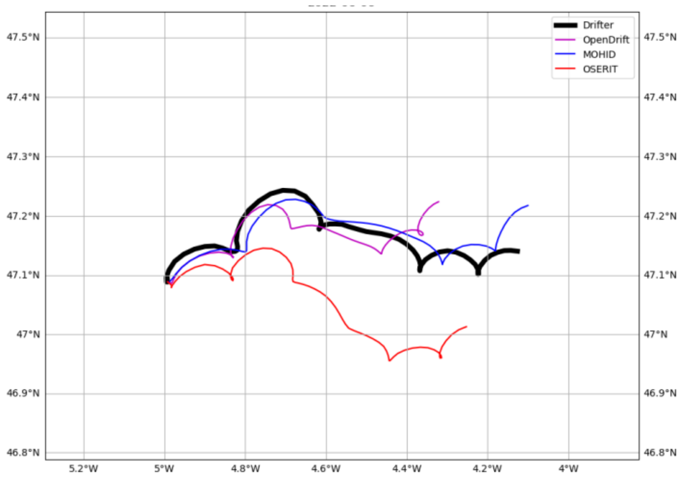
3-5 June



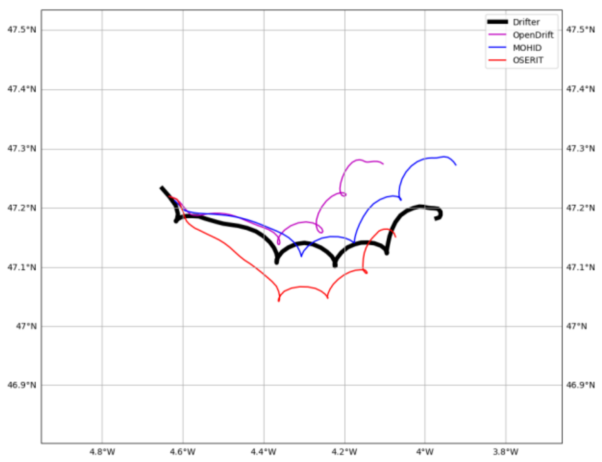
4-6 June



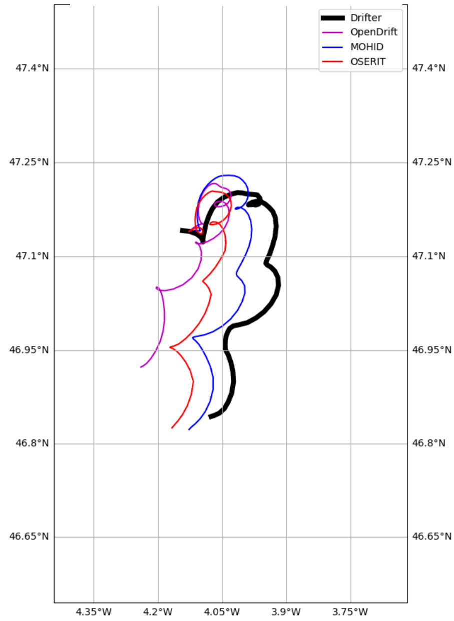
5-8 June

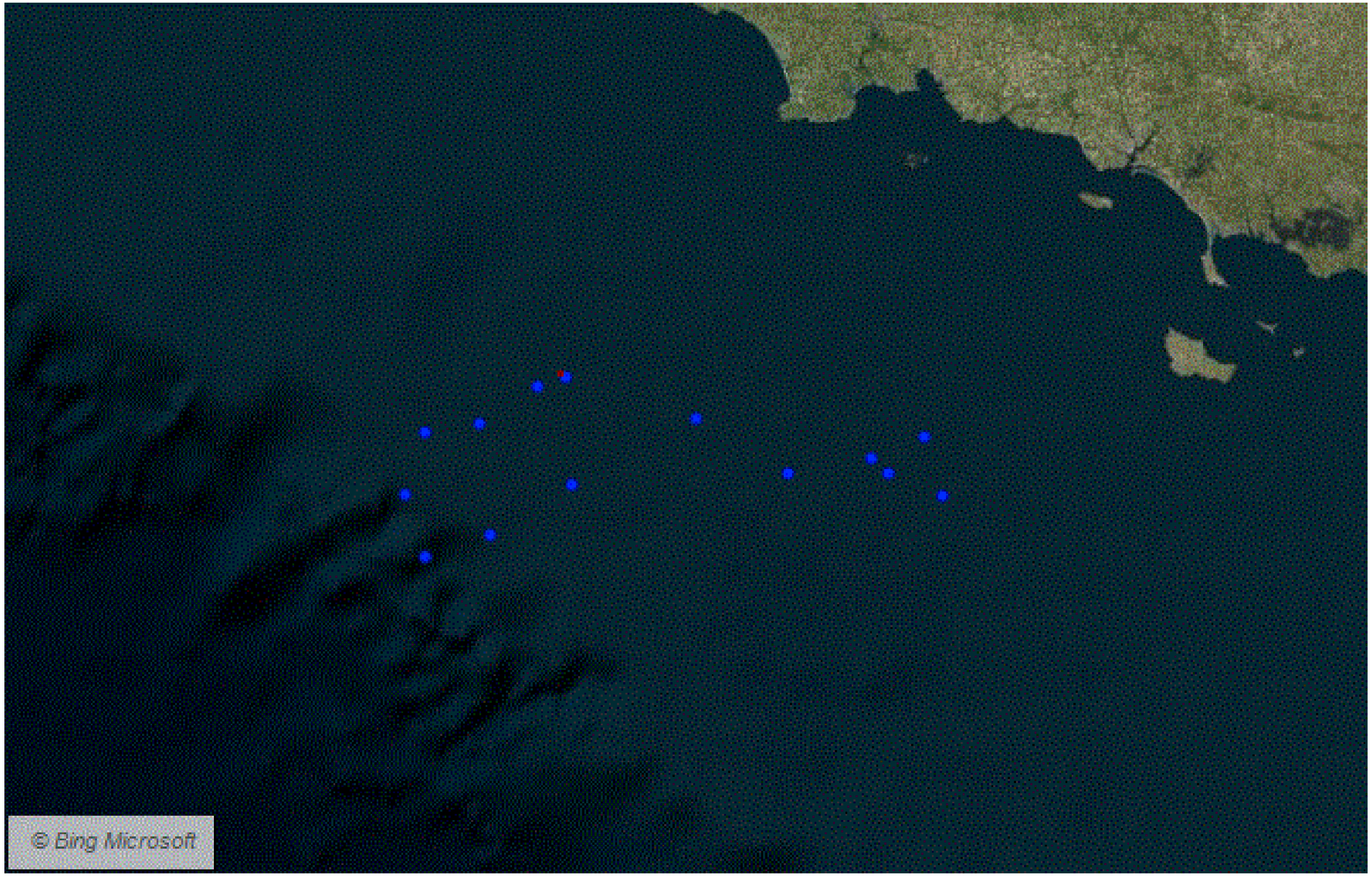


6-8 June



9-11 June



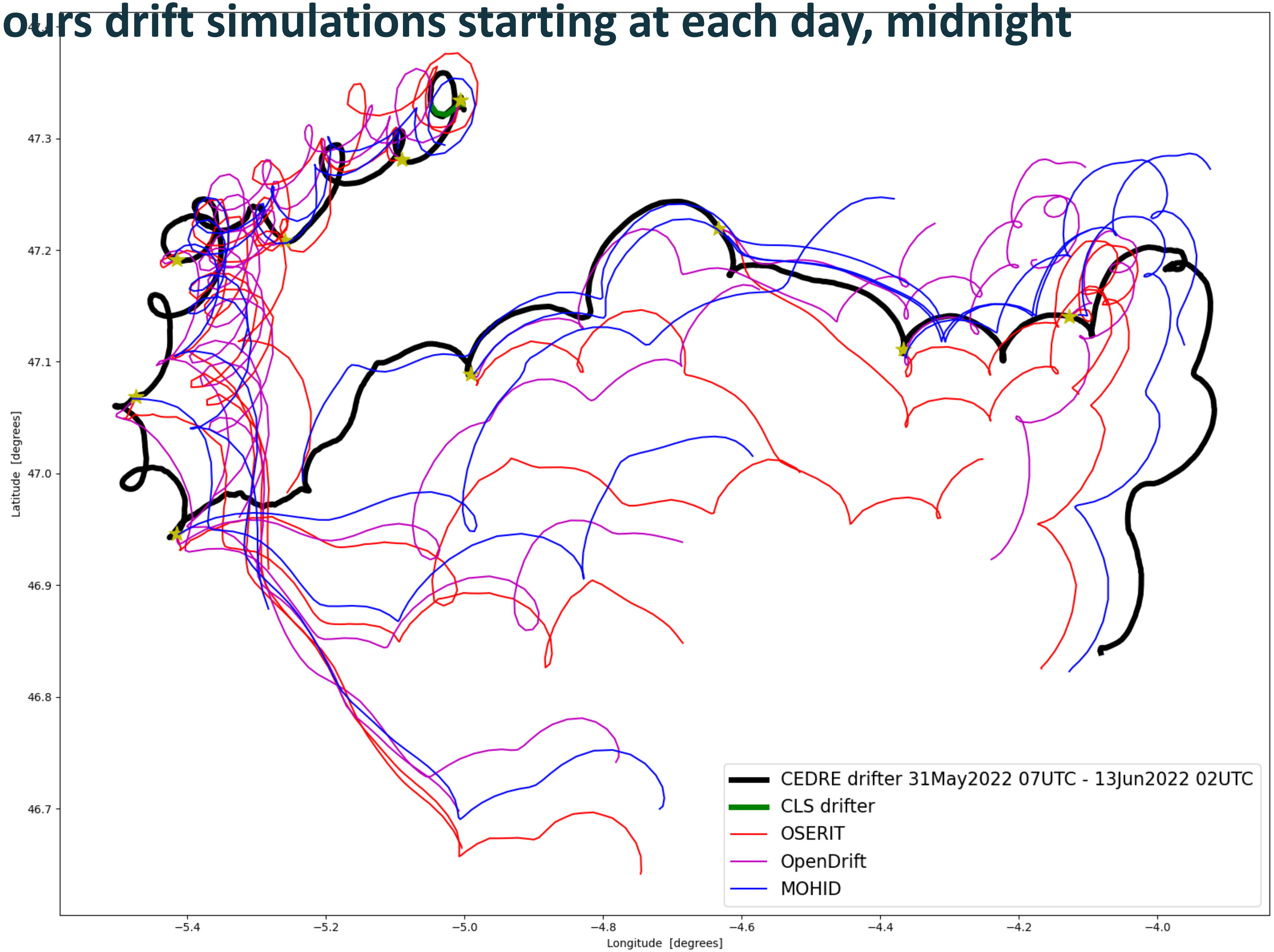


OpenFlows™
FLOOD™

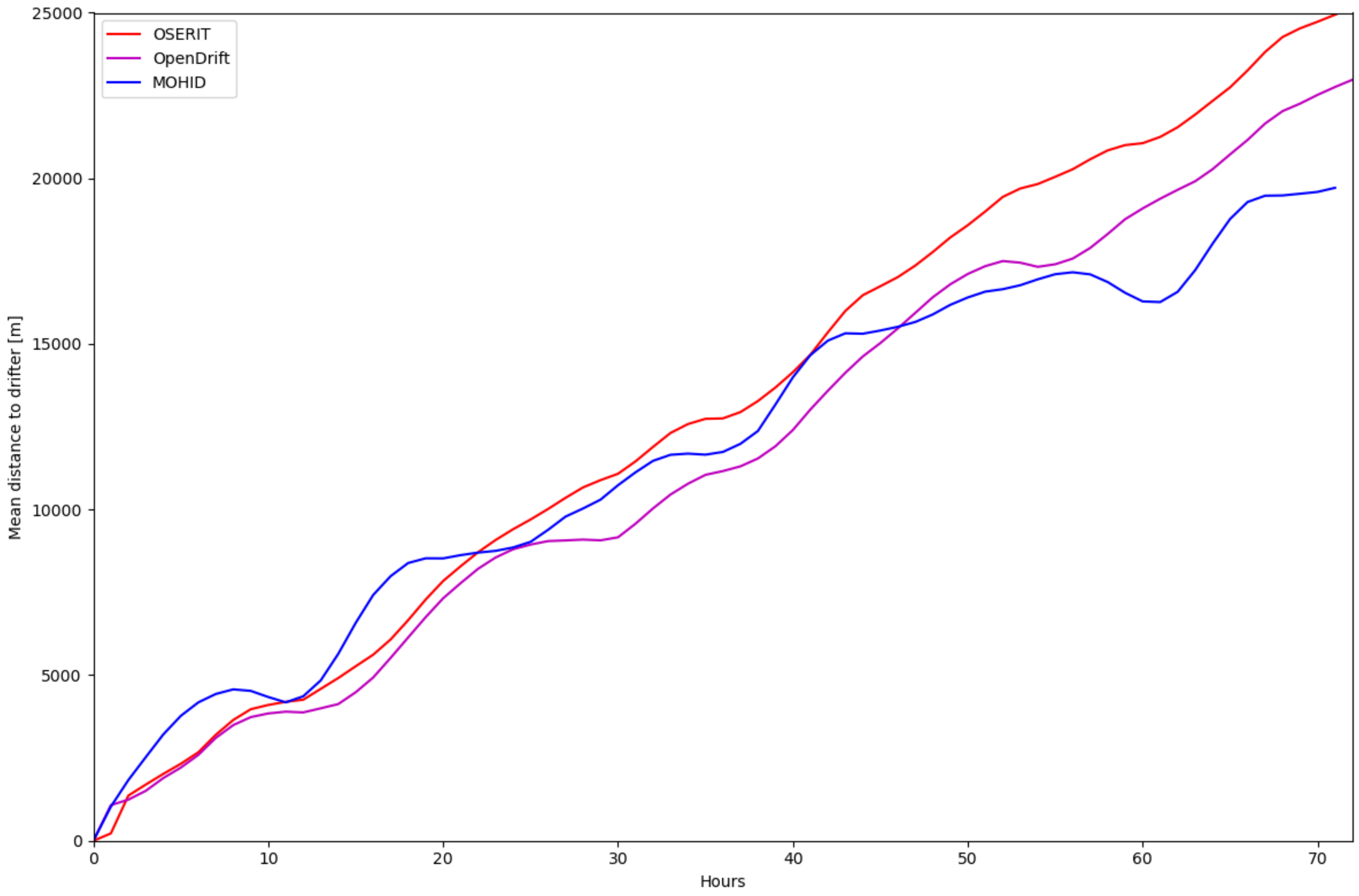
Sea trial - drift buoy

08:36:00
31-05-2022

72 hours drift simulations starting at each day, midnight



OSERIT, MOHID and OpenDrift:
Average error on drift increased by ~350 m/hour



Take home message

- Validation against buoys trajectory has been performed.
  - Models can simulate drift trajectory for 2-3 days.
  - Accuracy of trajectory forecast is mainly limited by accuracy of the met-ocean forcings.
  - A multi-model approach can provide some insights to decision maker.

Sea trial

Co-funded by the European Union Civil Protection

➢ *Previous info*

- Field trial scheduled for May 31 and June 1
- Several spills around this location : 47°20'30" N / 05°00"30 W
- Run the models on the following spills :
- **- soya oil (may 31/ 11:00 local time) - 3 m^3**
  - Butyl acetate (123-86-4) (may 31 / 12:00 local time) - 1 m^3
  - Aceton (37-34-1) (may 31 / 16:00 local time) - 1 m^3
  - Toluen (108-88-3) (june 1 / 16:00 local time) - 1 m^3
- Continuous spills of few minutes (from 5 to 10 minutes) sea surface
- Cedre will use the following metocean datasets : IBI copernicus / ARPEGE europe Météo-France

Sea trial

➢ *On the field trial day*

- E-mail with the spill location and meteocean information

- Please find the location of the spill (N-butyl acetate, 1 m3)
- Start of spill : 12h36 local time / 10h36 UTC ; 47°20.298N ; 005°00.147W
- End of spill : 12h43 local time / 10h43 UTC ; 47°20.262N ; 005°00.061W
- Waves : 0
  Winds : 2kt ; 260°
- Currents estimate : (no measurements) : 0.5kt NW (surface speed : 0.5kt ; bottom speed : 1.1kt)

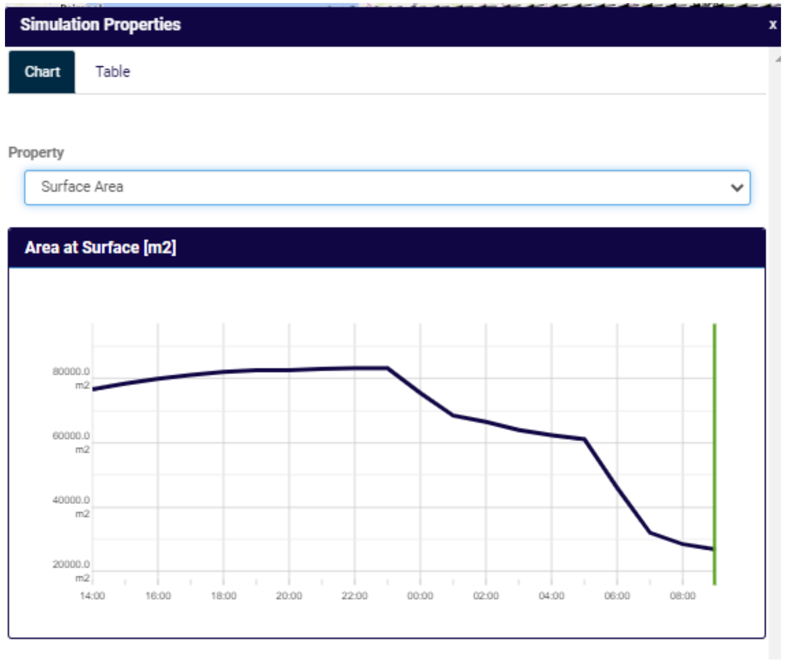
Sea trial – MOHID spill simulations

- Simulations performed on the day of the field trial with the previous information
- Metocean datasets used in the simulations: IBI copernicus \ GFS 0.25º

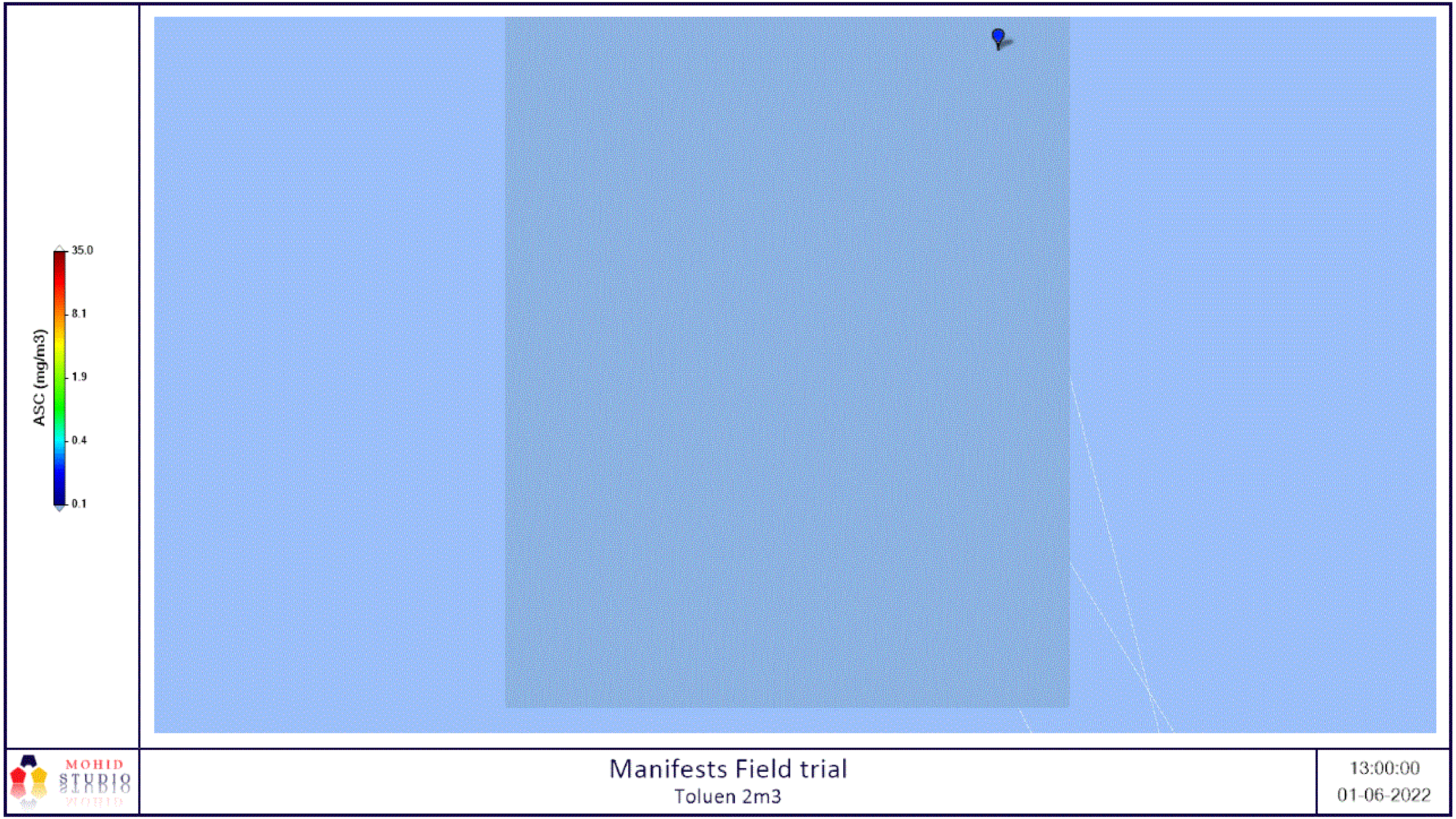
- Mohid Simulation Resume
- Name : Toluen_20220601_day
- Substance : HNS Spill
- Localization : -5.008 47.342
- Emission Type : continuous (10 minutes spill; 2m3)
- Start Date : 2022-06-01 14:00 UTC
- End Date : 2022-06-02 09:00 UTC
- Expected Run Duration : 9.5 minutes
-
- Currents at Emission point - IBI Model currents: 0.19 m/s (0.36Kt)
- Wind at Emission point - GFS 0.25º: 4.51 m/s (0.77kt) NW

Sea trial – MOHID spill simulations

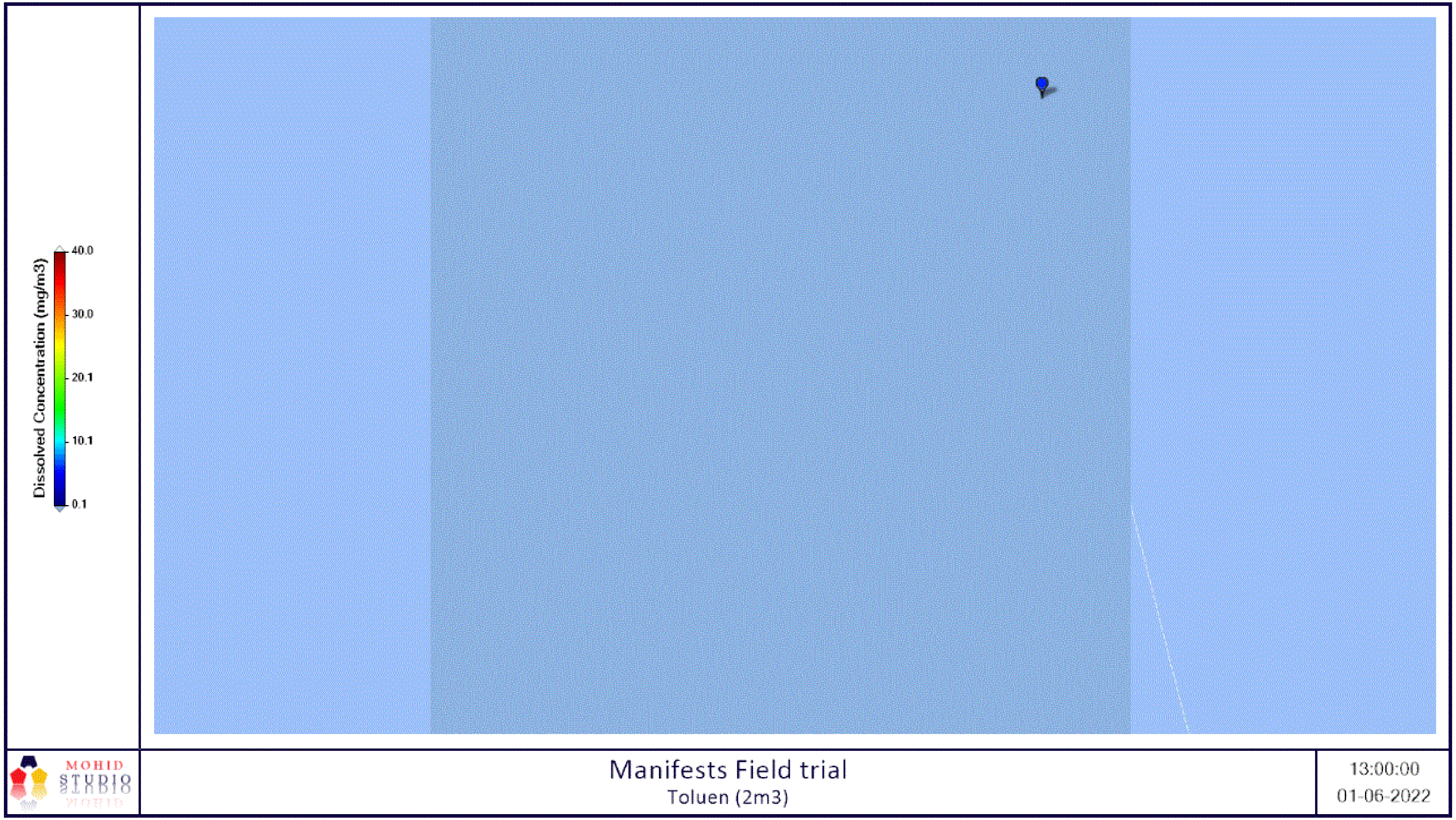
- HNS Spill - Toluen $2m^3$



Field trial – Toluen 2m3 – Air surface concentration

- 

Field trial – Toluen 2m3 – Dissolved concentration



Simulation scenario

- On April 23, in Tofiño (Vigo Estuary), a vessel containing 4,000 tons of anhydrous ammonia (Class 2.3) begins to leak product. 1 hour losing product.
- Wind NW (315º) Force 6, 22 knots (11.3 m/s)
- Vigo: 42º13.71 N, 08º46.72 W (42.2285, 8.7787)
- In Vigo, the vessel loses 60 m3 of anhydrous ammonia.

NAME	: Ammonia Anhydrous
DT_HNS_INTPROCESSES	: 60
DENSITY	: 681.8
VISCOSITY	: 0.173859
MOLECULARWEIGHT	: 17.031
VAPORPRESSURE	: 881527
HNSWINTERFACIALTENSION	: -999
WATERSOLUBILITY	: 531000
OWPARTITIONCOEF	: 0.23
AIR_DEGRADATIONRATE	: -999
WATER_DEGRADATIONRATE	: -999
SEDIMENT_DEGRADATIONRATE	: -999


Air Surface Concentration (mg/m3)
338
253
169
84
0
Moaña
Redondela
Cangas
Ria de Vigo
Vigo
Mondariz
La Car
Reguengo
Áreas
Puenteareas
Porriño
Nigrán
Bayona
Gondomar
Salceda de Caselas
Arbo
Salvatierra de Miño
Pader
Túy
Pias
Tangil
Oia
Tomiño
Cerdal
Abedim
Pene 1374
Fontoura
Vila Nova da Cerveira
Rosal
© Bing Microsoft
OpenFlows™ FLOOD™
Vigo
Ammonia Anhydrous
09:00:00
23-04-2024


Dissolved Concentration (mg/m3)
31.7
23.8
15.9
7.9
0.0
DONON
Hio
Darbo
Cangas
Tirán
Ria de Vigo
BARREIRAS
A CALZADA
Vigo
Lavadores
Alcabre
Goya
VILOURA
Navia
Comesaña
Matamá
Castrelos
Beade
Oya
Corujo
Valladares
© Bing Microsoft
OpenFlows™ FLOOD™
Ria de Vigo
Anhydrous ammonia
09:00:00
23-04-2024

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