D4.3 - Models intercomparison

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1. Introduction

1.1. Context

Maritime transport represents more than 80% of the international trade volume (UNCTAD, 2017). Apart from crude oil, tanker trades of refined petroleum products, chemicals and gas have increased by 4% over the 2019-2021 period, with a 5.6% growth in Liquefied Natural Gas (LNG) trade (UNCTAD, 2022). The volume of hazardous and noxious substances (HNS) is thus constantly rising with an increased risk of accidental spillages potentially associated with marine pollutions, whether in ports or in the open sea. In the event of an incident and a spill in the environment, information on the fate of the chemical(s) involved is essential to better anticipate the risks incurred by responders and populations, the impacts on the environment as well as the appropriate response techniques (Mamaca et al., 2009).

Chemicals accidentally spilled into the marine or aquatic environment generally undergo physical-chemical modifications that will characterize their behaviour and fate. As observed by Mamaca et al. (2004) and Le Floch et al. (2011), these modifications are dependent on the intrinsic parameters of the product involved, the *in situ* environmental parameters (temperature, density and salinity of the water) and the met-ocean conditions (e.g. sea state, wind speed, marine currents). A few hours following the spill short-term effects may thus occur such as spreading, natural dispersion in the water column (dissolution, emulsification) and evaporation into the atmosphere. Longer term degradation (e.g. polymerisation, biodegradation) and sedimentation processes can then follow, depending on the persistence and the nature of the substance.

One of the main concerns is that around 2,000 different types of HNS are regularly shipped in bulk or package forms (Purnell, 2009) which thus make difficult to capture their behaviour if accidentally released in the environment.

Of the wide variety of HNS traded, volatile and gaseous substances are particularly problematic for marine pollution response authorities. The release of such substances at sea can indeed lead to the formation of toxic, flammable, or explosive gas plumes – sometimes invisible to the naked eye – that can travel large distances and pose risks over a wide area in relatively short timescales. Yet, key information on the risks that responders or rescue teams could take when intervening, or those that could impact coastal communities and the environment when allowing a shipping casualty to dock at a place of refuge remain poorly known. The MANIFESTS EU-project is part of this context.

1.2. Objectives of the study

Models have been used for several decades as a decision support tool to assess marine pollution risks and plan response actions. By simulating pollutant behaviour, models provide insights on how pollutants may spread and affect organisms and ecosystems, and help identify effective response measures such as booms, skimmers, and dispersants. Models optimize resource deployment during response efforts, avoiding wastage and improving effectiveness. They provide a quantitative basis for decision-making, reducing bias and subjectivity in planning and response. Models also help organizations prepare for future incidents by informing response plans and policies and by providing guidance for prevention and response.

However, a small number of models can simulate the behaviour of gaseous and volatile pollutant released at sea. Among these are 4 models developed and/or operated by MANIFESTS partners. These models are:

- OSERIT, developed and operated by RBINS, Belgium
- MOHID, developed and operated by IST, Portugal
- OpenDrift, developed and operated by MET Norway
- CHEMMAP, a commercial model developed by RPS and operated by Cedre.

These 4 models belong to the general model category based on Lagrangian particles, but they differ by the numerous implementation choices. The purpose of MANIFESTS Task 4.3 was to perform an in-depth model inter-comparison exercise that would help on the one hand investigating the strengths and weaknesses of Lagrangian particles models in general and on the other hand understanding and documenting the impacts of the implementation choices in the different models. Doing so, we were hoping to provide new keys to help maritime authorities correctly interpreting model results for simulation involving gaseous or volatile HNS. This inter-comparison exercise is not aimed at identifying the best model (out of the four intercompared models).

To achieve these goals, the task participants progressed in 3 steps.

The first step was a paperwork exercise. The developers of OSERIT, MOHID and OpenDrift transparently presented their model, the implemented parameterisations and algorithms and explained several implementation choices. These discussions took place during four internal workshops. RPS engineers attended two of these workshops and provided general but still useful comments on the CHEMMAP model. These in-depth exchanges were extremely interesting and provided the background information necessary to correctly analysis the results of the benchmark simulations performed at steps 2 and 3. The outcome of the workshops are summarized in section 3.

During the second step of this exercise, the ability of the different models to simulate the competition between the evaporation, dissolution, and volatilization of a floater-evaporator-dissolver substance (butyl acrylate) was benchmarked for 8 contrasted met-ocean conditions.

Finally, during the third step, the ability of the models to simulate drift, fate, and behaviour of 10 different volatile substances in 2 contrasted met-ocean conditions have been benchmarked. The 28 simulations that have been studied during step 2 and step 3 are presented in section 4 and in the annexes (section 7).

2. General presentation of the models

2.1. OSERIT

OSERIT is a multipurpose Lagrangian particles model able to simulate the trajectory of floating objects adrift at sea as well as the drift, fate, and behaviour of acute marine pollution events by oil and other harmful and noxious substances (HNS) (Dulière et al., 2012; Legrand et al., 2017). The model employs external forcing from various sources to simulate drift and atmospheric dispersion and considers several parameters, such as wind, wave, current, and temperature. Lagrangian particles move in a 3D space and are influenced by the value of the parameters at their location. For instance, airborne particles are affected solely by wind, while those at the surface are impacted by wind, current, and waves. In contrast, particles in the water column are only affected by current and waves. Additionally, there are many more factors at play, including turbulent kinetic diffusion and buoyancy (only for particles in the water).

To compute the fate, the pollutant volume is equally divided between the different Lagrangian particles; the pollutant volume being itself subdivided at the level of a particle as a function of the chemical compound (or pseudo-compound). Each of the chemical compounds in the particle can be in several states: liquid (slick or droplets), emulsified, evaporated, dissolved, and degraded. The model is also able to simulate mixture, when they are non-azeotropic and there is no chemical reaction: each component of the mixture is treated as separated compounds. To track accurately the change of state of chemicals, the weathering module of OSERIT have been improved in the framework of the MANIFESTS project (Lepers and Legrand, 2022). It includes among other, evaporation, dissolution, and volatilization. Finally, because the state of chemical compounds influences the drift behaviour of a Lagrangian particle, the pollutant mass is periodically redistributed between neighbouring particles to minimize the number of different states active in each particle. This also assures the conservation of mass of the pollutant during the entire simulation.

2.2. MOHID

MOHID chemical spill model (Fernandes, 2014; Soares et al., 2020) is integrated in the Lagrangian component of MOHID model (a public-domain / open-source water modelling system – www.mohid.com). MOHID is a three-dimensional water modelling system, developed by MARETEC (Marine and Environmental Technology Research Center) at Instituto Superior Técnico (IST) which belongs to University of Lisbon. This modelling system allows the adoption of an integrated modelling philosophy, not only of processes (physical and biogeochemical), but also of different scales (allowing the use of nested models) and systems (estuaries, watersheds, open-sea, rivers), due to the adoption of an object-oriented programming philosophy. MOHID has been applied to different study cases, such as coastal and estuarine areas, as well as oceanic processes and reservoirs, and it has showed its ability to simulate complex features of the flows.

MOHID Lagrangian transport module uses the concept of tracer, assuming that the spilled contaminant can be represented as an amount of several different small tracers / spillets, and tracked as they move in three-dimensional space over time. This software is used in several different studies, as oil and HNS spills, floating containers, dispersion of plumes in submarine outfalls, sediments transport, etc. MOHID Lagrangian module can be run simultaneously with the hydrodynamic model (currents, water temperature, salinity, etc.), or in “offline” mode. In both modes, this model can digest currents, water properties, wave parameters and atmosphere properties from different model providers. Additionally, MOHID Lagrangian module allows backtracking / modelling, as well as a multi-solution approach (Fernandes et al., 2013) generating computational grid on-the-fly and using the available information from the multiple met-ocean forecasting solutions available).

The spilled mass is tracked through phase changes and transport, with all reaction products assumed to move together – chemical reactions are not specifically addressed in the model. 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). The 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. The model tracks separately surface floating chemical, entrained droplets or suspended particles of pure chemical, chemical adsorbed to suspended particulates, and dissolved chemical. The phase changes are computed independently for each particle every time step, and 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. Therefore, a correct modelling using this kind of approach obviously requires a great number of particles in the simulation, to properly reproduce phase changes when slow processes / small mass transfers are involved.

Chemical mass is transported in three-dimensional space and time. The 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. The vertical movement is estimated by vertical advection from currents, rising velocity, sinking velocity, and turbulent dispersion. More details about the model can be found in (Fernandes, 2014) and (Soares et al., 2020).

2.3. OpenDrift

OpenDrift is a generic framework for trajectory simulations (Dagestad et al., 2018), with dedicated modules for specific applications such as oil spills, search and rescue etc. A new, very basic module for HNS has been developed within the MANIFESTS project, starting from the existing and well validated oil drift module OpenOil (Röhrs et al., 2018), and adding weathering processes for chemicals as described in Legrand et al. (2017). As such, the OpenDrift HNS module is expected to provide fairly similar results to the OSERIT model, however as learned within this project, the actual implementation of given algorithms and processes does have a significant impact, e.g., the order at which weathering, and entrainment processes are executed.

Particles can be in one of several states: liquid (slick or droplets), emulsified, evaporated, and dissolved, with transfer based on parameterizations as described for the OSERIT model above.

Particles in air are advected with the wind velocity, with an optional horizontal diffusivity as may be specified by the user.

Particles at the ocean surface (slick) are advected with surface current, Stokes drift, as well as 2% of the surface wind, as found empirically in many experiments (e.g., Brekke et al. (2021)). If surface Stokes drift is not available from a wave model, the wind drift factor can be increased from 2% to about 3.5%, providing very similar results in most cases. In addition to this horizontal advection, a constant horizontal diffusivity can be specified, providing spreading through random walk processes.

The wind drift factor is only applied to particles at the surface, and the Stokes drift is decreasing with depth as described in Breivik et al. (2016).

Surface particles/chemicals are entrained at the rate/probability at which breaking waves occur at the surface, proportional to wind speed over wave period, but with no entrainment for winds below 5 m/s. After entrainment, droplets are mixed vertically with a diffusivity obtained from ocean model or parameterized from wind if not available. This is performed in an inner loop also taking buoyancy into account, with schemas described in Nordam et al. (2019).

2.4. CHEMMAP

CHEMMAP is a HNS drift, behaviour and fate model solution developed and marketed by RPS: https://www.rpsgroup.com/services/oceans-and-coastal/modelling/products/chemmap/. Widely considered as the reference model on the market, CHEMMAP is a chemical discharge modelling and response system that predicts the transport, fate, and biological impacts of a wide variety of chemical substances in the marine environment and atmosphere. The model is applied worldwide for emergency response, risk assessment, contingency planning- including worst-case scenario, natural resource damage assessment, drills, and education as well as cost-benefit analysis.

CHEMMAP computes 3D chemical transport and fate in water and air and integrates algorithms for dissolution, evaporation, volatilization, sediment interaction, adsorption and shore-line interactions. Operated by Cedre, CHEMMAP is the only commercial solution used in this validation exercise.

3. Intercomparison model implementation

The first step of the model intercomparison was a paperwork exercise. During 4 workshops, the developers of OSERIT, MOHID and OpenDrift transparently presented their model, the implemented parameterisations and algorithms and explained several implementation choices and during two workshops, 2 experts from the RPS company gave us some general information on CHEMMAP.

The four models are very similar:

- They all are based on a Lagrangian particle approaches.
- They all compute 3D drift processes in the water column and have atmospheric dispersion capabilities, based on a Runge-Kutta algorithm.
- They all associate to each Lagrangian particle a fraction of the pollutant mass and follow its fate between different processes (evaporation, dissolution, degradation, volatilization, adsorption, sedimentation, etc).

But they have also significant differences in the model implementation. For instance,

- some models compute pollutant fate at the level of the Lagrangian particles, while others compute the same processes at the total level of the pollutants.
- some models accept HNS mixtures while others not.
- models usually implement different parameterisations for the different fate processes. These differences are often at the level of the calibration parameters, where some models use hardcoded values while others use formula depending on environmental parameters. For instance, the kinematic coefficient in the dissolution process is systematically one or two order of magnitude larger in MOHID than in OSERIT.
- time-stepping strategy is different. MOHID uses the same time step for drift and fate processes. OSERIT use different time-steps for drift and for fate processes (typically 10 sub-time steps for fate processes for 1 timestep for drift). OpenDrift uses sub-time steps for vertical displacements what the other model do not.
- All models estimate in diverse ways the slick surface area, the slick thickness, and the slick spreading. These differences have direct impacts on the computation of the evaporation and the dissolution rate of the surface slick.
- MOHID activates fate processes as a function of the SEBC classification. For instance, evaporation and dissolution will never be computed for a persistent floater; surface slick of a

dissolver-evaporator will instantaneously be dissolved in the water avoiding evaporation but increasing volatilisation; etc.

- MOHID is also the only model to subdivide the dissolved fraction into a fraction that remains close to the sea surface and that is still under the influence of wind and a second fraction that can go deeper in the water column.
- The models also resolve the fate processes in different orders.

All these implementation choices induced differences in the simulated drift, fate, and behaviour from one model to another.

In the hereunder text, we present the results of the systematic intercomparison of OSERIT, MOHID and OpenDrift implementations.

3.1. Horizontal drift

3.1.1. Surface drift

OSERIT use the Runge-Kutta 2 scheme with the current, the winds at 10 meters with a leeway coefficient ranging from 0.01 to 0.0315 and the surface stokes drift (for waves). A random walk perturbation is added on top, with a horizontal turbulent diffusivity coefficient (default of $1.5 m^2/s$).

The horizontal movement in MOHID is similar to OSERIT, it is controlled by current, Stokes drift and wind for the floating substance in the surface layer. There is also spreading and horizontal turbulence.

OpenDrift is similar to the two other models, with an Euler, Runge-Kutta 2 or Runge-Kutta 4 advection scheme relying on the current, stokes drift and wind drift. The random walk perturbation uses a parameter defined by the user, typically $100 m^2/s$.

3.1.2. Subsurface drift

For OSERIT, the subsurface drift is very similar to the surface one but without the wind, and with a exponential decay of the stokes drift with the depth. The random walk is the same as the one at the surface.

For OpenDrift, it is the same as for the surface drift but with the wind impact decreasing linearly to 0 at 10cm of depth, the same random walk and the stokes drift decreases following Breivik et al. (2016).

3.1.3. Atmospheric transport

The atmospheric transport in OSERIT is a simple advection with Runge-Kutta 2 with the wind at 10 meters.

For MOHID, the chemical is transported horizontally by the wind.

OpenDrift uses a Euler advection with the wind at 10 meters.

3.1.4. Atmospheric dispersion

In OSERIT, there is a Gaussian spreading of the chemical around each particle, with the spreading depending on the distance travelled and the atmospheric conditions (Turner, 1970).

For MOHID, the particles are subject to turbulent dispersion velocities in the horizontal and vertical direction.

In OpenDrift, there is a random walk perturbation with a user given diffusivity.

3.2. Vertical displacement in the water column

In OSERIT, vertical displacement is computed at the sum of the vertical advection, the buoyancy, and a random walk displacement scale from the vertical turbulent diffusivity term. The buoyancy is accounted for with Clift et al. (1978) (3 regimes).

In MOHID, the vertical movement is estimated in accordance with vertical advection from currents, rising velocity, sinking velocity and turbulent dispersion. The rising velocity can by estimated by two alternatives approaches; a double regime one (spherical-cap bubble and small spherical droplets) from Liungman and Mattsson (2011) or a three regimes formulation, as proposed by Zheng and Yapa (2000).

OpenDrift uses a random walk displacement loop with sub-time stepping of typically 60 seconds. This includes diffusivity (from ocean model or parametrized by wind), vertical advection and terminal velocity (buoyancy, gravity, drag, with two regimes from Tkalich (2002)).

3.3. Other processes

3.3.1. Stranding

In OSERIT, a particle is stopped when they hit the coastline in OSERIT. It is possible to deactivate this behaviour, in this case the particle position will not be update if it should cross the coastline.

When a particle reaches a grid cell close enough to the coastline in MOHID, it may become randomly beached. Once this is done, the particle may also be removed randomly on a rising tide or by offshore winds.

OpenDrift is similar to OSERIT, the particles are deactivated when they get to the shoreline. If this behaviour is deactivated, they will stay at the shore until there is an offshore drift.

3.3.2. Sedimentation

The implementation in OSERIT will stop when they hit the seabed. There is no resuspension implemented yet.

In MOHID, the chemically contaminated particles deposed at the seabed can be resuspended if the current velocity at the bottom is above a specified threshold (default = 0.2m/s).

In OpenDrift, particles are lifted or deactivated when they hit the seafloor. If the current velocity is above a given threshold (e.g., above 0.5 m/s), the particles will be resuspended.

3.3.3. Entrainment in the water column

The probability of entrainment in the water column in OSERIT is from Tkalich and Chan (2002).The intrusion depth of the particle is computed from a random value scaled by the significant waves height, such as in Guo and Wang (2009). This behaviour is applied both for breaking and non-breaking waves. Droplets size is computed from a log-uniform distribution.

In MOHID, the particles can migrate in the water column due to breaking waves. It can be estimated by the approach of Delvigne and Sweeney (1988) and the one of Delvigne and Hulsen (1994). Entrained droplet diameters can be optionally estimated based on three approaches:

- User defined definition
- Half of the mass median droplet diameter (Spaulding et al., 1992)
- Pseudo-randomly chosen diameter based on a diameter class distribution computed using Delvigne and Sweeney (1988) formulation

OpenDrift compute the entrainment in the water column according to Li et al. (2017), which is also used for droplet size, where Johansen (2015) is an optional alternative.

3.3.4. Resurfacing

Droplets in OSERIT can resurface if they hit the surface; dissolved or chemically dispersed (oil) particle cannot.

In MOHID, only droplets can resurface too.

For OpenDrift, the particles can only resurface by buoyancy such as described in Nordam (2019).

3.3.5. Oil sediment interaction

Only MOHID have a process implemented here. Contaminant in the water column is carried to the sea floor primarily by adsorption to suspended particles and subsequent settling.

3.3.6. Slick area

In OSERIT, surface slick spreading is computing from a random walk algorithm scaled on the pollutant viscosity (Garcia-Martinez and Flores-Tovar, 1999). The slick area is computed from a quadtree classification of the surface particles.

In MOHID, the implemented algorithm for this purpose determines random velocities assuming a uniform distribution inside a range (in directions x and y), proportional to spreading diffusion coefficients. The spreading diffusion coefficients Dx and Dy are in fact the rate of change of the surface area of an individual particle (m^2/s), previously presented and obtained from Kolluru's formulas solution (Kolluru et al., 1994).

3.3.7. Slick thickness

In OSERIT, the slick thickness is computed from the cell of the quadtree used to compute the surface area and the volume of HNS inside of it.

In MOHID, the thickness limit is defined according to MCAuliffe (1987).

In OpenDrift, the thickness may be calculated/updated during the simulation by averaging within boxes of defined size. However, the default entrainment algorithm (Li et al., 2017) does not need oil thickness to work properly.

3.3.8. Slick spreading

For OSERIT, the slick spreading is represented as the random walk displacement of surface particles scaled on the pollutant viscosity (as in Garcia et al. (1999)).

Surface spreading is modelled at three different levels in MOHID:

- the initial area of the surface slick (based on Al-Rabeh, et al. (2000)), which is randomly populated by MOHID with Lagrangian particles
- the increasing surface area of individual particle (adapted from Mackay, et al., (2006))
- 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))

OpenDrift assumes the spreading is negligible compared to horizontal drift/diffusion and no other process is implemented.

3.4. Fate processes

3.4.1. General remark

Fate processes are computed by quadtree cell using a sub-time stepping scheme in OSERIT.

MOHID includes the vertical entrainment from breaking waves, evaporation from surface, and volatilization from water column, dissolution, partitioning / sedimentation (adsorption to sediments), resuspension and degradation.

3.4.2. Evaporation

In OSERIT, the evaporation can be modelized using the Jones (1997) or the Brighton (1985) parametrization. It affects only surface particles.

The evaporation in MOHID is based on Mackay and Matsugu (1973), where the rate of mass flux to the atmosphere increases with vapor pressure temperature wind speed and surface area.

For OpenDrift, the evaporation is based on NOAA ADIOS/PyGNOME[1].

3.4.3. Dissolution

The dissolution in OSERIT is computed as in Hines and Maddox (1985). This algorithm computes the dissolution rate as a function of the Reynolds number.

Dissolution is estimated for spillets in the surface and in droplets dispersed in the water column. The approach is based on a mass flux assuming a well-mixed layer with most of the resistance to mass transfer lying in a hypothetical stagnant region close to chemical. The dissolution in the slick is based on the hypothesis of a flat plate (the slick), and the droplets in water column are assumed to be

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[1] https://gnome.orr.noaa.gov/doc/pygnome/index.html

spherical, with the dissolution treated as a mass flux across the surface area of a sphere, according to Mackay & Leinonen (1977).

3.4.4. Volatilization

OSERIT computes the volatilization as in (Lyman et al., 1990).

In MOHID, volatilization from the water column is calculated from the chemical's vapor pressure and solubility. The procedure in the model is as outlined by Lyman et al., (1982), based on Henry's Law and mass flux being controlled by diffusion in both the water and the air near the interface .

3.4.5. Emulsification

In OSERIT, emulsification is computed following Scory (2005) and is primarily designed for oils.

For OpenDrift, it is using NOAA ADIOS/PyGNOME.

3.4.6. Degradation

The degradation in OSERIT is computed with the half-life of the HNS, for each half-life of time simulated half of the HNS will be degraded (if there are no other weathering processes).

For MOHID, the degradation of a chemical is abstracted as occurring at different environments (atmosphere, water column and sediment) by different processes (biological, chemical, or photochemical). Since this degradation processes are not specifically addressed in this model (spilled mass is modelled in terms of transport and phase changes), a constant decay rate specific to the environment where the mass exists is assumed, in order to determine the degradation / loss of chemical to some other form no longer of concern (Mackay et al., 2006).

In OpenDrift, the degradation is not implemented, excepted for biodegradation of oil where it follows Adcroft et al. (2010).

4. Academic study cases

To ensure the highest possible accuracy in comparing model processes, a series of test cases is essential. These test cases enable models to be compared with one another by providing identical inputs and examining differences in outputs. To minimize the influence of external variables, real-world data was not utilized in the test cases. In real-world data there are many variable fluctuating at the same time, and models may use different forcing providers, which can introduce further variations. Therefore, using controlled test cases ensures that the comparison of model processes is as precise as possible.

In this study, a total of 28 test cases were conducted across two series. The first series was named the "weathering" series, as it focused on studying the effects of weathering processes such as evaporation, dissolution, and volatilization. The test conditions were designed to keep the slick stationary, without the interference of wind, current, or waves and with the same HNS. The weathering processes were activated separately and then all together to better understand their combined impact. To further understand the influence of temperature on these processes, simulations were duplicated at two different temperatures. Detailed information on the conditions used for these simulations is provided in Table 1.

Table 1:Configuration of the academic cases with weathering but no drift. 1000 m3 of Butyl Acrylate was released, and simulated for 72 hours.

	Weathering process activated	Air temperature [°C]	Water temperature [°C]
Case 1	Evaporation	5	5
Case 2		20	20
Case 3	Dissolution	5	5
Case 4		20	20
Case 5	Evaporation + Dissolution	5	5
Case 6		20	20
Case 7	Evaporation + Dissolution + Volatilization	5	5
Case 8		20	20

The first series of test cases (Figure 57) gave us the general indications in model similarities and differences. For instance, the tested version of MOHID has systematically underestimated the evaporation rate with respect to the other models, while the tested version of OSERIT has systematically underestimated the dissolution rate with respect the other models. However, when evaporation, dissolution and volatilization are all activated, all the models qualitatively produce comparable results; the apparent longer persistence of the slick by MOHID being explained by the fact that the Lagrangian particles containing “dissolved pollutant available for volatilisation” are flagged as “surface” particles. In OSERIT, the considerable influence of temperature on evaporation is explained by the fact OSERIT adjusts the vapour pressure of the pollutant following the Clausus-

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Clapeyron relation. MOHID performs the same adjustments, but in our tests, this relation on temperature mainly impacts volatilization, a slower fate process. In CHEMMAP, no dependence on temperature has not been observed, but we may not exclude this is due to an omission by the model operator. This first series of test case illustrates the fact that our model intercomparison can only highlights similarities and differences in the different models but cannot lead to a model ranking.

The second set of simulations involved comparing the model predictions under varying conditions, including two different wind speeds and two different current speeds, while utilizing five different HNS. This allowed for a more realistic evaluation of models' differences while still maintaining a simple enough environment to easily interpret the results. A detailed description of the conditions and HNS used for these simulations can be found in Table 2.

Table 2: Configuration of the 20 academic cases with drift and weathering (5 chemicals x 2 wind speeds x 2 current speeds)

Duration of simulation	72 hours
Wind direction	Eastwards
Wind speeds	5 and 15 m/s
Current direction	Northwards
Current speeds	0.2 and 0.8 m/s
Significant waves height	As a function of wind speed
Air temperature	5 degrees
Water temperature	5 degrees
Volume	1000 m3
Chemicals	Acetone, Xylene, Toluene, Methanol, Butyl acetate

For sake of clarity, the main findings of these 20 academic tests are illustrated for a few scenarios; results for all scenarios being presented in Annex.

4.1. Slick spreading: area and persistence

Slick area and slick persistence time are the first 2 parameters studied in this intercomparison exercise. In case of real incidents, maritime authorities have only a limited response options to contain and recover HNS spilled in the marine environment. In general, recovery is only possible for substances that float or sink as the main behaviour and stay a sufficient long time at the sea surface or the see bed to plan operation; mobilize the necessary equipment; reach the polluted area; and start the response operation (Alcaro et al., 2021). So slick persistence and area are 2 key elements of information for responders.

Figure 1 presents the surface slick area (km²) as a function of time for the 20 weathering and drift academic cases. The 5 columns correspond respectively to acetone (DE), Xylene (FE), Toluene (E), Methanol (DE) and butyl acetate (FED). The four lines respectively corresponds to “slow wind-slow current” conditions, “fast wind-slow current” conditions, “slow wind-fast current” conditions and “fast wind-fast currents”, respectively. MOHID results are displayed in blue; OSERIT results in red; OpenDrift results in pink; CHEMMAP results in green. The lessons learnt from this exercise are the following:

- Again, the apparent longer persistence of the slick by MOHID is explained by the fact that the Lagrangian particles containing “dissolved pollutant available for volatilisation” are flagged as “surface” particles.
- For all the 20 cases, the persistence times simulated by OSERIT, OpenDrift and CHEMMAP qualitatively remain within the same range.
- For all tested chemicals, the maximal slick surface area simulated by the different models have a dependence on the met-ocean conditions. For OSERIT, strong wind conditions led to larger slick surface, while in CHEMMAP and MOHID, strong winds led to smaller slick surface.

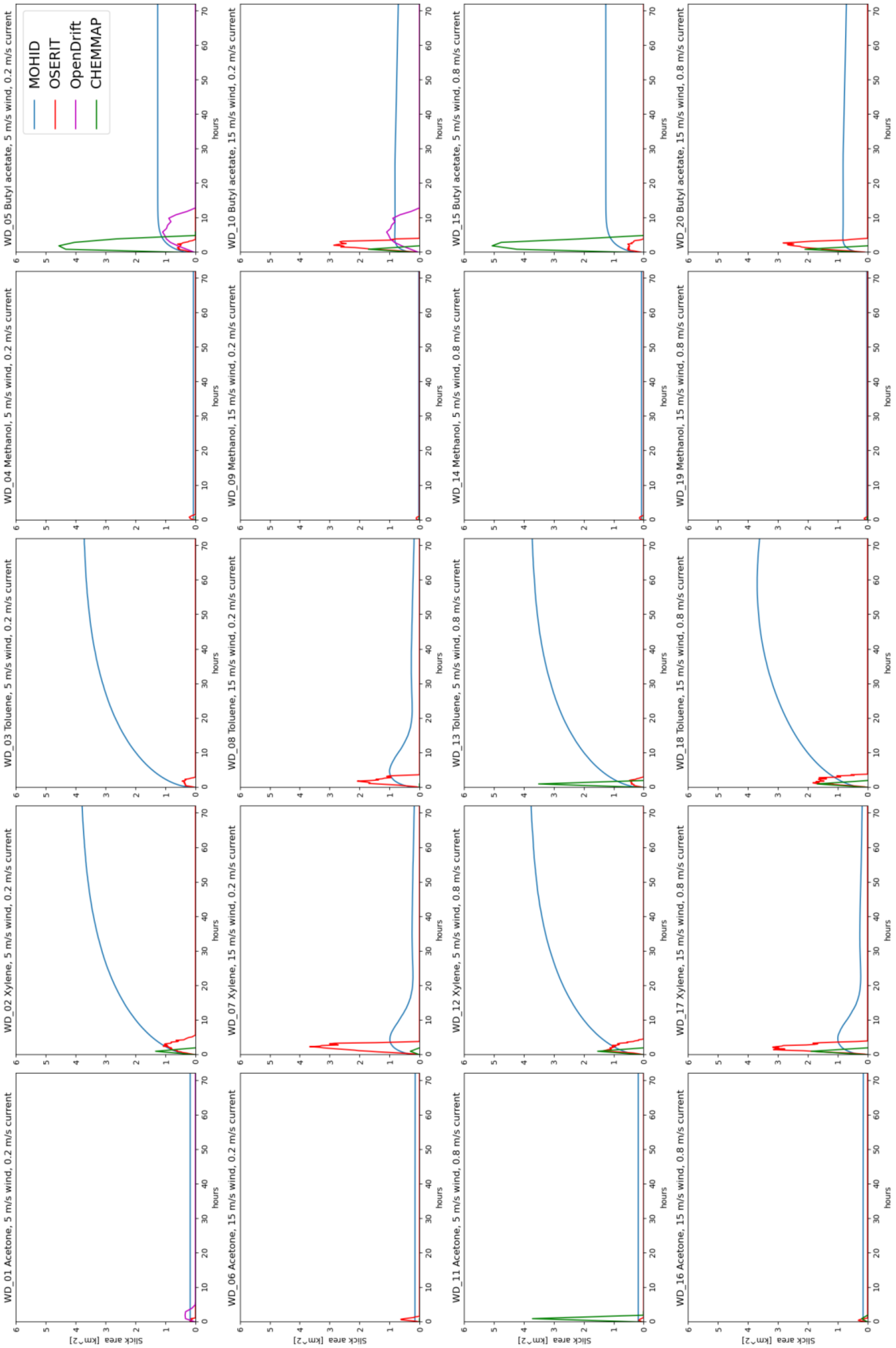


Figure 1 Area for the slick in the simulations in square kilometers of MOHID (blue), OSERIT (red), OpendDrift (purple) and CHEMMAP (green) for the weathering drift cases

4.2. Evaporation-Dissolution-Volatilisation

To explain the observed difference in the simulated maximal slick surface, one need to further analyse how the different models simulate the competition between evaporation, dissolution, and volatilisation. This can be done by analysing mass balance graphs. These graphs show how the different fate processes impacts the mass distribution of a pollutant in its different phases: surface slicks, droplets in the water column, dissolved in the water column, evaporated, degraded, adsorbed on sediments, etc. Because there is no uniformization between the different models in the definition of the mass fraction categories, this study uses the following colour code for the mass balance graphs: black represents the mass fraction in the surface slick; blueish colours represent mass fraction evaporated and/or volatilised in the atmosphere; greenish colours represent mass fraction dissolved in the water column; and reddish colours represented degraded mass fractions.

In this section we will restrict ourselves to present and discuss the case of acetone (DE) and butyl acetate (FED) for the slow wind-slow current conditions and for the fast wind-slow current conditions.

4.2.1. Acetone

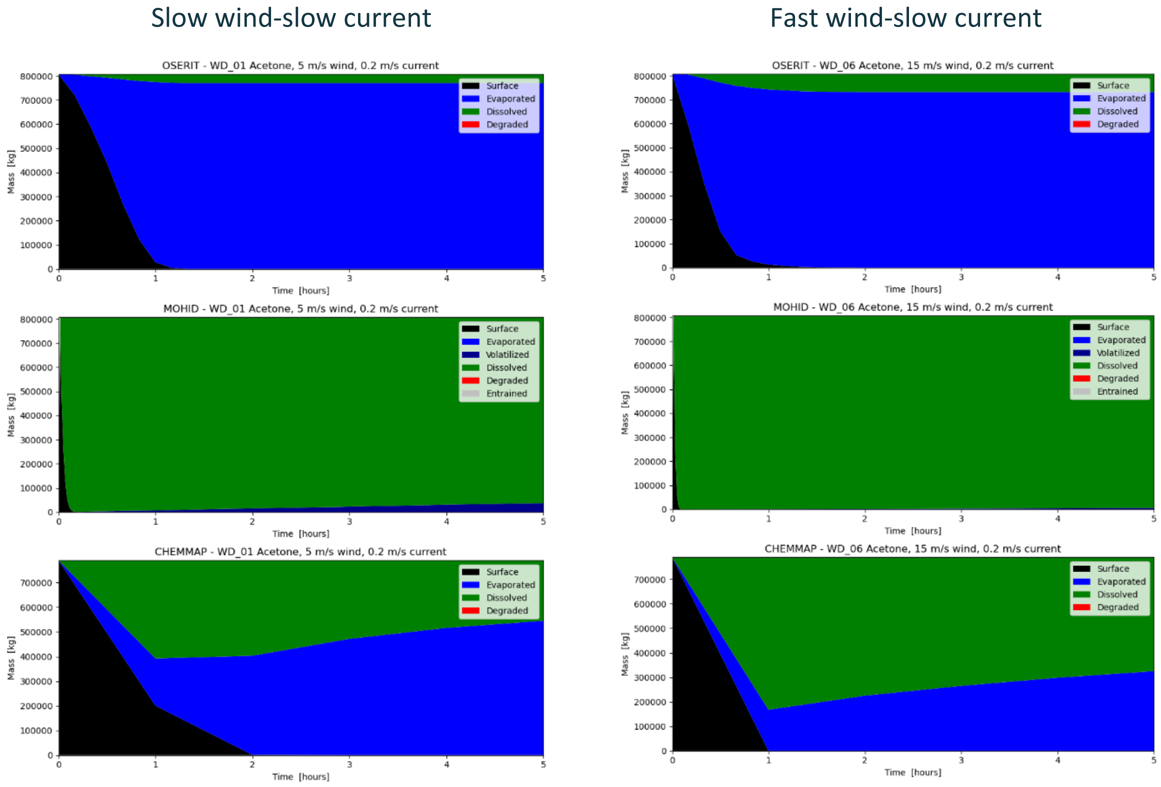
According to the SEBC classification, acetone is a dissolver-evaporator substances.

For all models, the initial situation is a surface slick of 1000m³ of acetone. The mass balance graphs for acetone is rather different for MOHID, OSERIT and CHEMMAP:

- In MOHID, because the dominant behaviour of acetone is dissolver, the full volume of the acetone slick is almost instantly converted as “dissolved” in less than 10 minutes. In the slow wind-slow current condition, most of the dissolved volume remains close to the sea surface available for volatilization. In the fast wind-slow current condition, the intrusion depth of dissolved particles in increased by the larger significant waves height, reducing the amount of acetone available for the volatilization.
- In CHEMMAP, only hourly outputs are available, what introduced a biais on the graphs. For the slow wind-slow current simulation, one can estimate that the slick persistence time is of about 1h20. During this first period, evaporation and dissolution seems to be of equal importance. Roughly speaking, 40% of the acetone has been evaporated during the first 80

minutes of the simulation and 60% of the acetone dissolved. In the part of the simulation, only volatilization occurs at apparently a larger rate than in MOHID. The same behaviour can be observed for the fast wind-slow current simulation. However, due to higher waves, a larger fraction of the slick is entrained in the water column, which reduce the total amount of acetone available for evaporation and increase the total amount of acetone available for dissolution. The surface slick persistence can be estimates to 30-40 minutes. In this simulation, the volatilization rate is much larger than in MOHID but decreased with respect to the slow wind-slow current simulation.

- For OSERIT, the dissolution rate depends on the chemical solubility but also on the Reynolds number. The latter is much lower in slow current condition than in fast current condition. Without surprised, the dissolution process is inhibited in OSERIT than in MOHID and CHEMMAP. Consequently, evaporation dominates. However, the slick persistence time as simulated by OSERIT and CHEMMAP remains of the same order of magnitude. In the second part of the simulation, volatilization rate in OSERIT and MOHID are also of the same order of magnitude but applied on different volume of dissolved acetone.


Slow wind-slow current

Fast wind-slow current

Figure 2: Mass balance graphs for acetone for respectively the OSERIT model (top), MOHID (middle) and CHEMMAP (bottom). In OSERIT and MOHID, the timesteps has been decreased to 1 minute. For CHEMMAP, only hourly outputs are available. The persisentence time of the slick is therefore artificially increased in the mass balance graphs of CHEMMAP.

4.2.2. Butyl Acetate

According to the SEBC classification, Butyl Acetate is a Floater-Evaporator-Dissolver. According to this classification, dissolution can occur but is not the leading fate process.

For all models, the initial situation is a surface slick of 1000m³ of Butyl Acetate. The mass balance graphs for Butyl Acetate are also rather different for MOHID, OSERIT and CHEMMAP:

- In MOHID, the evaporation process has not been activated because at 5°C, the vapour pressure of Butyl Acetate is below the thresholds value of the SEBC classification... Otherwise stated, MOHID handles Butyl Acetate at 5°C as a Dissolver pollutant. This explains why MOHID forecast a dissolution of 80% to 100% of Butyl Acetate at 5°C, depending on the met-ocean condition. Even at low temperature, MOHID simulates the volatilisation processes. Despite the relatively small vapour pressure of Butyl Acetate, up to 85% of the dissolved butyl acetate can volatilize after 72 hours if in case the dissolved fraction remains close to the sea surface (slow-wind – slow current simulation).
- As expected, in CHEMMAP dissolution is slower for Butyl acetate than for Acetone. For the slow wind-slow current simulation, evaporation largely dominates, and dissolution remains limited (<10%). The persistence time is of 4 hours. For the fast wind-slow current simulation, a larger fraction of the slick is entrained in the water column, which reduce the total amount of Butyl The persistence time decrease to less than 1 hour. In both simulations, the volatilization rate is much larger than in MOHID.
- For OSERIT, the dissolution rate depends on the chemical solubility but also on the Reynolds number. The latter is much lower in slow current condition than in fast current condition. Even activated, the dissolution process is totally inhibited in the OSERIT simulations of butyl acetate with slow current: buthyl acetate density being only of 889 kg/m³ at 5°C, droplets entrained in the water column are also hardly dissolved. Despite this behaviour difference, persistence time of the slick as simulated OSERIT and CHEMMAP remains comparable.

slow wind – slow current

Fast wind-slow current

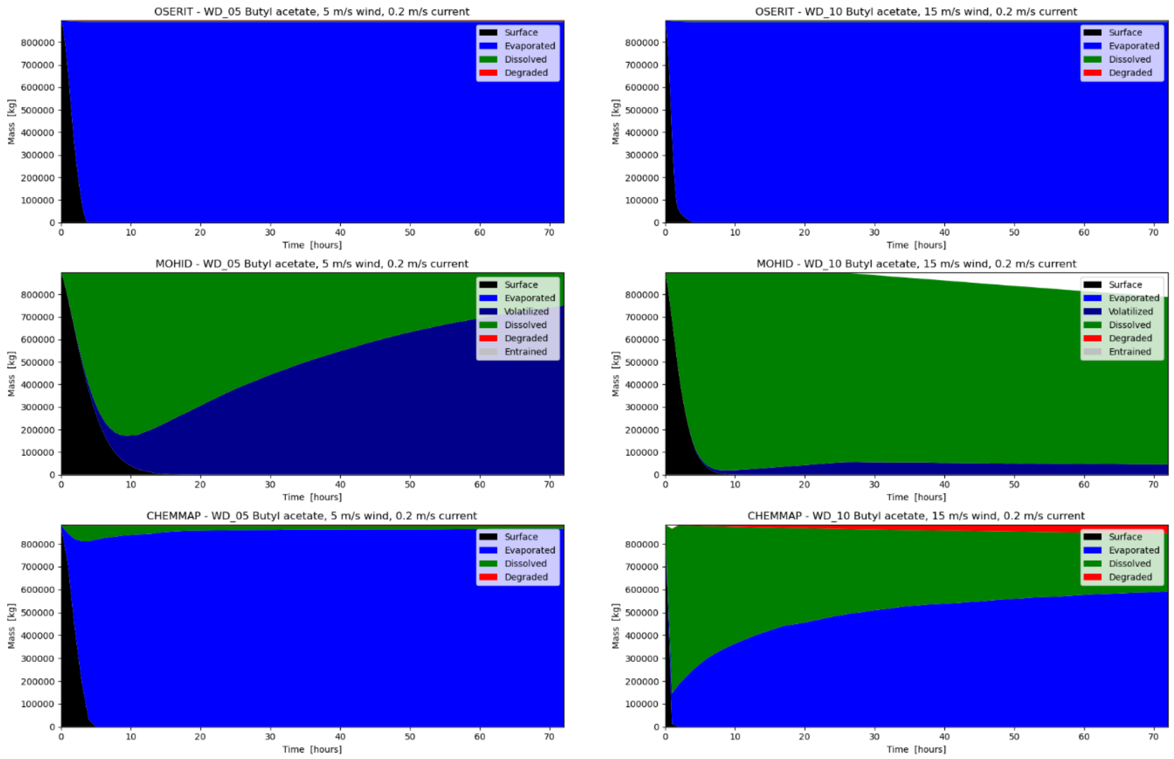


Figure 3: : Mass balance graphs for Butyl Acetate for respectively the OSERIT model (top), MOHID (middle) and CHEMMAP (bottom). In OSERIT and MOHID, the timesteps has been decreased to 1 minute. For CHEMMAP, only hourly outputs are available. The white colour in MOHID graphs is explained by the fact that some airborne particles have left the model domain.

4.3. Drift: Impact of current, wind and waves

Horizontal drift is implemented in a similar way in OSERIT, MOHID, OpenDrift and CHEMMAP. Figure 4 presents the results for the simulation of Butyl acetate with slow wind-slow current conditions.

- As expected, no significant difference is observed for the surface slick drift, as long as the persistence time are comparable. The surface drift is maybe slightly faster in CHEMMAP and windage coefficient maybe slightly smaller in OpenDrift.
- Although the dispersion rate is larger in CHEMMAP, the dissolved fraction in OSERIT, OpenDrift and CHEMMAP are drifting in the same direction and velocity. For MOHID, one can clearly sea the separation of the dissolved pollutant fraction that remains close to the sea surface (and there under wind influence) and the deeper dissolved fraction that drifts only with currents.

- In all the models, the airborne particles drift similarly. However, the elongated HNS clouds as simulated by MOHID, CHEMMAP and CHEMMAP are produced by the continuous volatilisation process. Volatilization having been inhibited in OSERIT for this simulation, the OSERIT cloud is only due to the surface slick evaporation during the first 4 hours.

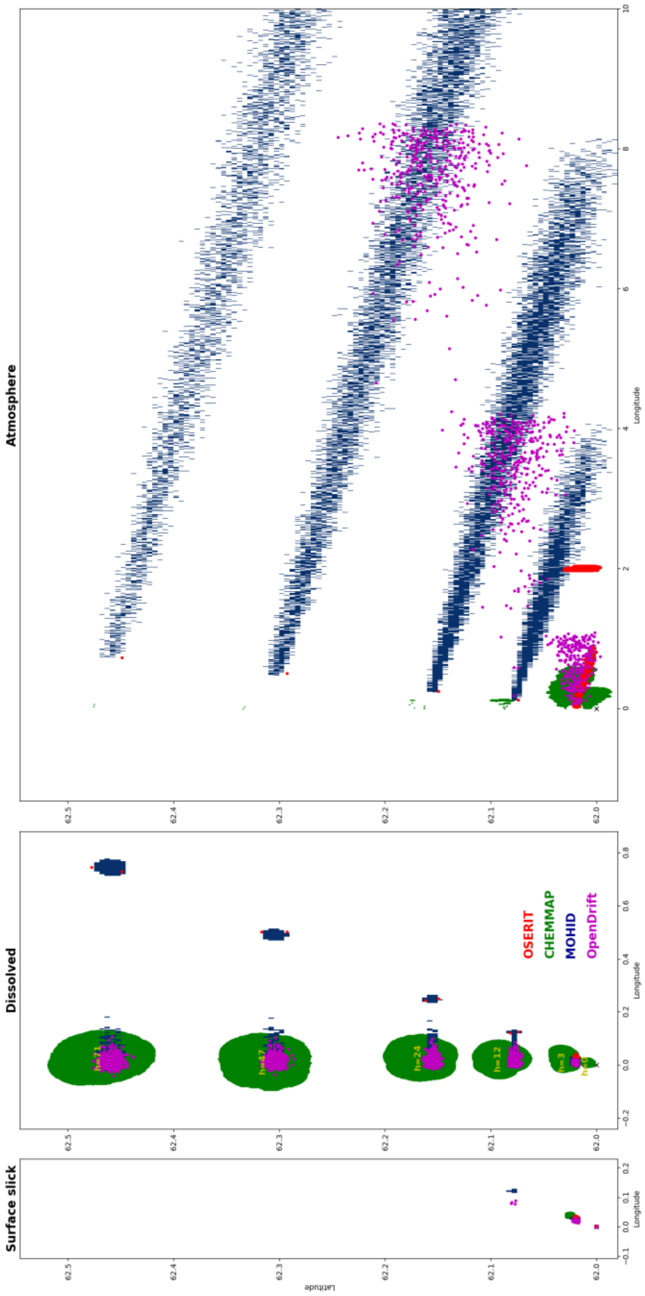


Figure 4: Intercomparison on drift processes for butyl acetate :Snapshot of pollutant locations at different time steps for the airborne fraction (top), dissolved fraction (middle), surface slick (bottom). Attention the map scale changed between the different level

5. Conclusion

This report presents the outcome of an intercomparison exercise between 4 state-of-the-art HNS drift, fate, and behaviour models: OSERIT developed by RBINS (Belgium), MOHID developed by IST (Portugal), OpenDrift developed by MetNorway (Norway) and CHEMMAP developed by RPS (USA) but operated by Cedre (France).

Although these models have been developed following the same general principles, numerous implementations differences have been highlighted in sections 2 and 3. For instance, no models use the same parametrisation for the same fate process. Most of the time, the parameterisations differ by their calibration coefficients, by some simplification assumptions or on the contrary by the inclusion of some empirical formulas that should generalize some behaviour for a wider range of met-ocean conditions.

Most if not all fate processes parameterisations have been introduced in the 1970's and the 1980's. The observation datasets used for developing and calibrating the parametrisations are no more available. Most of the time, modellers do not even know which chemicals have been tested and following which experimental protocol. This situation leads to huge uncertainties about the accuracy of the parametrisations used in the different models. This observation is a call to (re-)perform these experimental tests and share their results in an new open and sustainable database, that store all necessary metadata (including protocols).

This intercomparisons exercise was however extremely interesting. Modellers have learnt a lot from each other. We have been working in a fully transparent and open-minded way. We have challenged each other and had to deepen our understanding of our respective models to correctly intercompare and interpret our simulations results. Doing so, we have identified opportunities of improvements. We will surely investigate these opportunities in the coming months and years. This means that this report must be seen as a snapshot for the model versions available late 2022, early 2023. This observation is also a call to periodically redo this intercomparison exercise.

To conclude, we have some consolidated messages for the end-users of our model simulations:

- We, modellers, are confident in our drift algorithms and the met-ocean forcing is now the largest source of uncertainty in our simulated trajectories.
- All the models predict consistent persistence time of the surface slicks.

- The different parametrisations implemented in the models generates huge different results for the competition between evaporation, dissolution, and volatilisation. This means users should not yet blindly trust model forecast of the pollutant concentration in the air and the water column. There are no solid arguments to trust more one model than another. This means that, with the current knowledge, HNS drift, fate, and behaviour simulations can only be interpreted by trained experts. Whenever possible, theses experts should get access to simulations from different models. This pleads for a reinforced collaboration between neighbouring countries.

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7. Annex: simulation results

7.1. Weathering drift cases description

In the Table 3 all the conditions which are varying for each weathering-drift case

Table 3 : Parameters of the weathering-drift testcases

Number of the case	***windspeed***	***current speed***	***HNS***
1	*5*	*0.2*	*Acetone*
2	*5*	*0.2*	*Xylene*
3	*5*	*0.2*	*Toluene*
4	*5*	*0.2*	*Methanol*
5	*5*	*0.2*	*Butyl acetate*
6	*15*	*0.2*	*Acetone*
	15	*0.2*	*Xylene*
8	*15*	*0.2*	*Toluene*
9	*15*	*0.2*	*Methanol*
10	*15*	*0.2*	*Butyl acetate*
11	*5*	*0.8*	*Acetone*
12	*5*	*0.8*	*Xylene*
13	*5*	*0.8*	*Toluene*
14	*5*	*0.8*	*Methanol*
15	*5*	*0.8*	*Butyl acetate*
16	*15*	*0.8*	*Acetone*
17	*15*	*0.8*	*Xylene*
18	*15*	*0.8*	*Toluene*
19	*15*	*0.8*	*Methanol*
20	*15*	*0.8*	*Butyl acetate*

7.2. Mass budget

As showed from the figures presented, the persistence time of the slick at the surface appears to be similar in each models. However, the impact of different weathering processes on HNS varies between the models. In MOHID, dissolution plays a predominant role in the weathering of HNS, whereas in OSERIT, evaporation is the main influencing factor. CHEMMAP, on the other hand, exhibits a more balanced effect of the two processes. Additionally, when the temperature is low, MOHID deactivates evaporation, which further strengthens the dominance of dissolution. It is worth noting that volatilization occurs at a slower pace than evaporation in these models.

7.2.1. First 5 hours

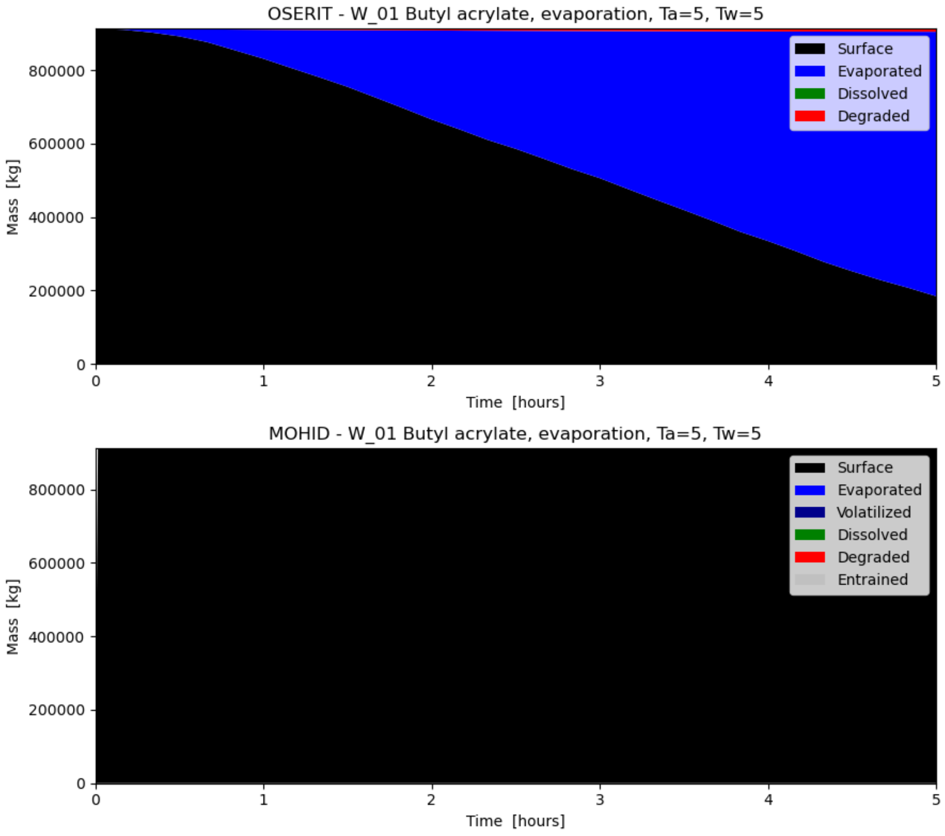

Figure 5 : Mass balance for the first 5 hours for the weathering testcase 1. OSERIT is on top and MOHID at the bottom, only the evaporation is activated and the air and water temperature are 5°C

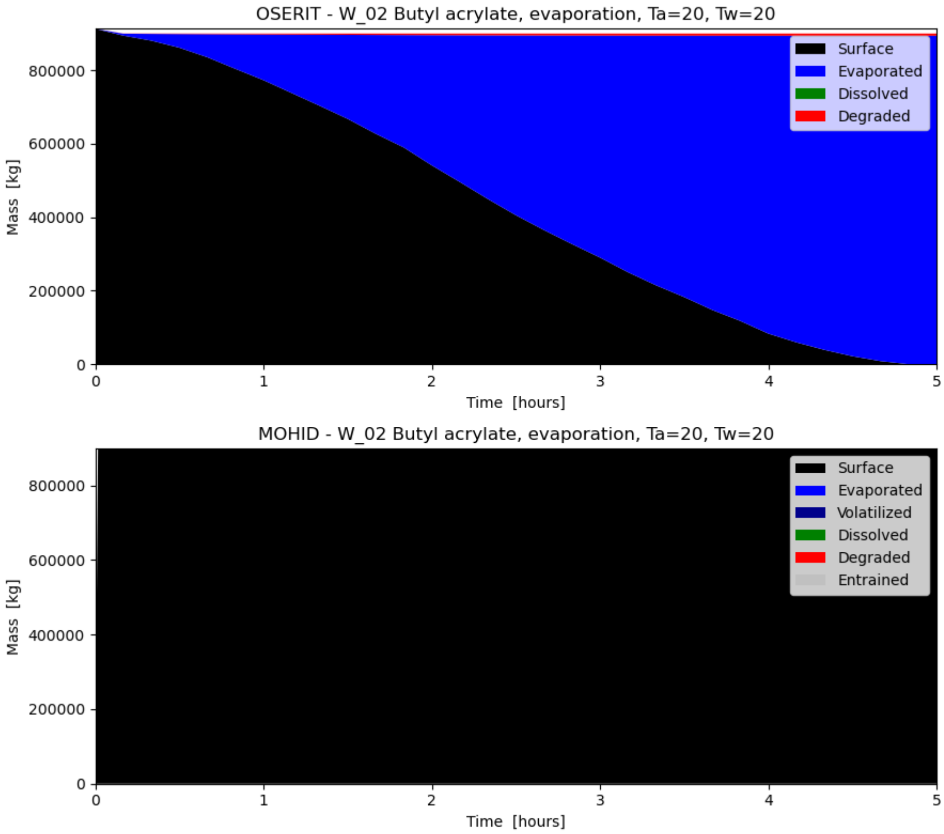

Figure 6: Mass balance for the first 5 hours for the weathering testcase 2. OSERIT is on top and MOHID at the bottom, only the evaporation is activated and the air and water temperature are 20°C

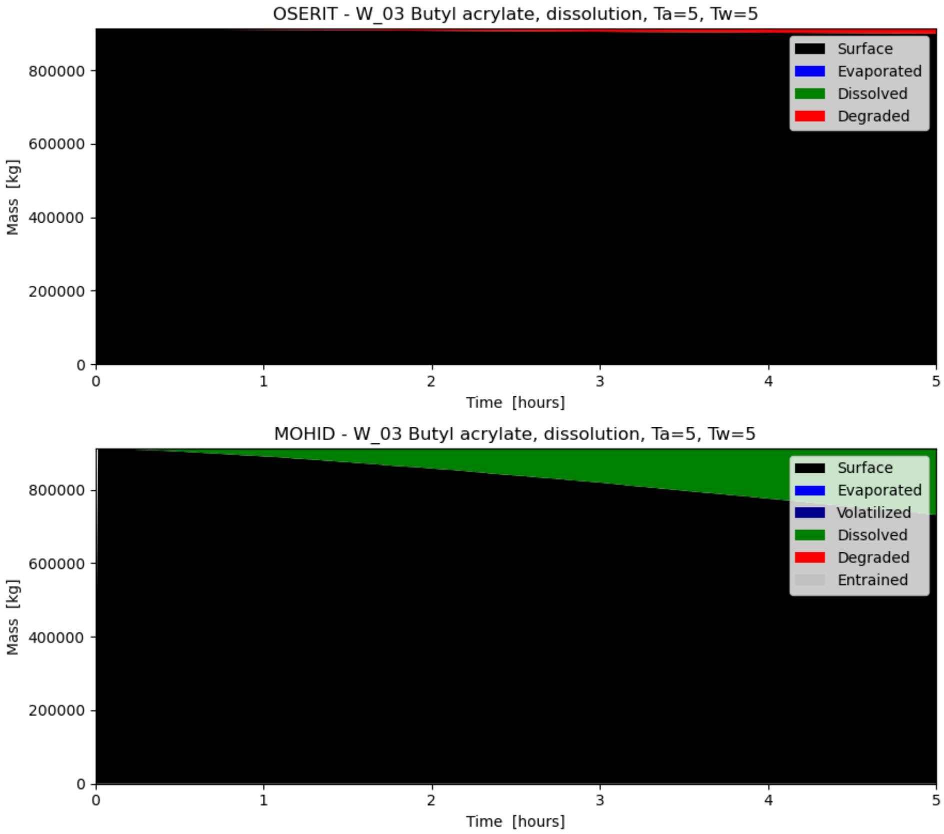

Figure 7 : Mass balance for the first 5 hours for the weathering testcase 3. OSERIT is on top and MOHID at the bottom, only the dissolution is activated and the air and water temperature are 5°C

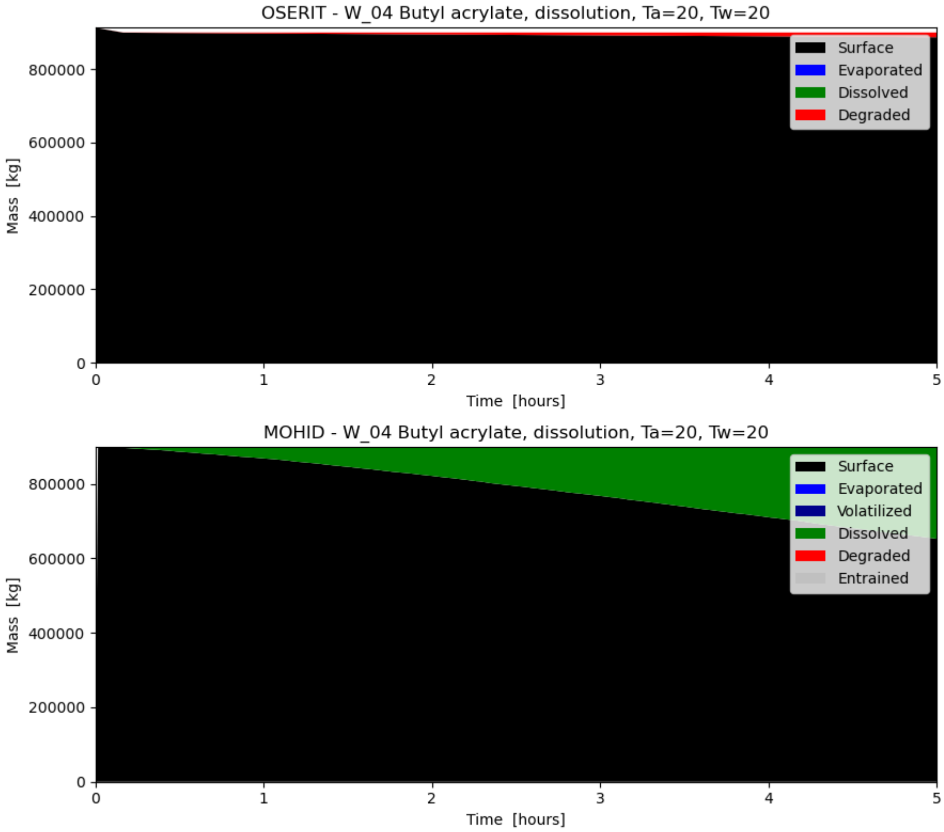

Figure 8 : Mass balance for the first 5 hours for the weathering testcase 4. OSERIT is on top and MOHID at the bottom, only the dissolution is activated and the air and water temperature are 20°C

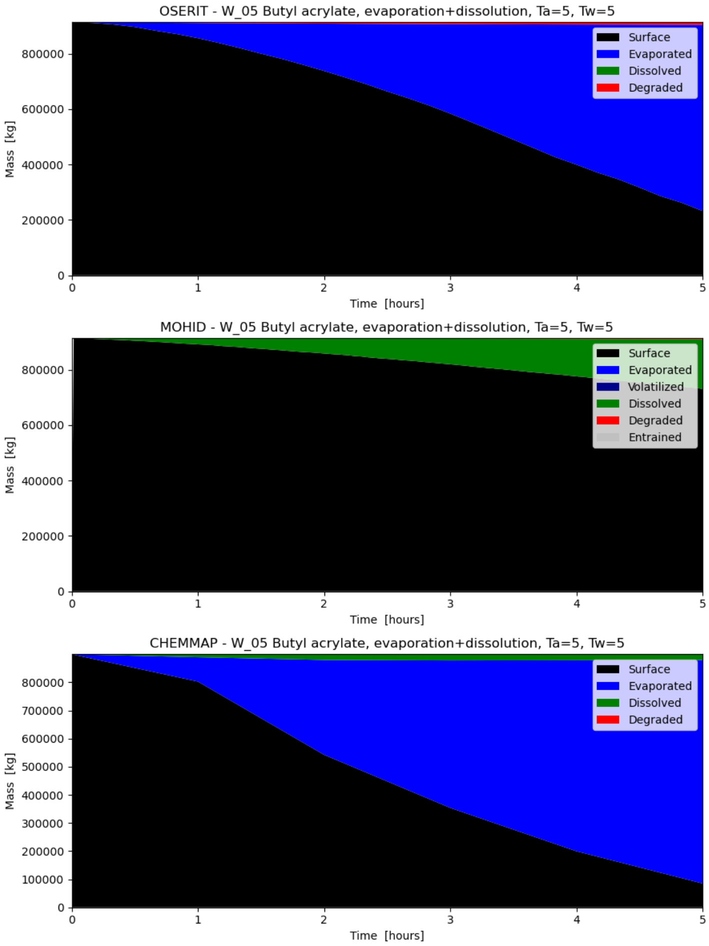

Figure 9 : Mass balance for the first 5 hours for the weathering testcase 5. OSERIT is on top and MOHID in the middle and CHEMMAP at the bottom, the dissolution and the evaporation are activated and the air and water temperature are 5°C

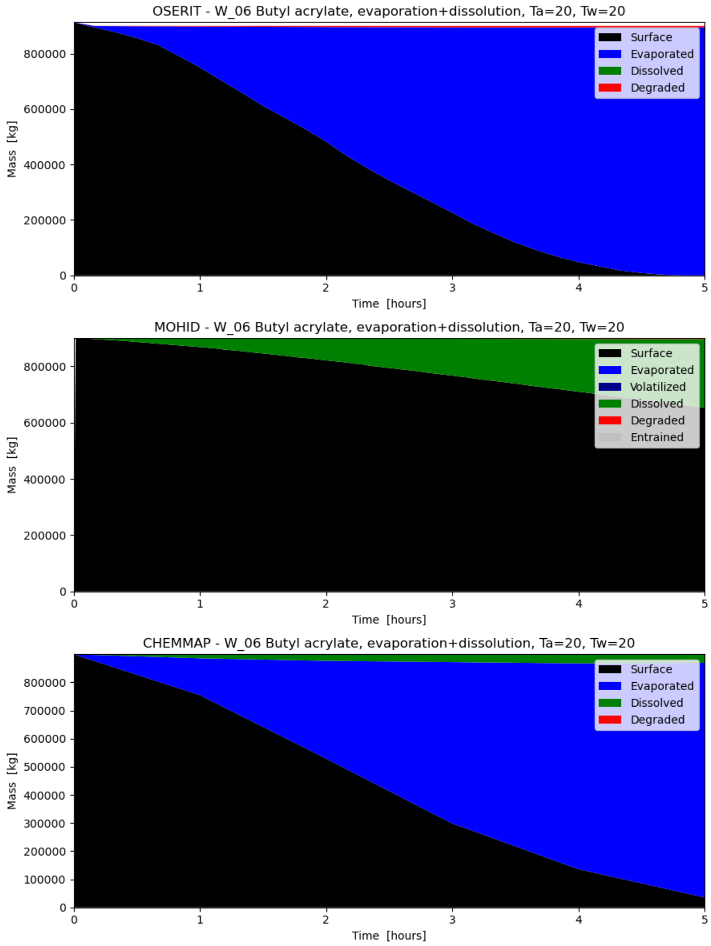

Figure 10 : Mass balance for the first 5 hours for the weathering testcase 6. OSERIT is on top and MOHID in the middle and CHEMMAP at the bottom, the dissolution and the evaporation are activated and the air and water temperature are 20°C

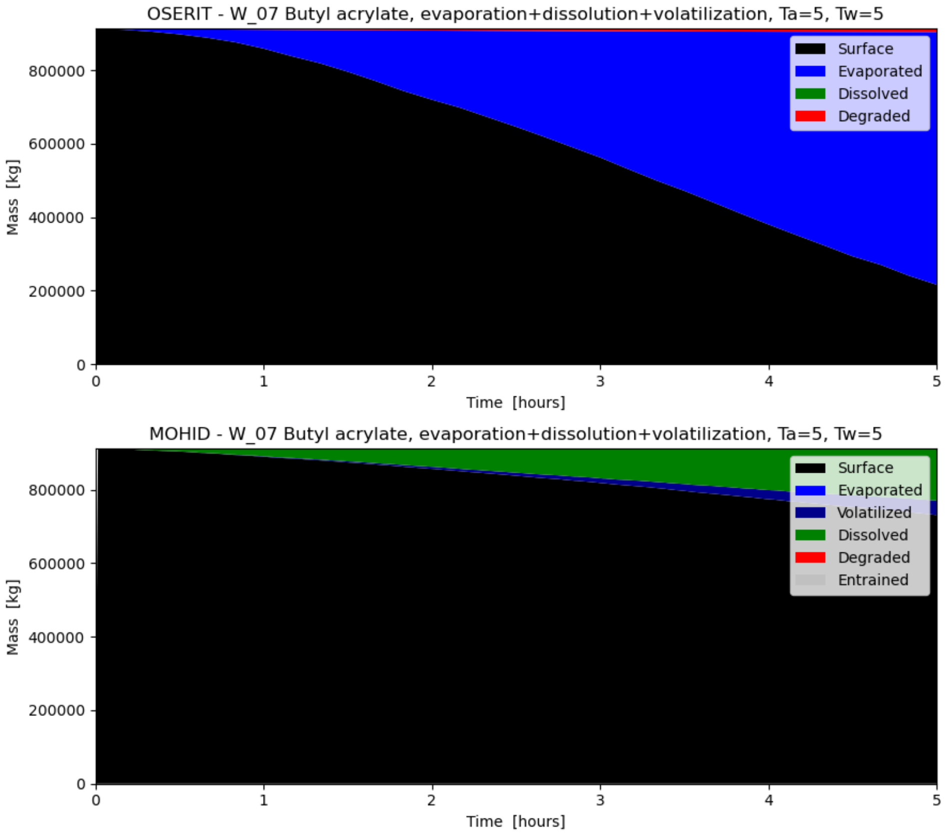

Figure 11 : Mass balance for the first 5 hours for the weathering testcase 7. OSERIT is on top and MOHID at the bottom, the dissolution, volatilization and the evaporation are activated and the air and water temperature are 5°C

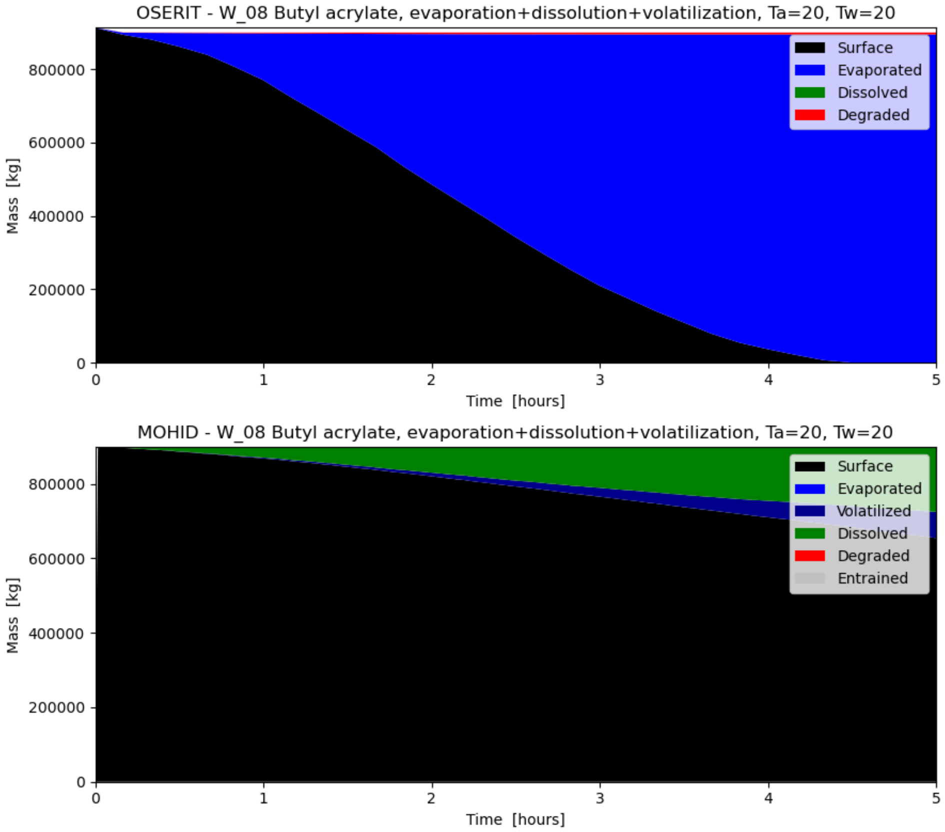

Figure 12 : Mass balance for the first 5 hours for the weathering testcase 8. OSERIT is on top and MOHID at the bottom, the dissolution, volatilization and the evaporation are activated and the air and water temperature are 20°C

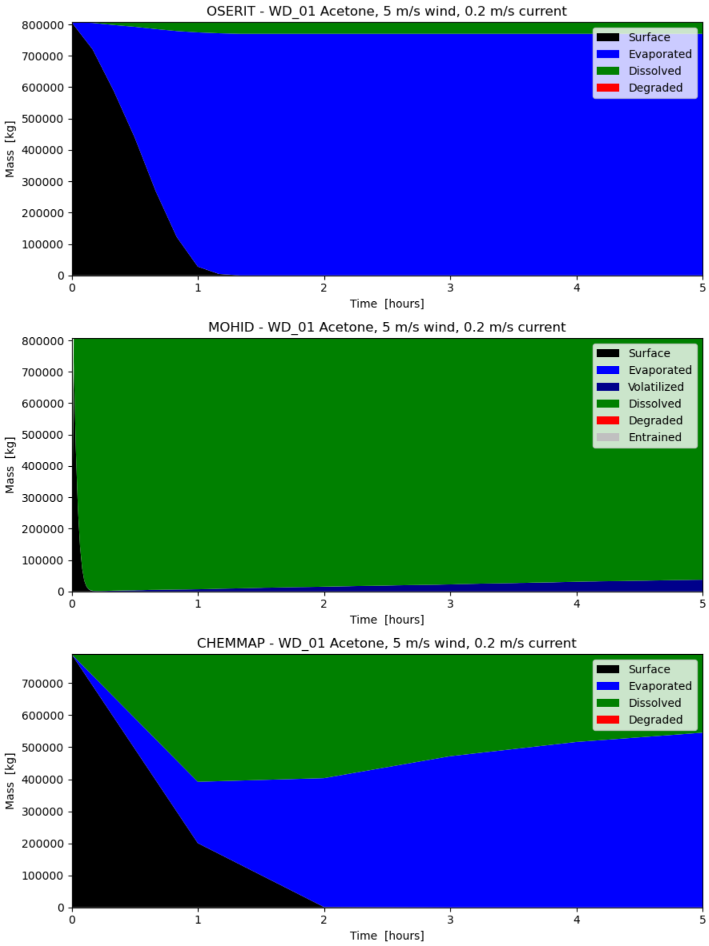

Figure 13 : Mass balance for the first 5 hours for the weathering drift testcase 1. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Acetone, the wind is of 5 m/s and the current of 0.2 m/s

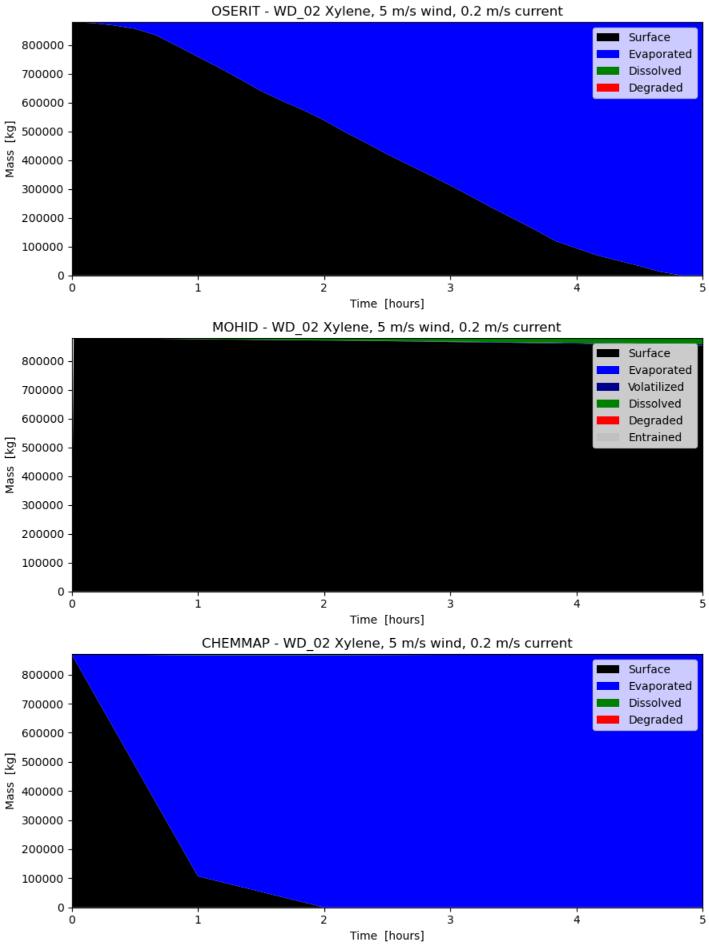

Figure 14 : Mass balance for the first 5 hours for the weathering drift testcase 2. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Xylene, the wind is of 5 m/s and the current of 0.2 m/s

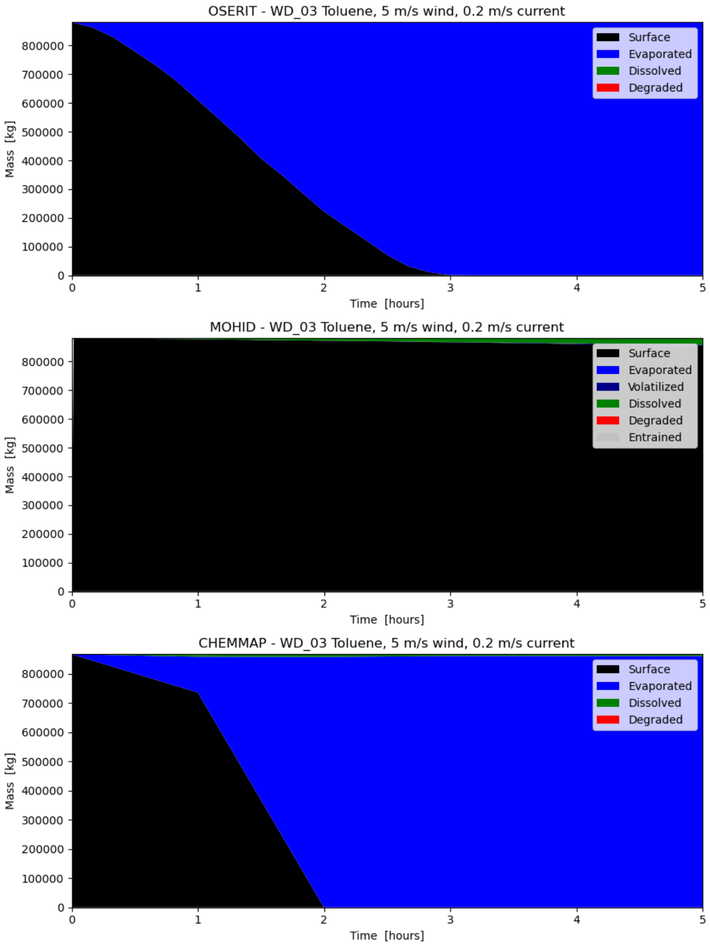

Figure 15 : Mass balance for the first 5 hours for the weathering drift testcase 3. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Toluene, the wind is of 5 m/s and the current of 0.2 m/s

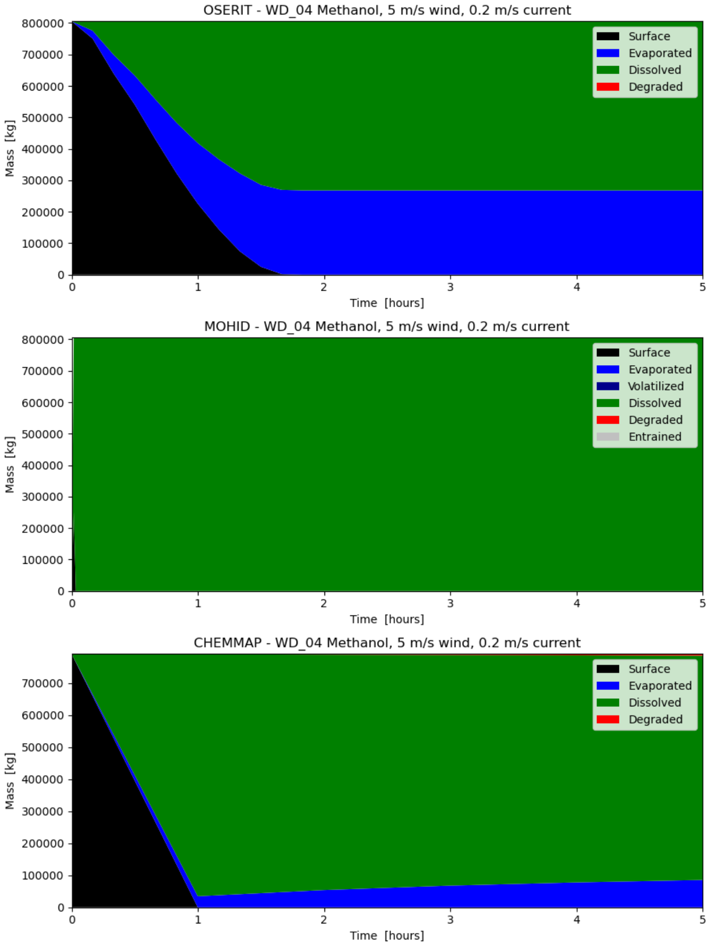

Figure 16 : Mass balance for the first 5 hours for the weathering drift testcase 4. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Methanol, the wind is of 5 m/s and the current of 0.2 m/s

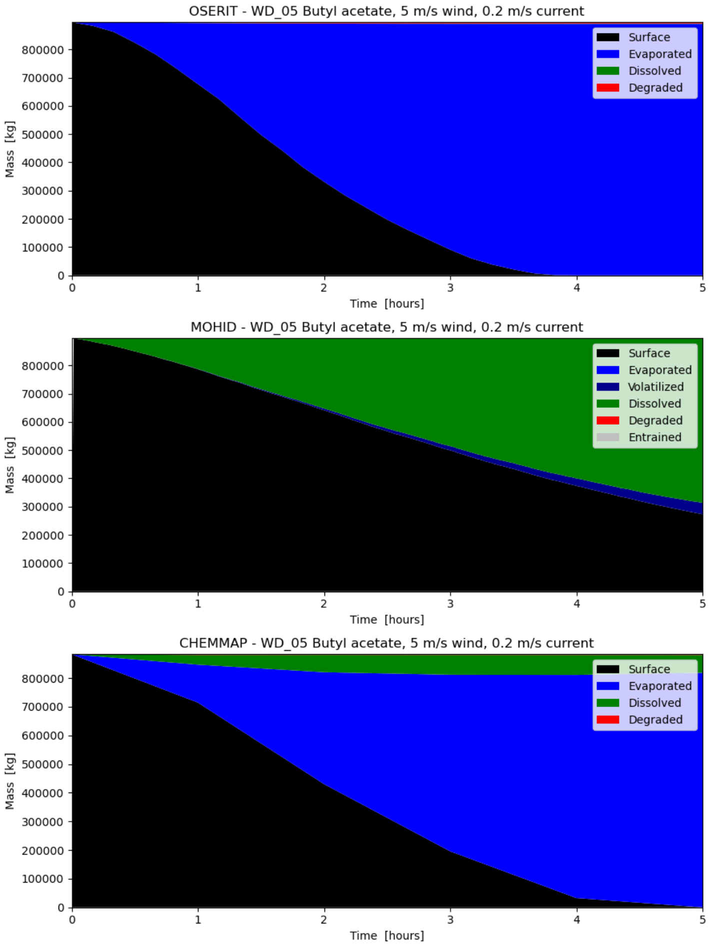

Figure 17 : Mass balance for the first 5 hours for the weathering drift testcase 5. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Butyl acetate, the wind is of 5 m/s and the current of 0.2 m/s

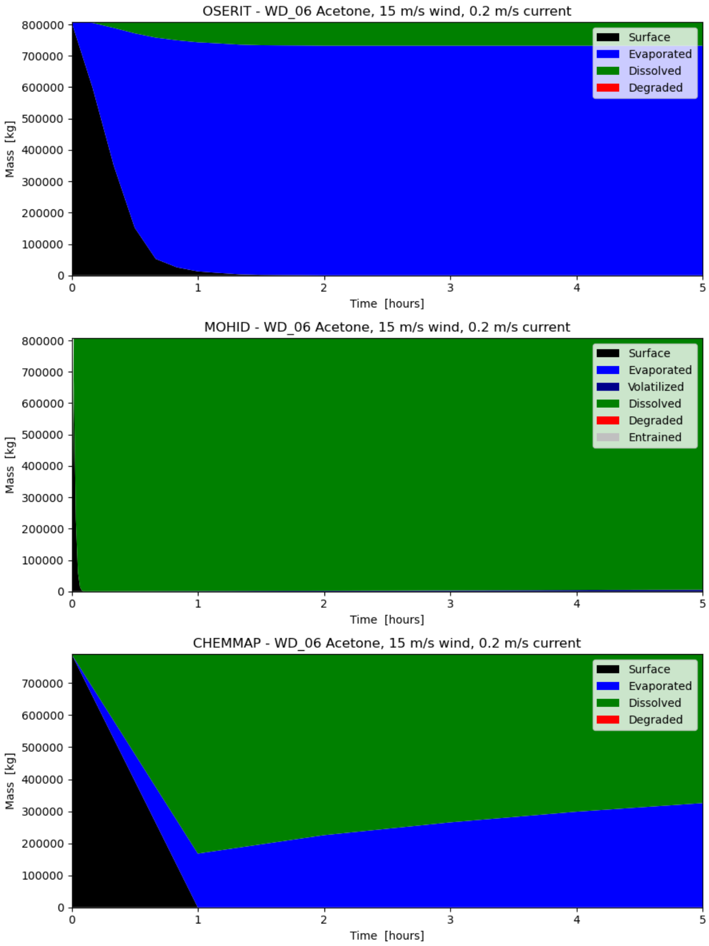

Figure 18 : Mass balance for the first 5 hours for the weathering drift testcase 6. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Acetone, the wind is of 15 m/s and the current of 0.2 m/s

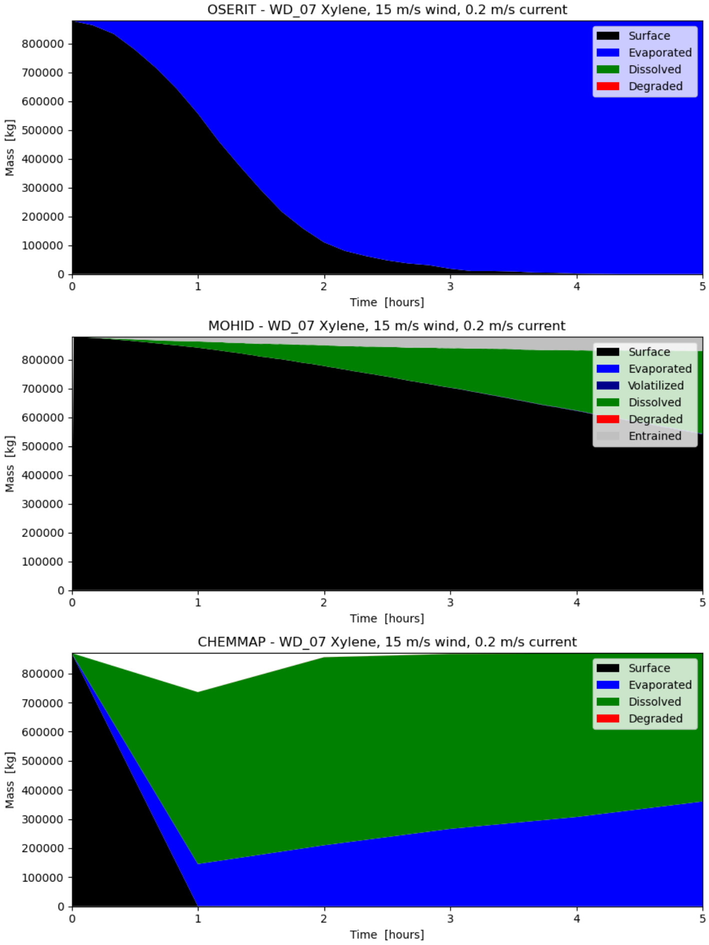

Figure 19 : Mass balance for the first 5 hours for the weathering drift testcase 7. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Xylene, the wind is of 15 m/s and the current of 0.2 m/s

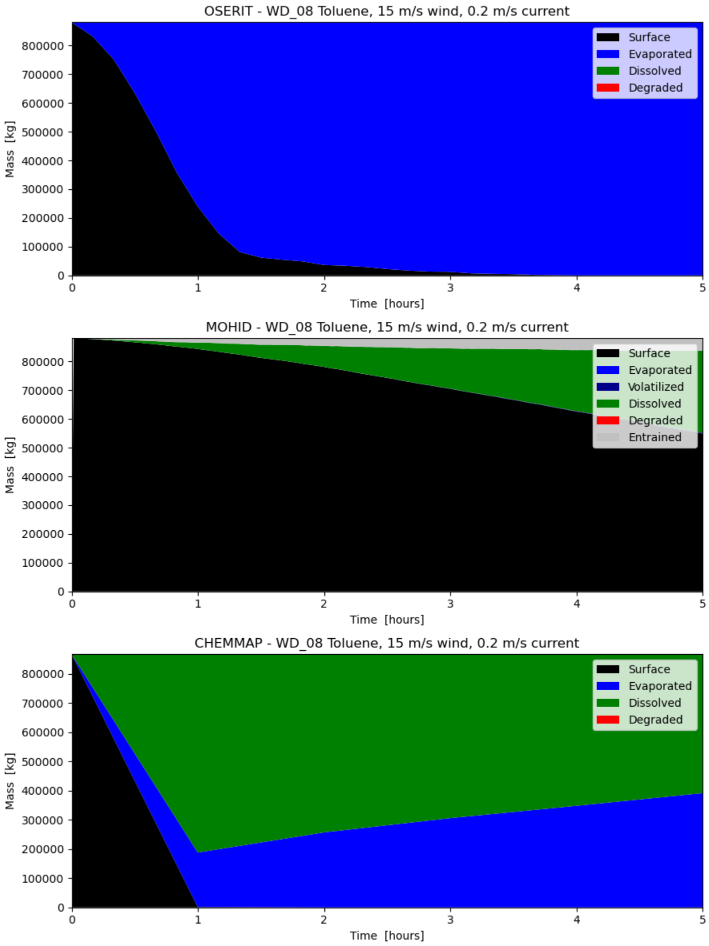

Figure 20 : Mass balance for the first 5 hours for the weathering drift testcase 8. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Toluene, the wind is of 15 m/s and the current of 0.2 m/s

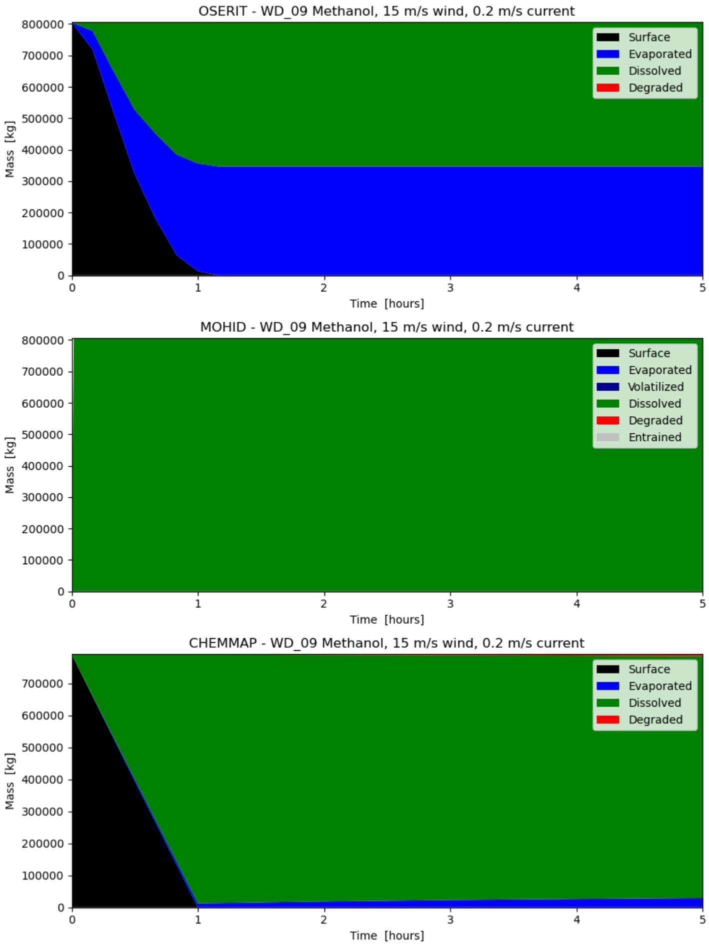

Figure 21 : Mass balance for the first 5 hours for the weathering drift testcase 9. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Methanol, the wind is of 15 m/s and the current of 0.2 m/s

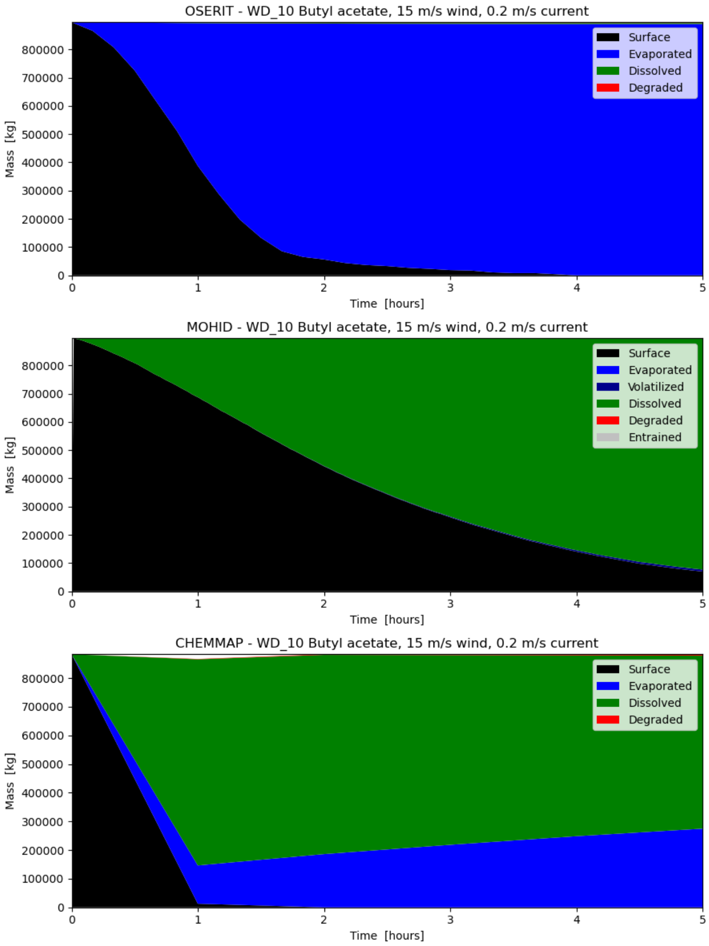

Figure 22 : Mass balance for the first 5 hours for the weathering drift testcase 10. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Butyl acetate, the wind is of 15 m/s and the current of 0.2 m/s

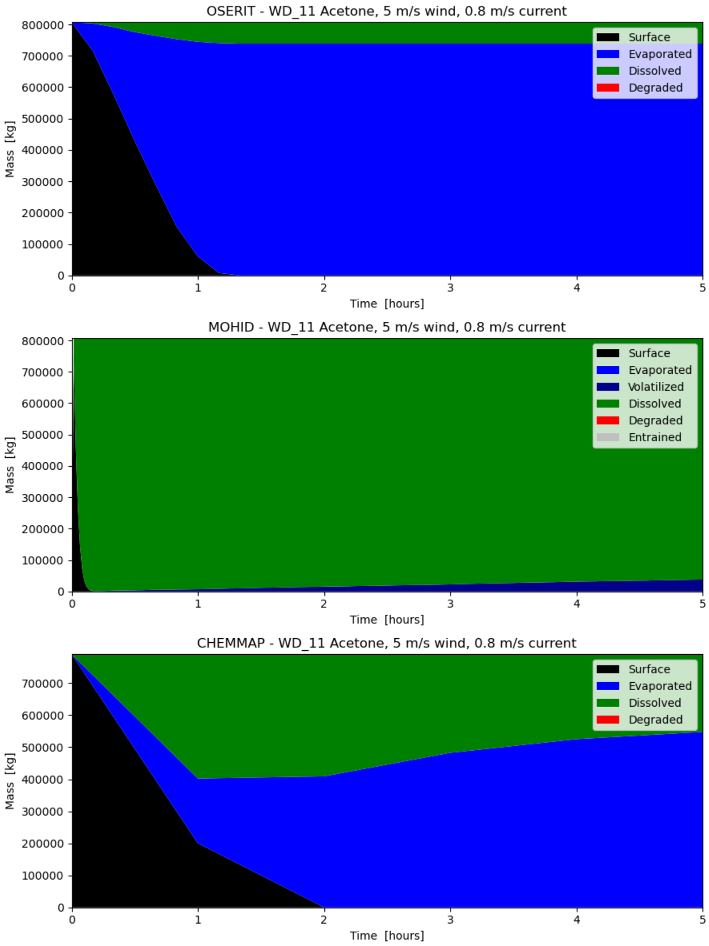

Figure 23 : Mass balance for the first 5 hours for the weathering drift testcase 11. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Acetone, the wind is of 5 m/s and the current of 0.8 m/s

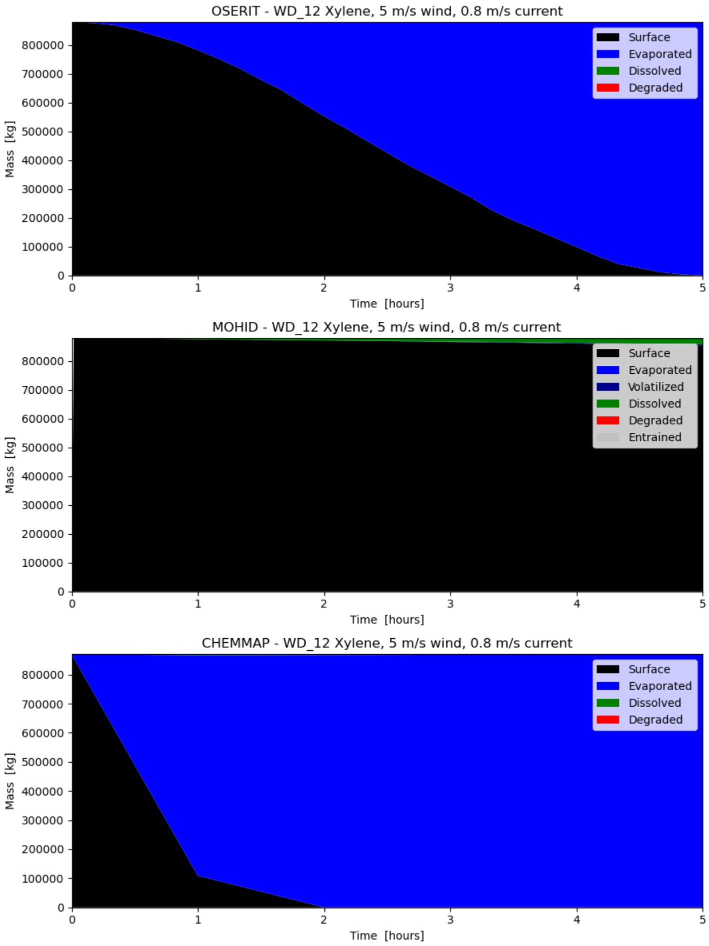

Figure 24 : Mass balance for the first 5 hours for the weathering drift testcase 12. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Xylene, the wind is of 5 m/s and the current of 0.8 m/s

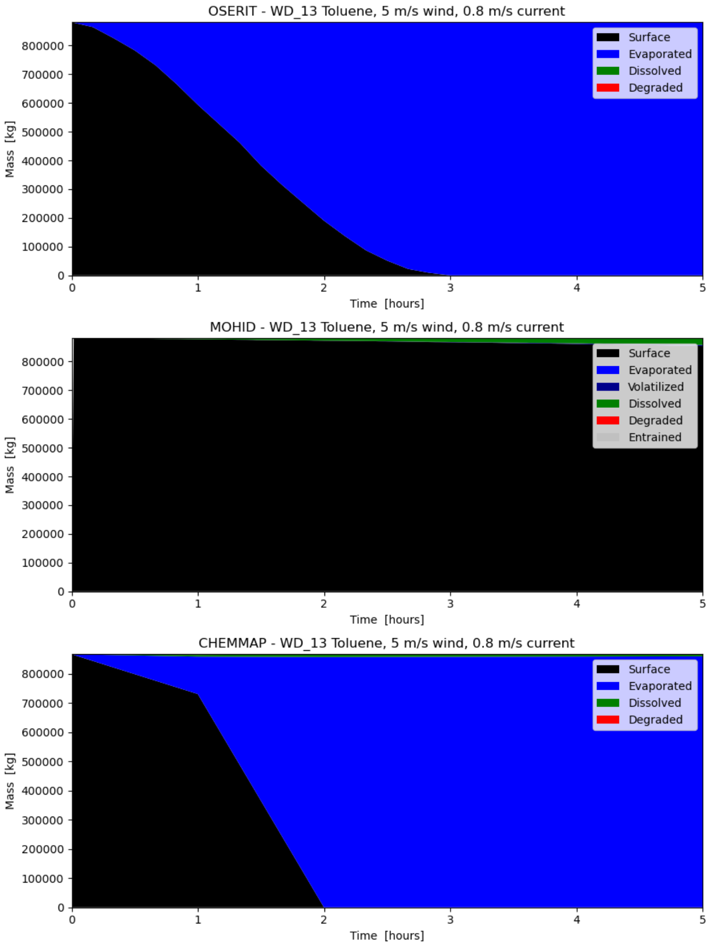

Figure 25 : Mass balance for the first 5 hours for the weathering drift testcase 13. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Toluene, the wind is of 5 m/s and the current of 0.8 m/s

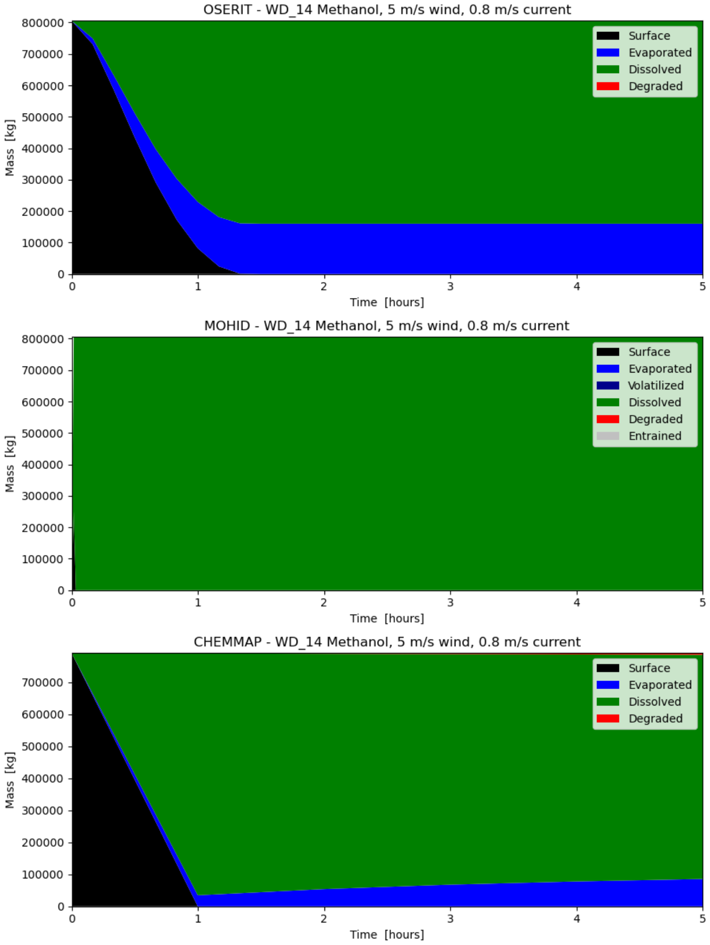

Figure 26 : Mass balance for the first 5 hours for the weathering drift testcase 14. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Methanol, the wind is of 5 m/s and the current of 0.8 m/s

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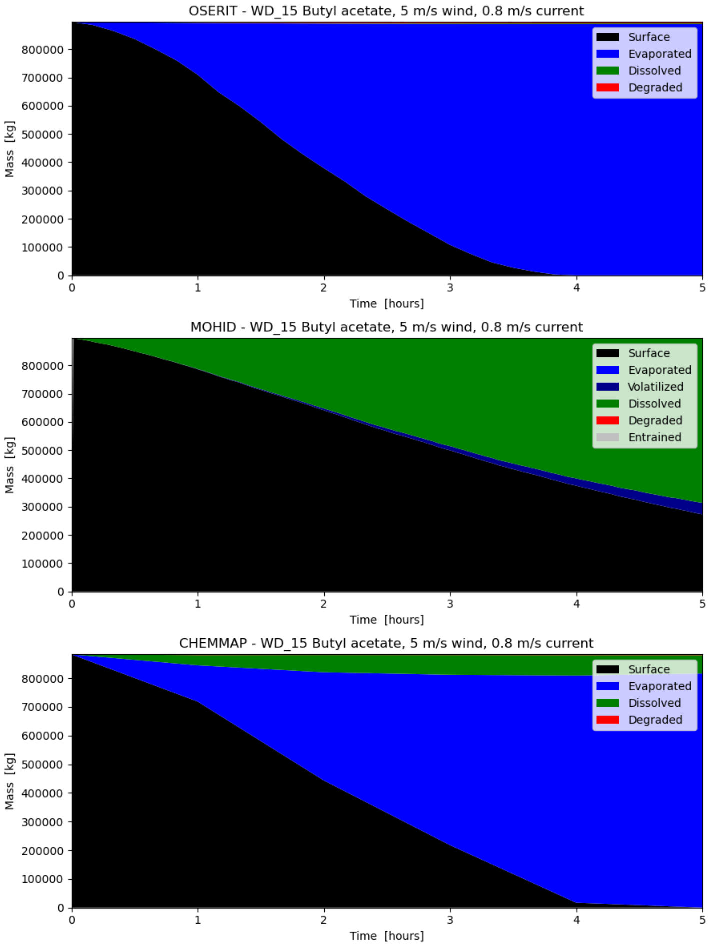

Figure 27: Mass balance for the first 5 hours for the weathering drift testcase 15. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Butyl acetate, the wind is of 5 m/s and the current of 0.8 m/s

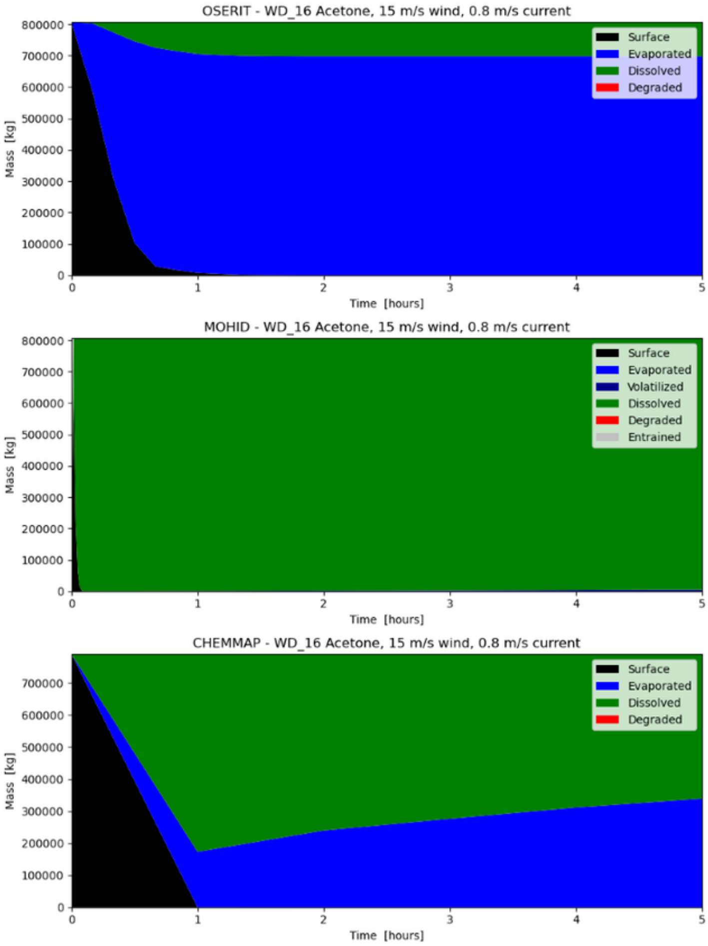

Figure 28 : Mass balance for the first 5 hours for the weathering drift testcase 16. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Acetone, the wind is of 15 m/s and the current of 0.8 m/s

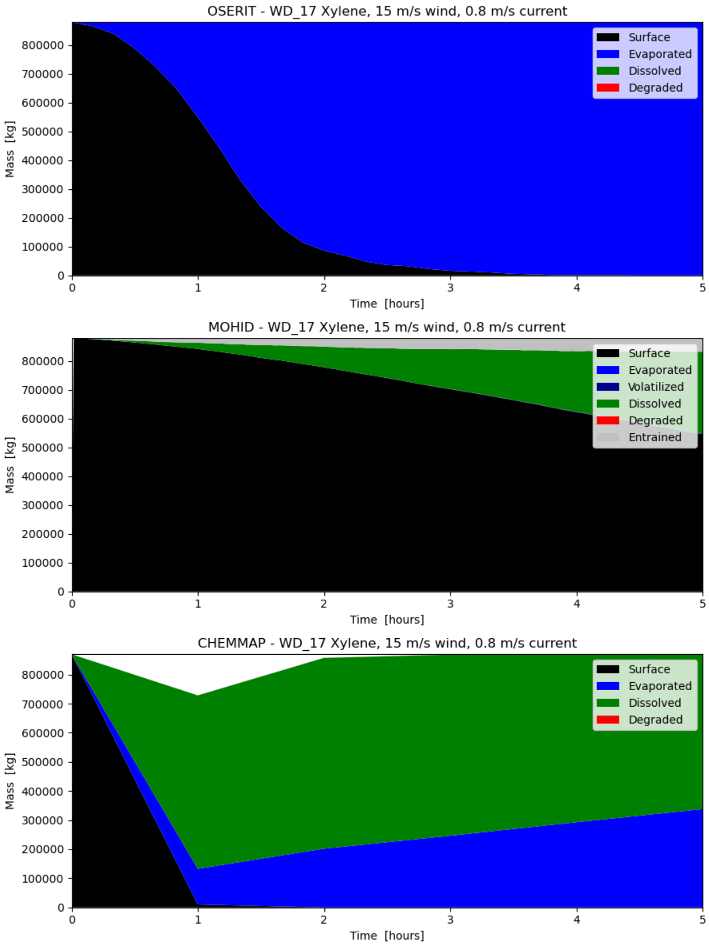

Figure 29 : Mass balance for the first 5 hours for the weathering drift testcase 17. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Xylene, the wind is of 15 m/s and the current of 0.8 m/s

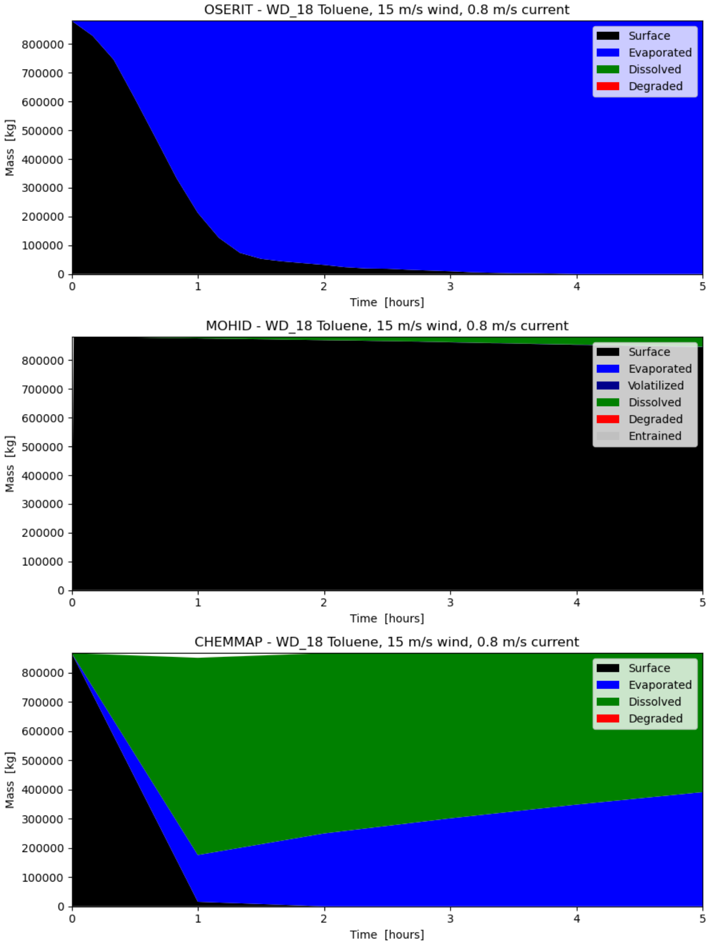

Figure 30 : Mass balance for the first 5 hours for the weathering drift testcase 18. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Toluene, the wind is of 15 m/s and the current of 0.8 m/s

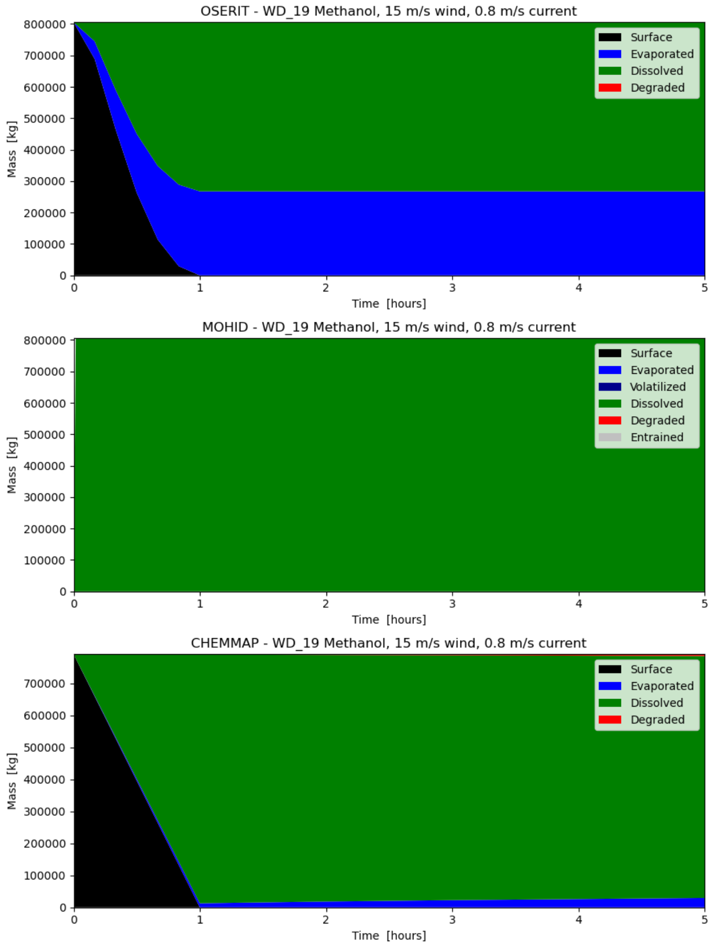

Figure 31 : Mass balance for the first 5 hours for the weathering drift testcase 19. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Methanol, the wind is of 15 m/s and the current of 0.8 m/s

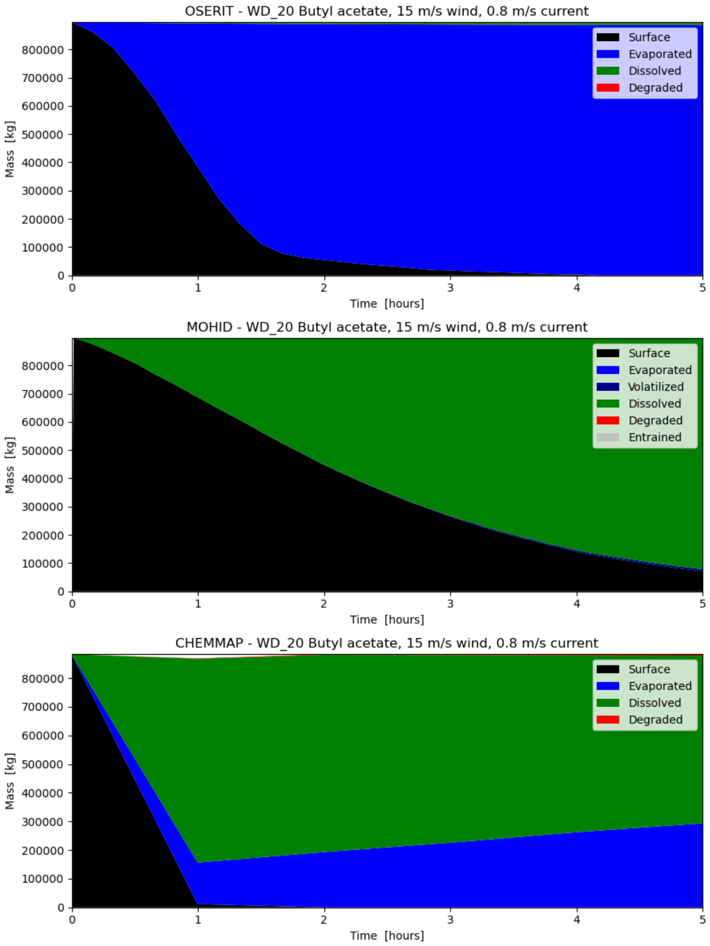

Figure 32 : Mass balance for the first 5 hours for the weathering drift testcase 20. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Butyl acetate, the wind is of 15 m/s and the current of 0.8 m/s

7.2.2. Entire simulation

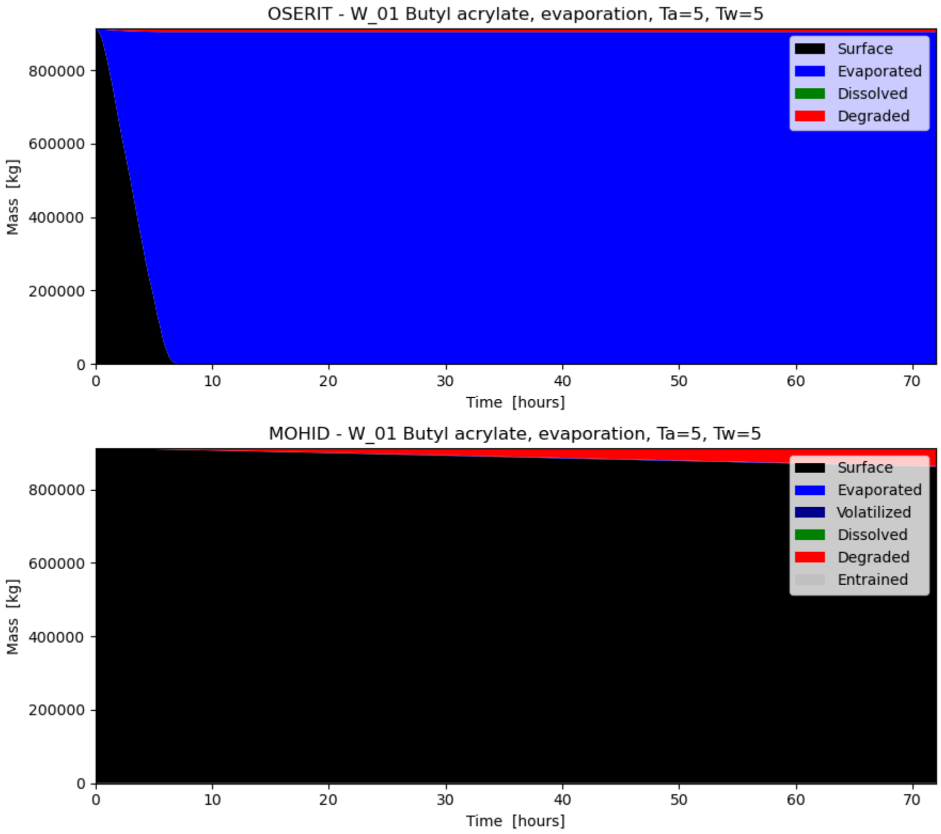

Figure 33 : Mass balance for the entire simulation for the weathering testcase 1. OSERIT is on top and MOHID at the bottom, only the evaporation is activated and the air and water temperature are 5°C

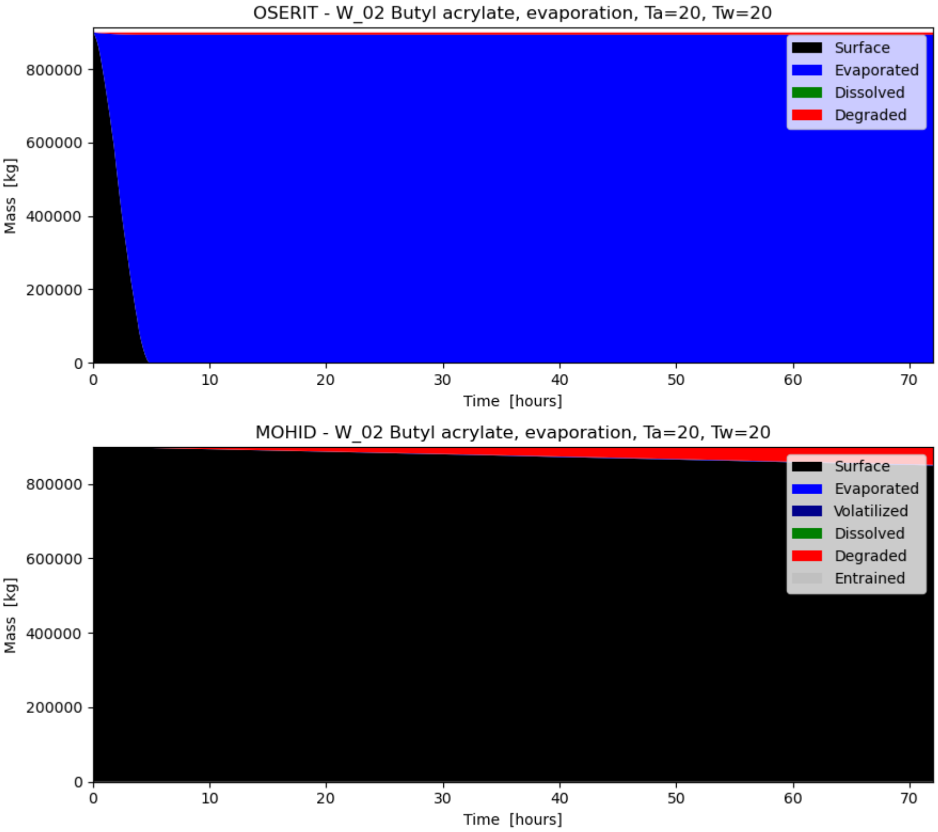

Figure 34 : Mass balance for the entire simulation for the weathering testcase 2. OSERIT is on top and MOHID at the bottom, only the evaporation is activated and the air and water temperature are 20°C

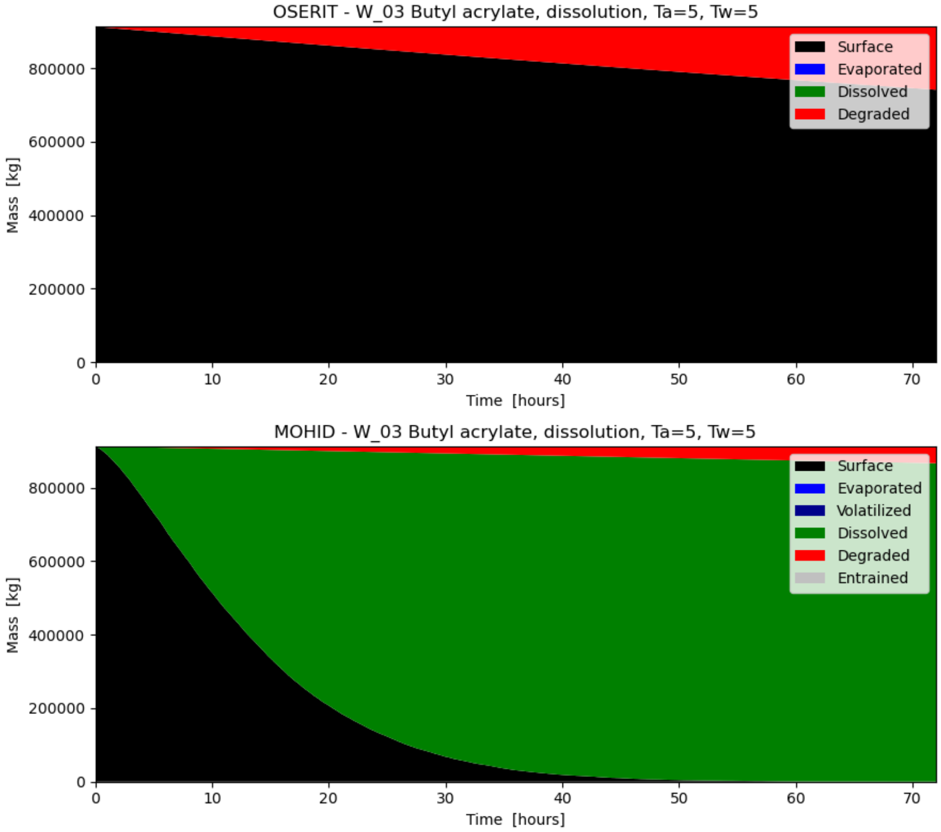

Figure 35 : Mass balance for the entire simulation for the weathering testcase 3. OSERIT is on top and MOHID at the bottom, only the dissolution is activated and the air and water temperature are 5°C

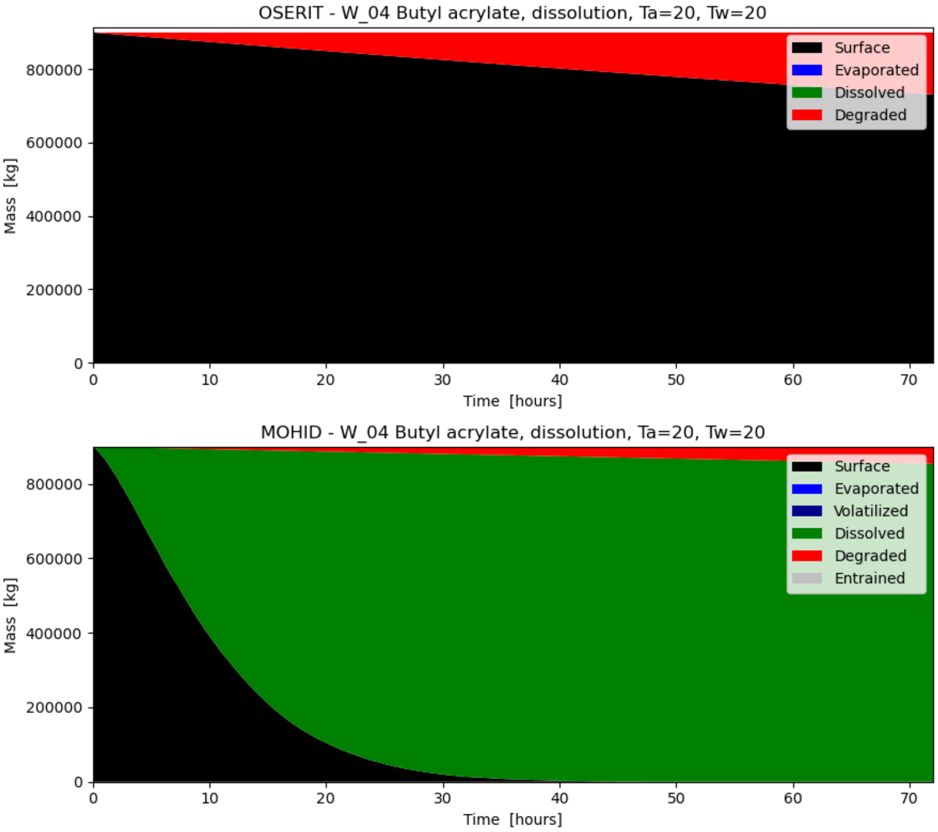

Figure 36 : Mass balance for the entire simulation for the weathering testcase 4. OSERIT is on top and MOHID at the bottom, only the dissolution is activated and the air and water temperature are 20°C

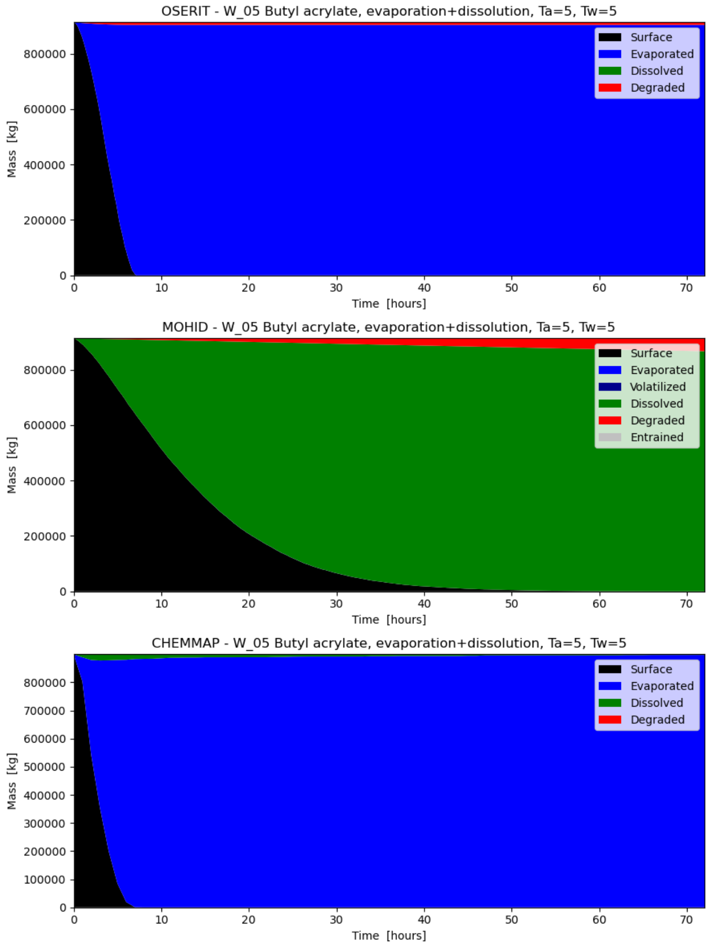

Figure 37 : Mass balance for the entire simulation for the weathering testcase 5. OSERIT is on top and MOHID in the middle and CHEMMAP at the bottom, the dissolution and the evaporation are activated and the air and water temperature are 5°C

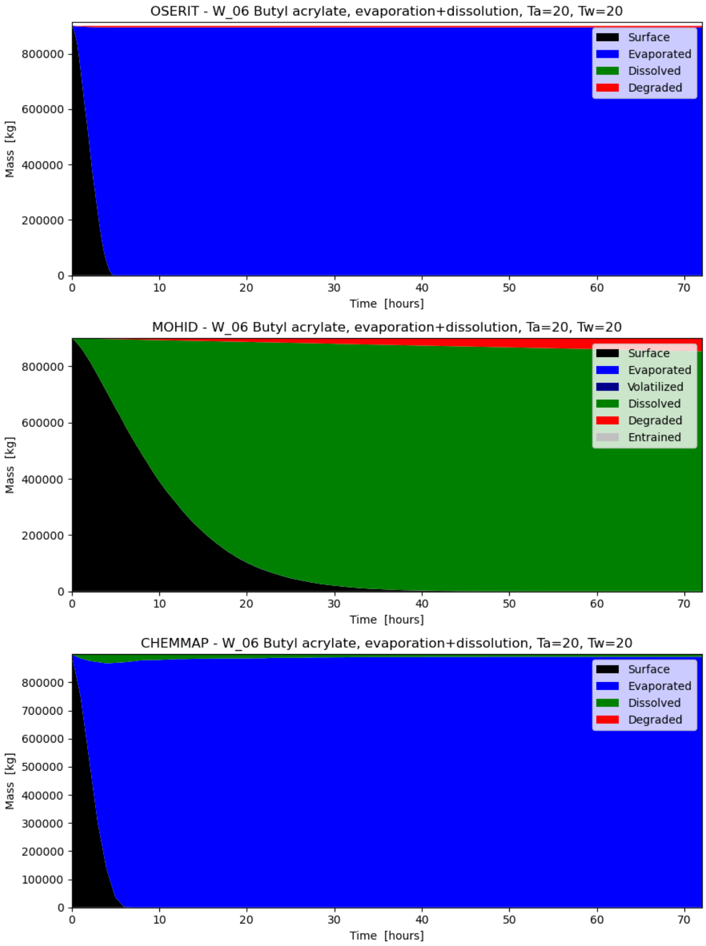

Figure 38 : Mass balance for the entire simulation for the weathering testcase 6. OSERIT is on top and MOHID in the middle and CHEMMAP at the bottom, the dissolution and the evaporation are activated and the air and water temperature are 20°C

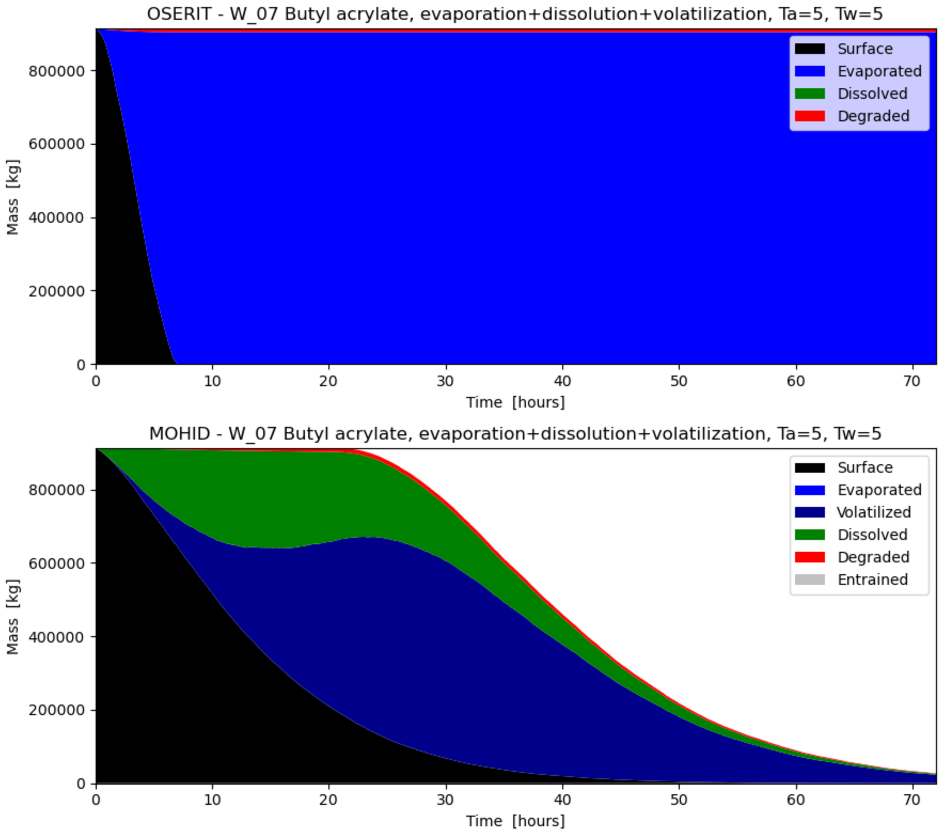

Figure 39 : Mass balance for the entire simulation for the weathering testcase 7. OSERIT is on top and MOHID at the bottom, the dissolution, volatilization and the evaporation are activated and the air and water temperature are 5°C

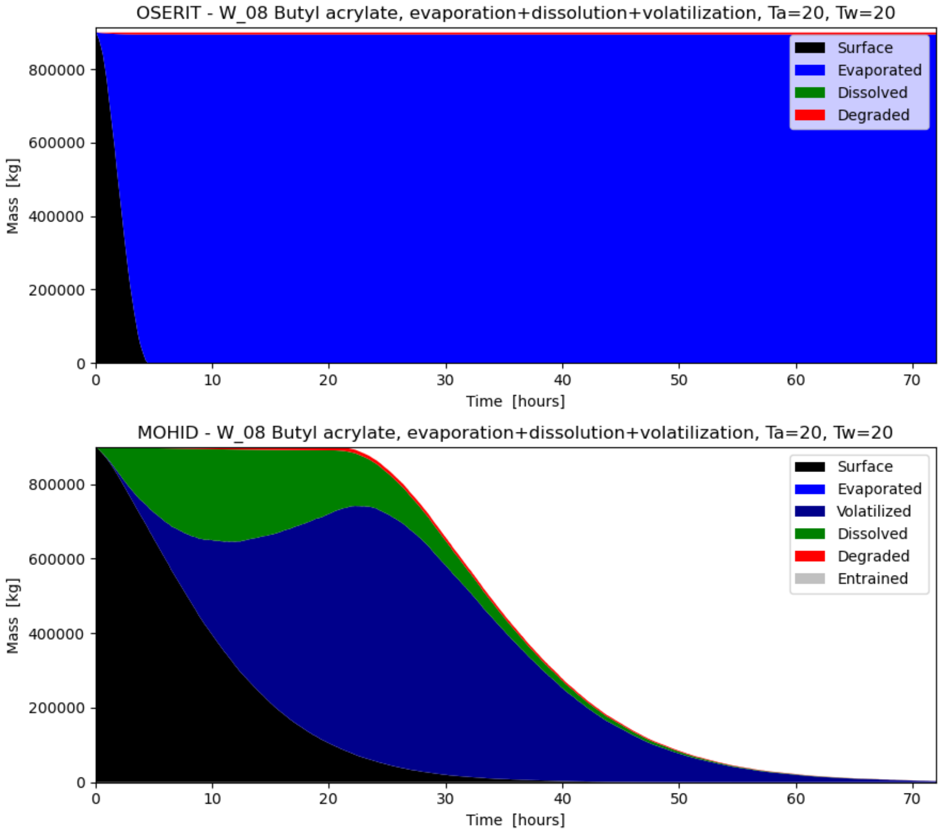

Figure 40 : Mass balance for the entire simulation for the weathering testcase 8. OSERIT is on top and MOHID at the bottom, the dissolution, volatilization and the evaporation are activated and the air and water temperature are 20°C

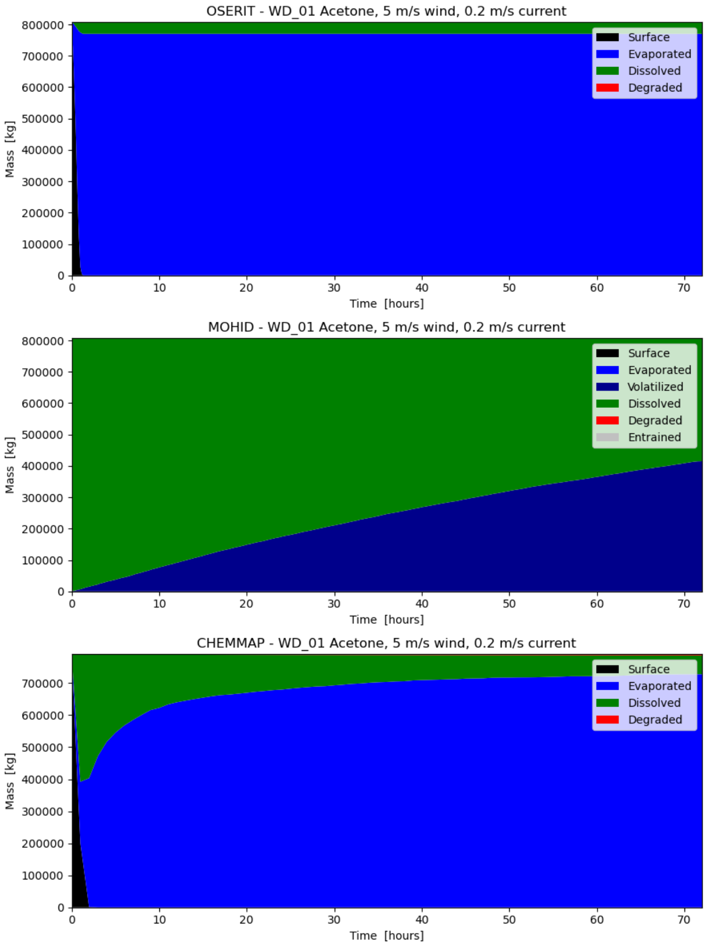

Figure 41 : Mass balance for the entire simulation for the weathering drift testcase 1. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Acetone, the wind is of 5 m/s and the current of 0.2 m/s

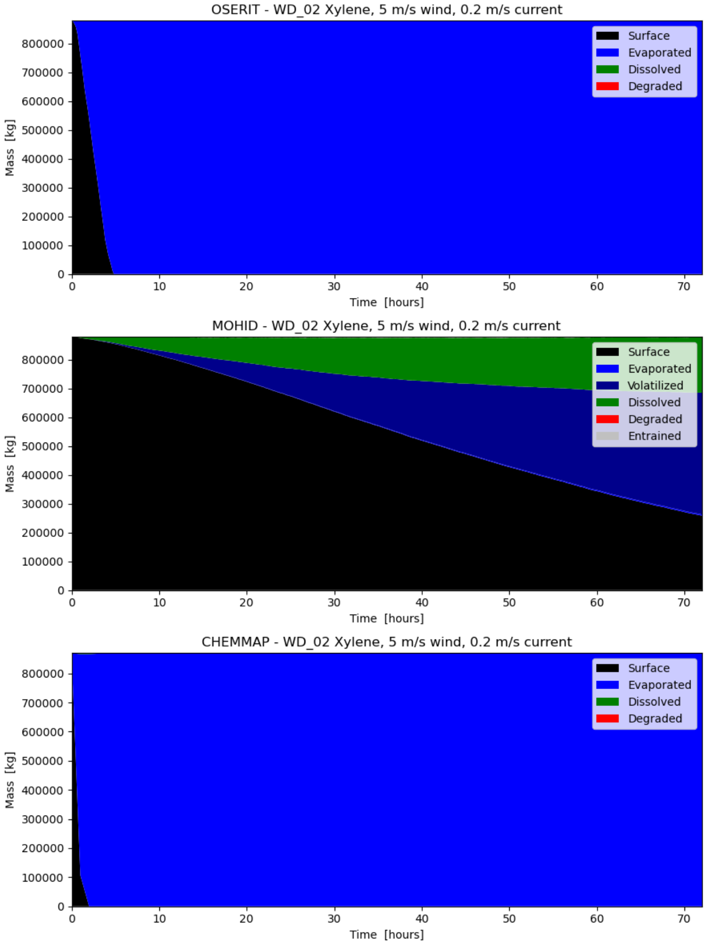

Figure 42 : Mass balance for the entire simulation for the weathering drift testcase 2. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Xylene, the wind is of 5 m/s and the current of 0.2 m/s

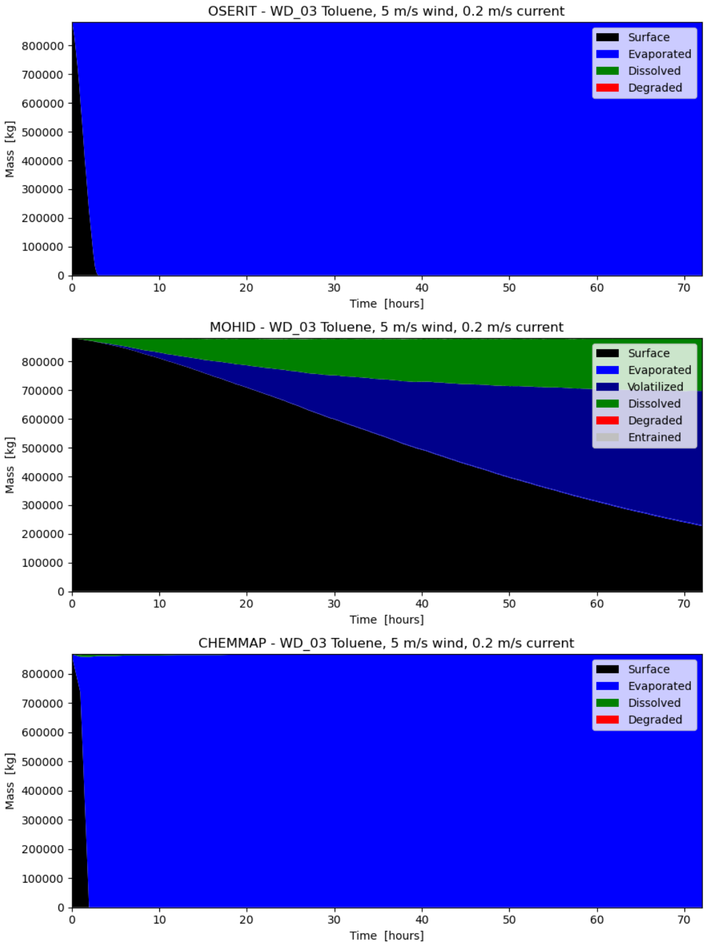

Figure 43 : Mass balance for the entire simulation for the weathering drift testcase 3. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Toluene, the wind is of 5 m/s and the current of 0.2 m/s

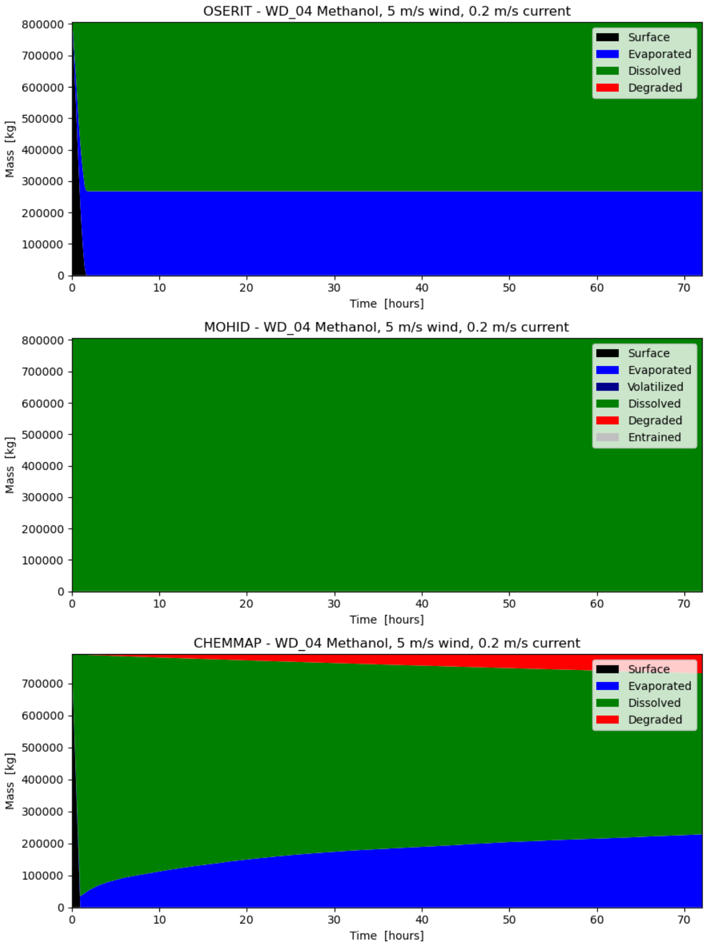

Figure 44 : Mass balance for the entire simulation for the weathering drift testcase 4. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Methanol, the wind is of 5 m/s and the current of 0.2 m/s

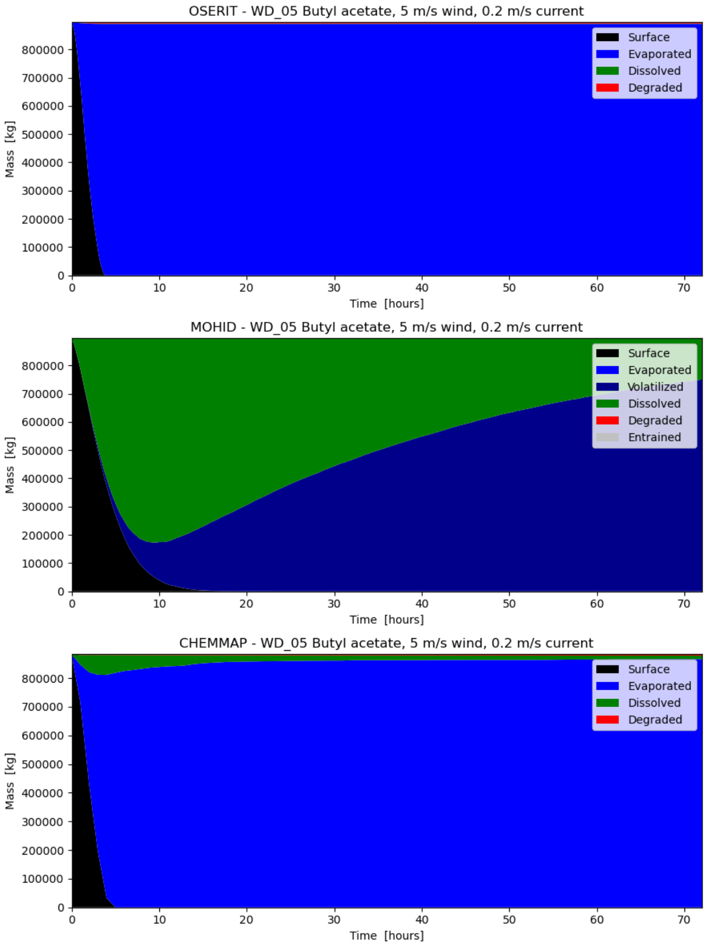

Figure 45 : Mass balance for the entire simulation for the weathering drift testcase 5. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Butyl acetate, the wind is of 5 m/s and the current of 0.2 m/s

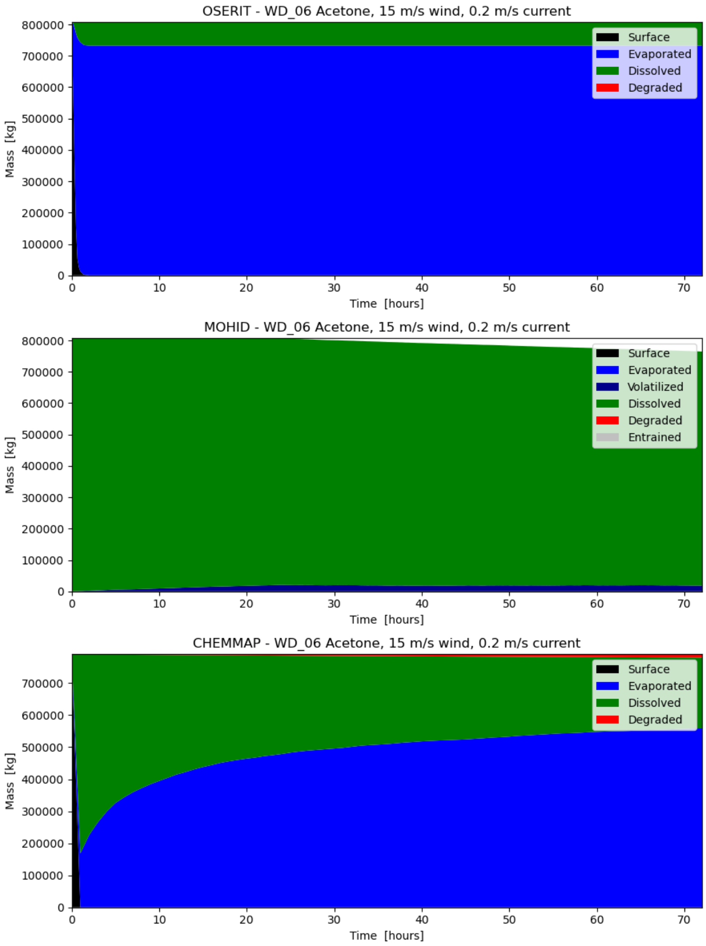

Figure 46 : Mass balance for the entire simulation for the weathering drift testcase 6. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Acetone, the wind is of 15 m/s and the current of 0.2 m/s

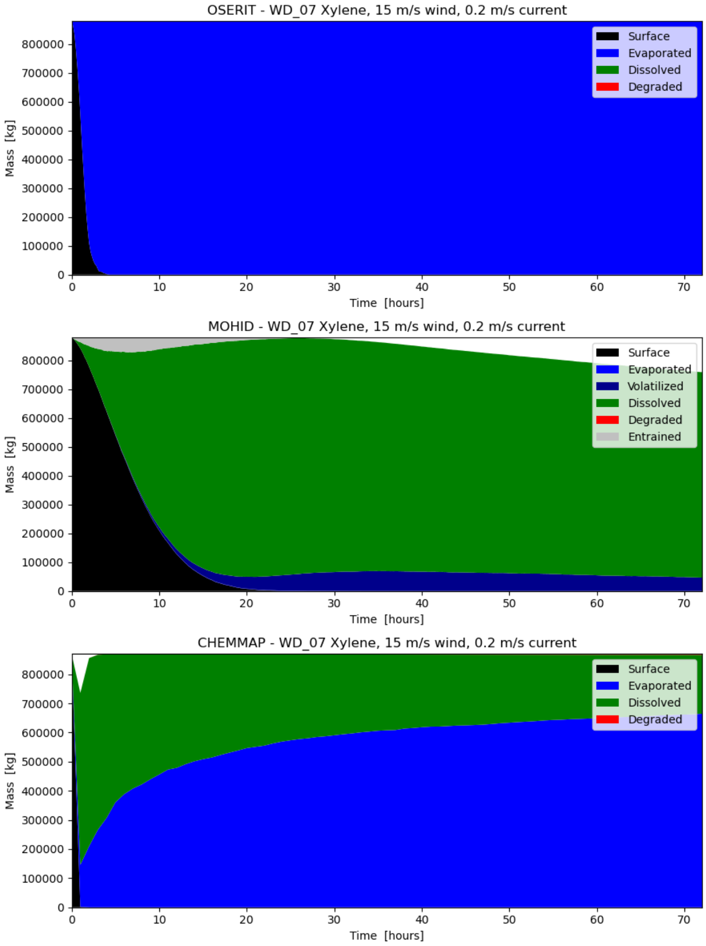

Figure 47 : Mass balance for the entire simulation for the weathering drift testcase 7. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Xylene, the wind is of 15 m/s and the current of 0.2 m/s

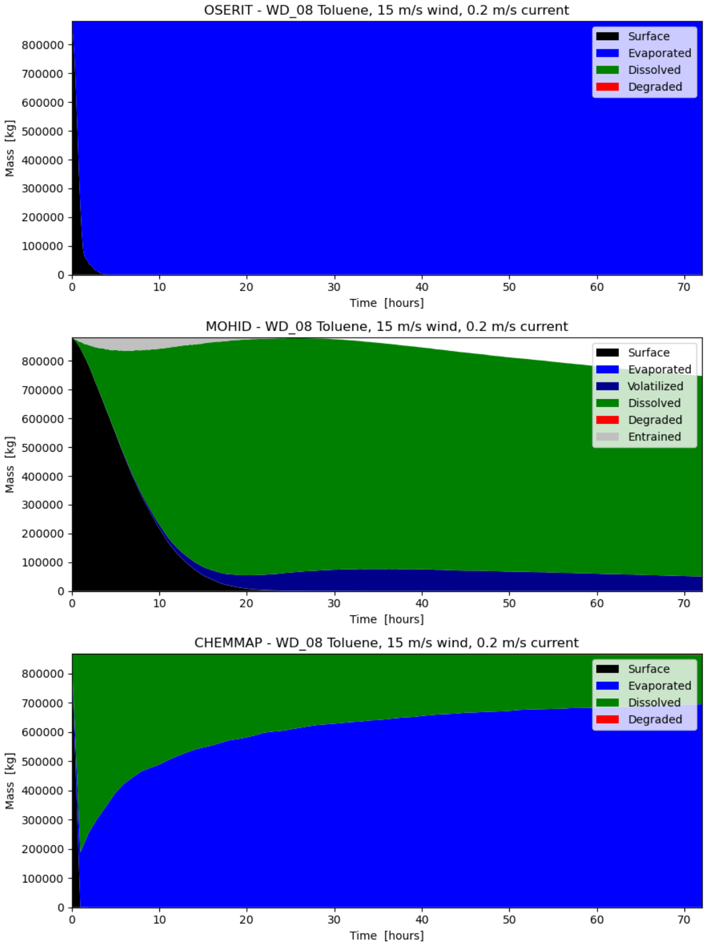

Figure 48 : Mass balance for the entire simulation for the weathering drift testcase 8. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Toluene, the wind is of 15 m/s and the current of 0.2 m/s

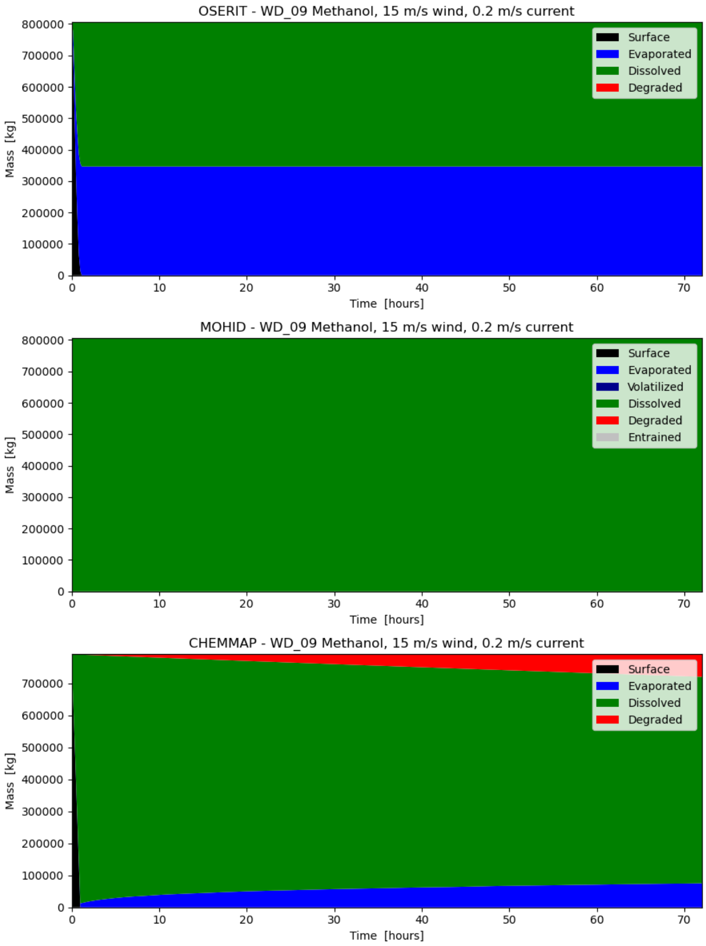

Figure 49 : Mass balance for the entire simulation for the weathering drift testcase 9. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Methanol, the wind is of 15 m/s and the current of 0.2 m/s

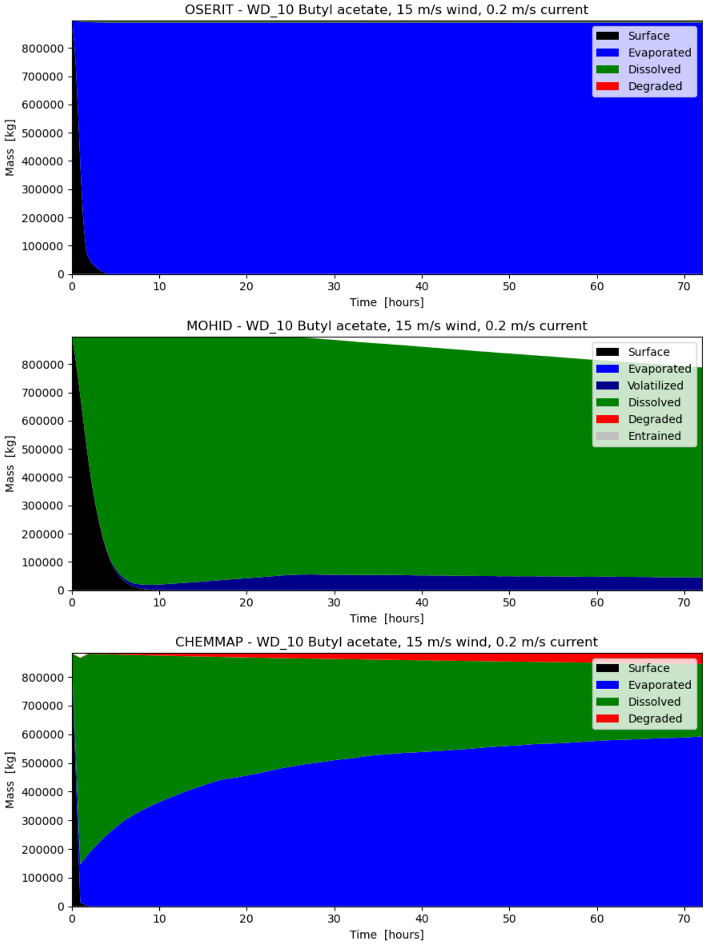

Figure 50 : Mass balance for the entire simulation for the weathering drift testcase 10. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Butyl acetate, the wind is of 15 m/s and the current of 0.2 m/s

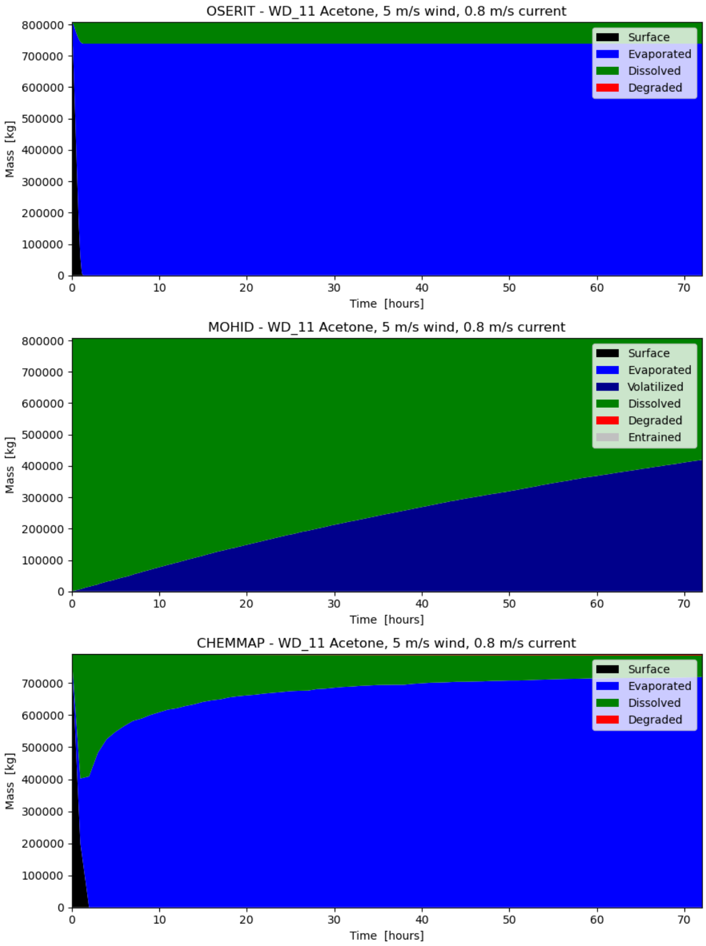

Figure 51 : Mass balance for the entire simulation for the weathering drift testcase 11. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Acetone, the wind is of 5 m/s and the current of 0.8 m/s

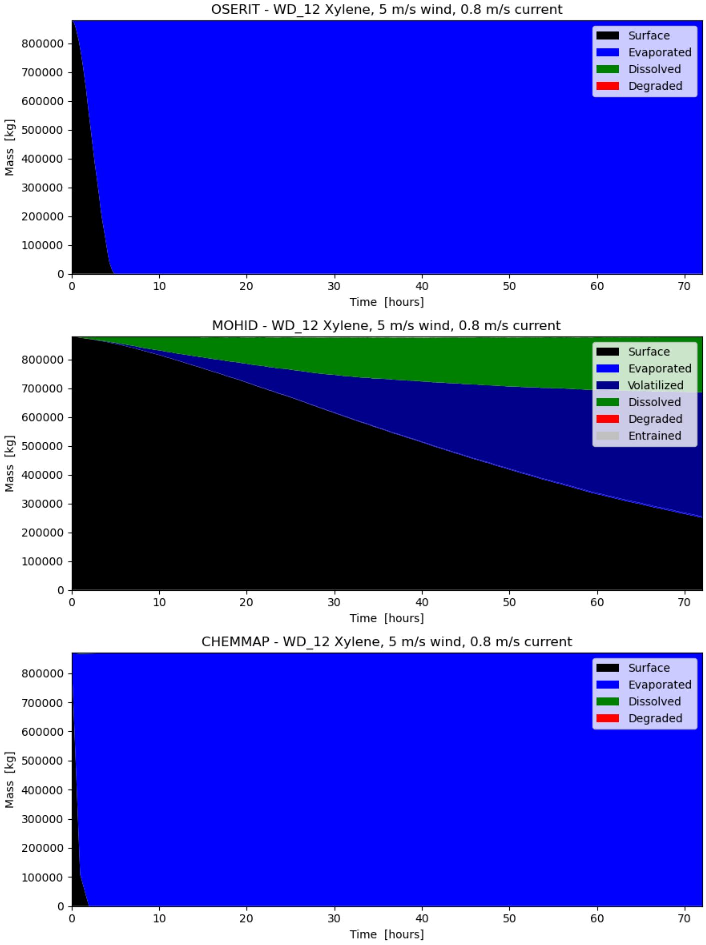

Figure 52 : Mass balance for the entire simulation for the weathering drift testcase 12. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Xylene, the wind is of 5 m/s and the current of 0.8 m/s

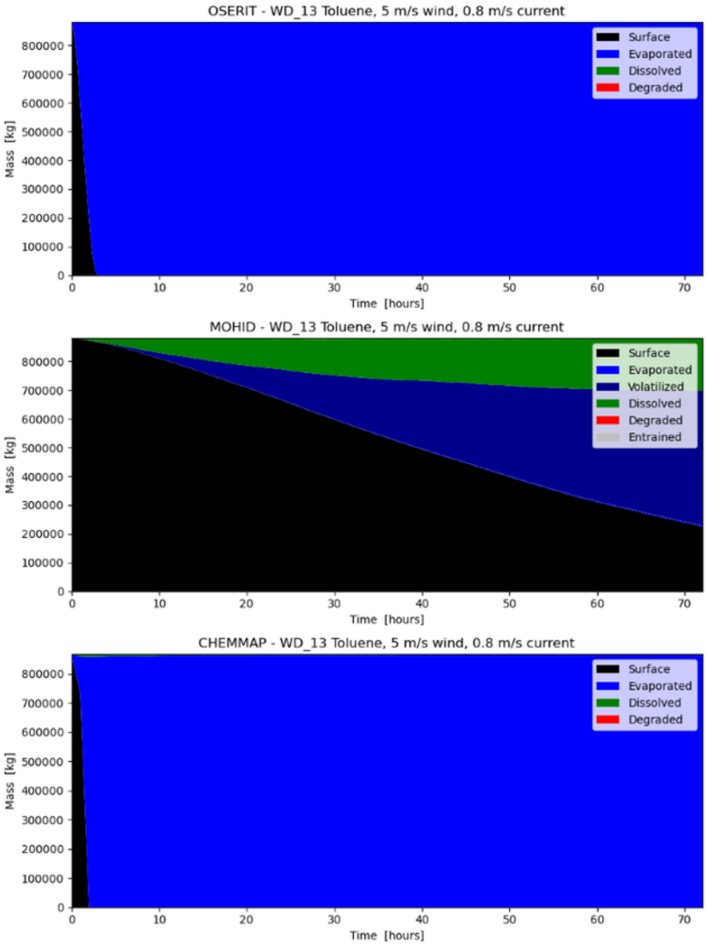

Figure 53 : Mass balance for the entire simulation for the weathering drift testcase 13. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Toluene, the wind is of 5 m/s and the current of 0.8 m/s

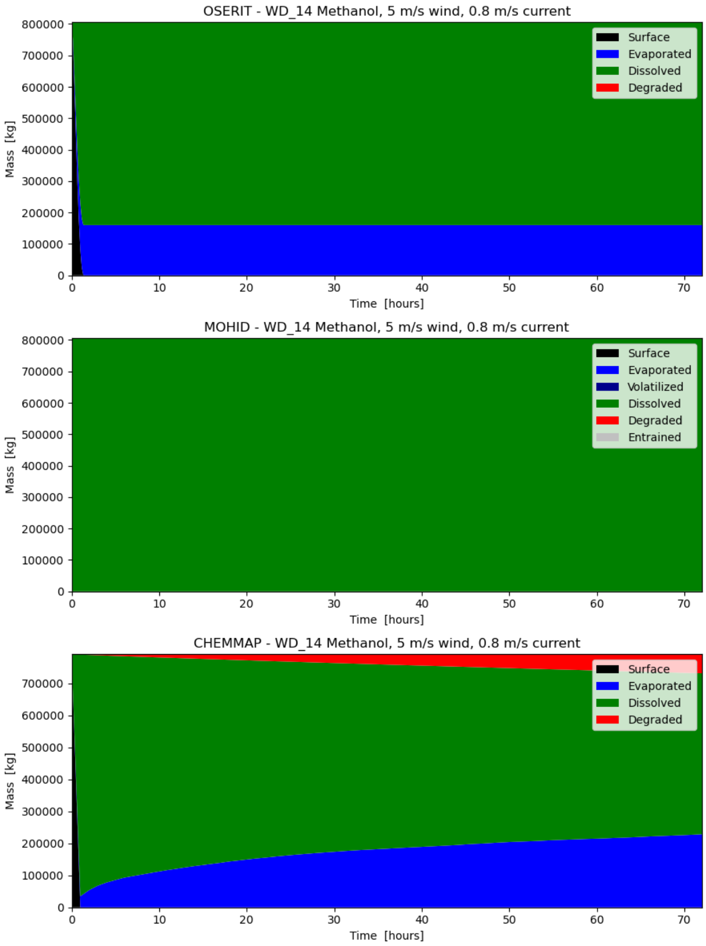

Figure 54 : Mass balance for the first 5 hours for the weathering drift testcase 14. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Methanol, the wind is of 5 m/s and the current of 0.8 m/s

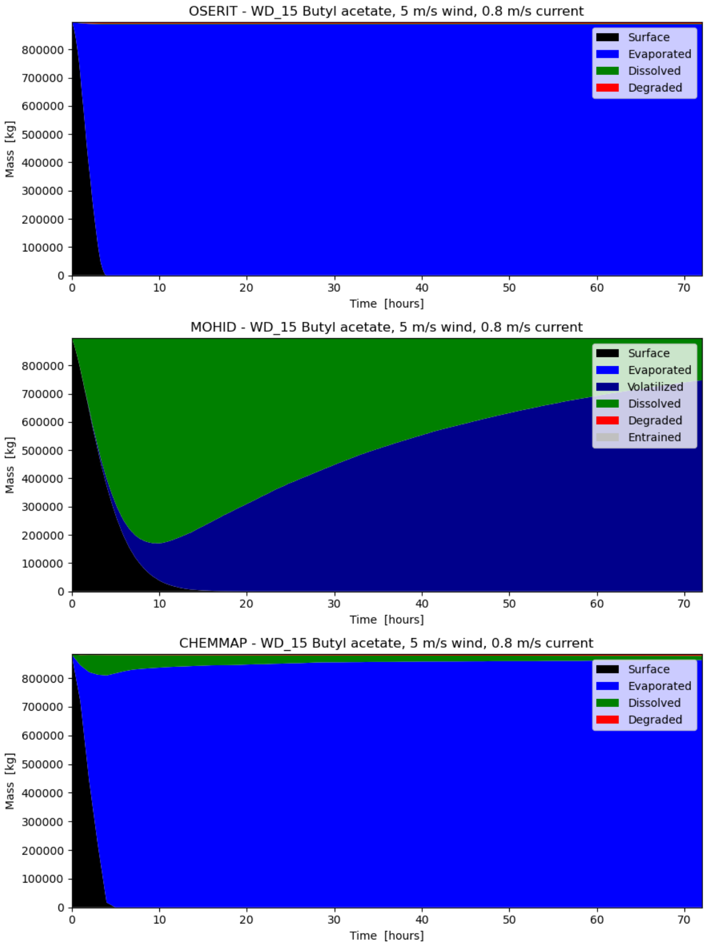

Figure 55 : Mass balance for the entire simulation for the weathering drift testcase 15. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Butyl acetate, the wind is of 5 m/s and the current of 0.8 m/s

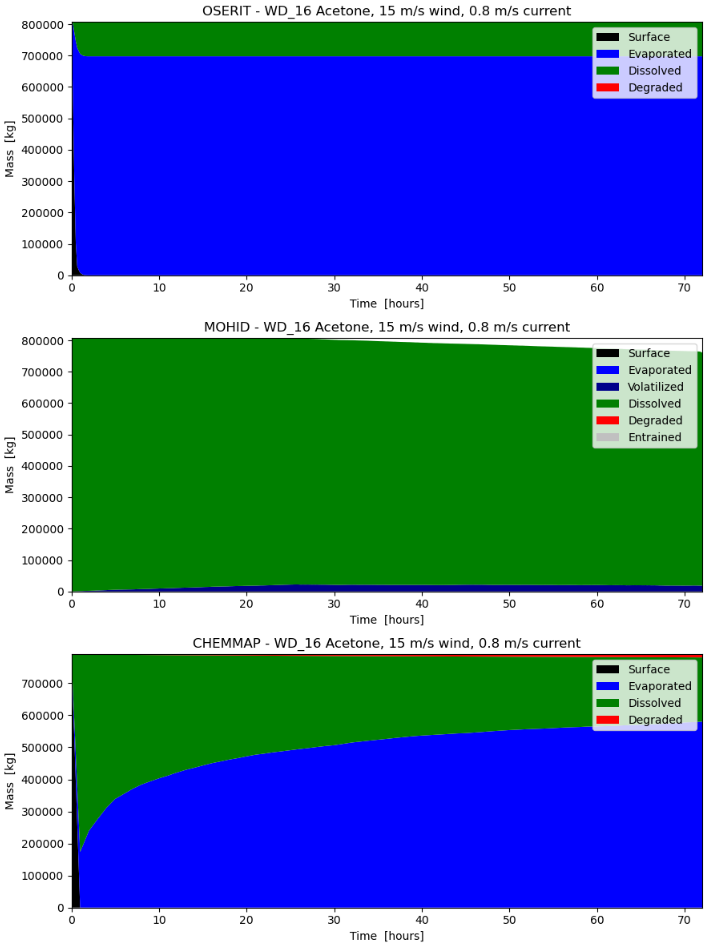

Figure 56 : Mass balance for the entire simulation for the weathering drift testcase 16. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Acetone, the wind is of 15 m/s and the current of 0.8 m/s

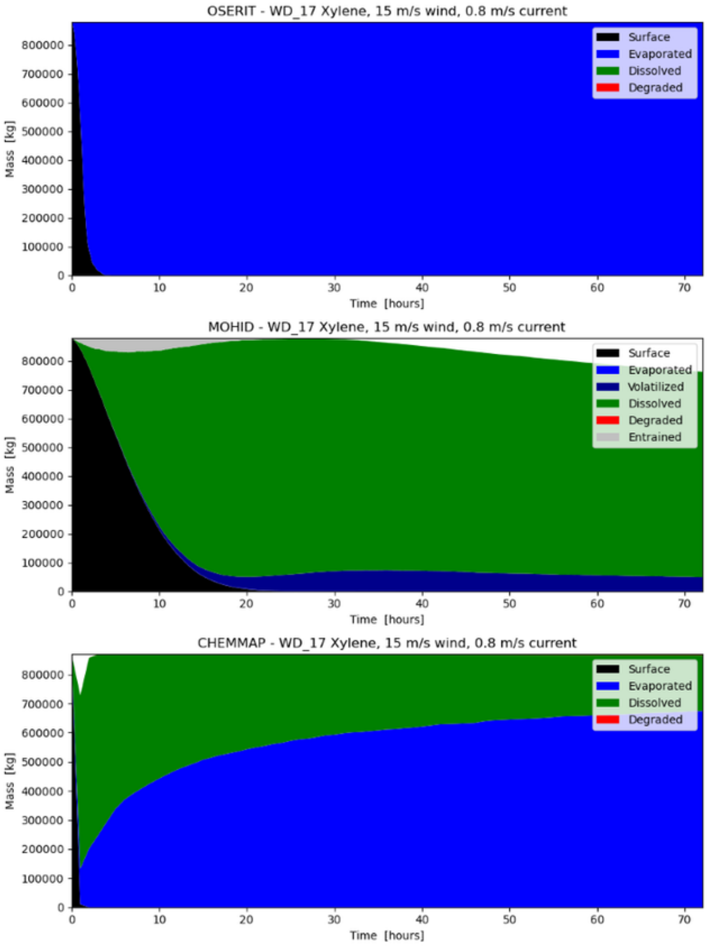

Figure 57 : Mass balance for the entire simulation for the weathering drift testcase 17. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Xylene, the wind is of 15 m/s and the current of 0.8 m/s

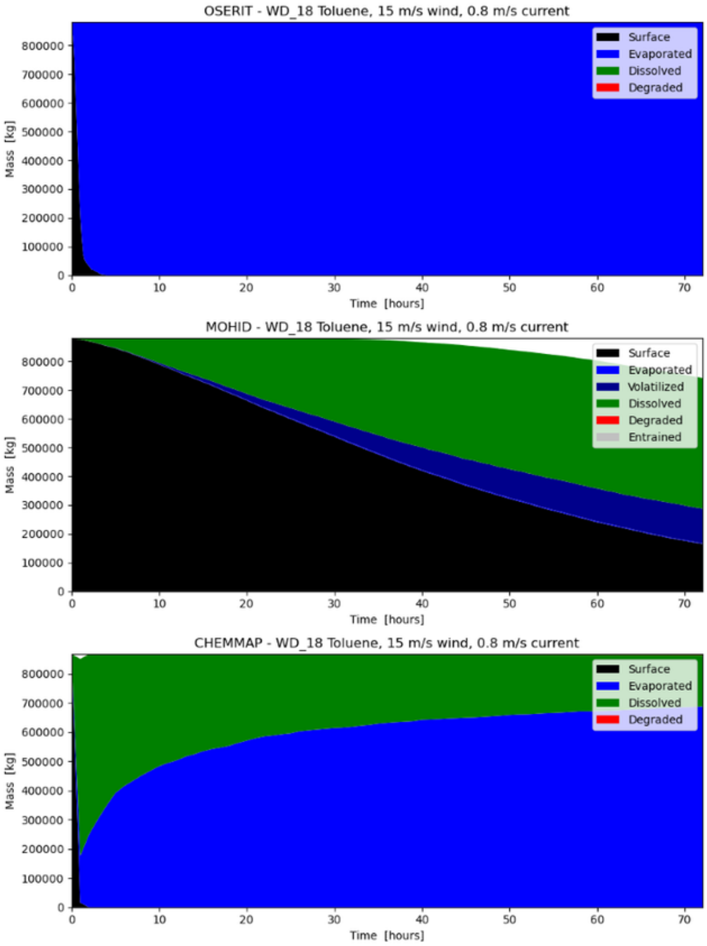

Figure 58 : Mass balance for the entire simulation for the weathering drift testcase 18. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Toluene, the wind is of 15 m/s and the current of 0.8 m/s

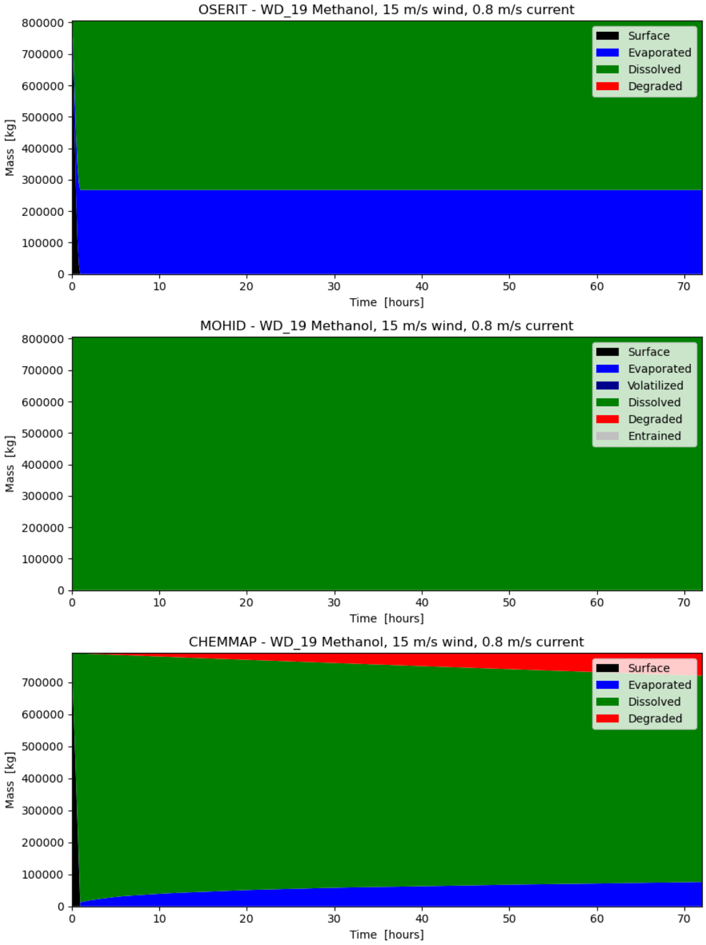

Figure 59 : Mass balance for the entire simulation for the weathering drift testcase 19. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Methanol, the wind is of 15 m/s and the current of 0.8 m/s

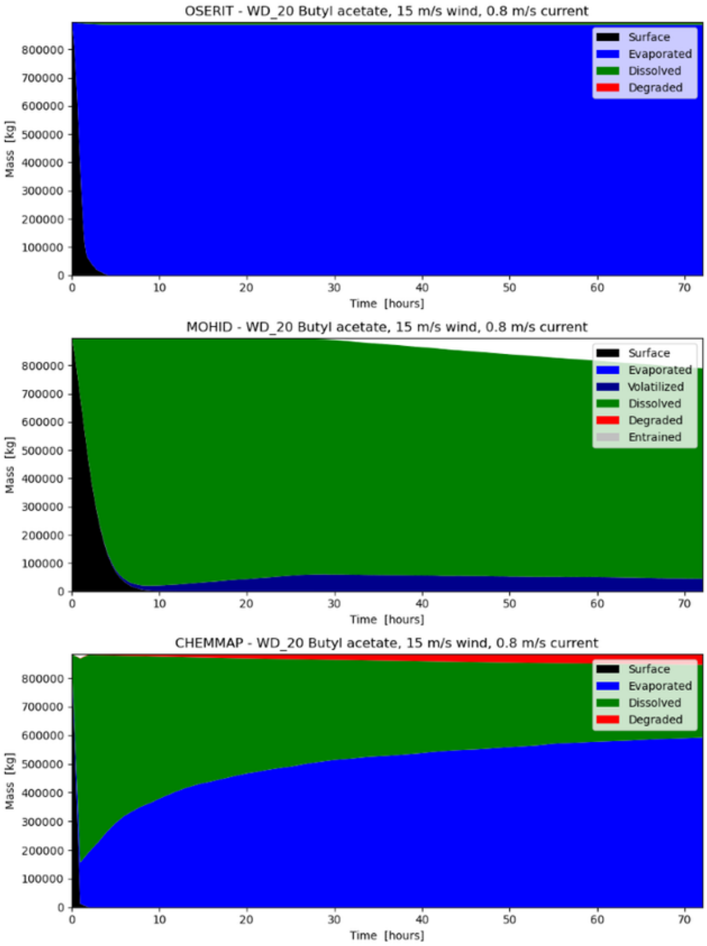

Figure 60 : Mass balance for the entire simulation for the weathering drift testcase 20. OSERIT is on top MOHID at the middle and CHEMMAP at the bottom, the HNS is Butyl acetate, the wind is of 15 m/s and the current of 0.8 m/s

7.3. Area and persistence

Initially, the surface slick area appears to be similar in each of the models for the first few hours. However, as the simulation progresses, differences in how the models compute the area can lead to some variation. Towards the end of the simulation, MOHID generally reports a higher slick area due to the lesser impact of evaporation, while in the absence of evaporation, OSERIT reports a much higher value.

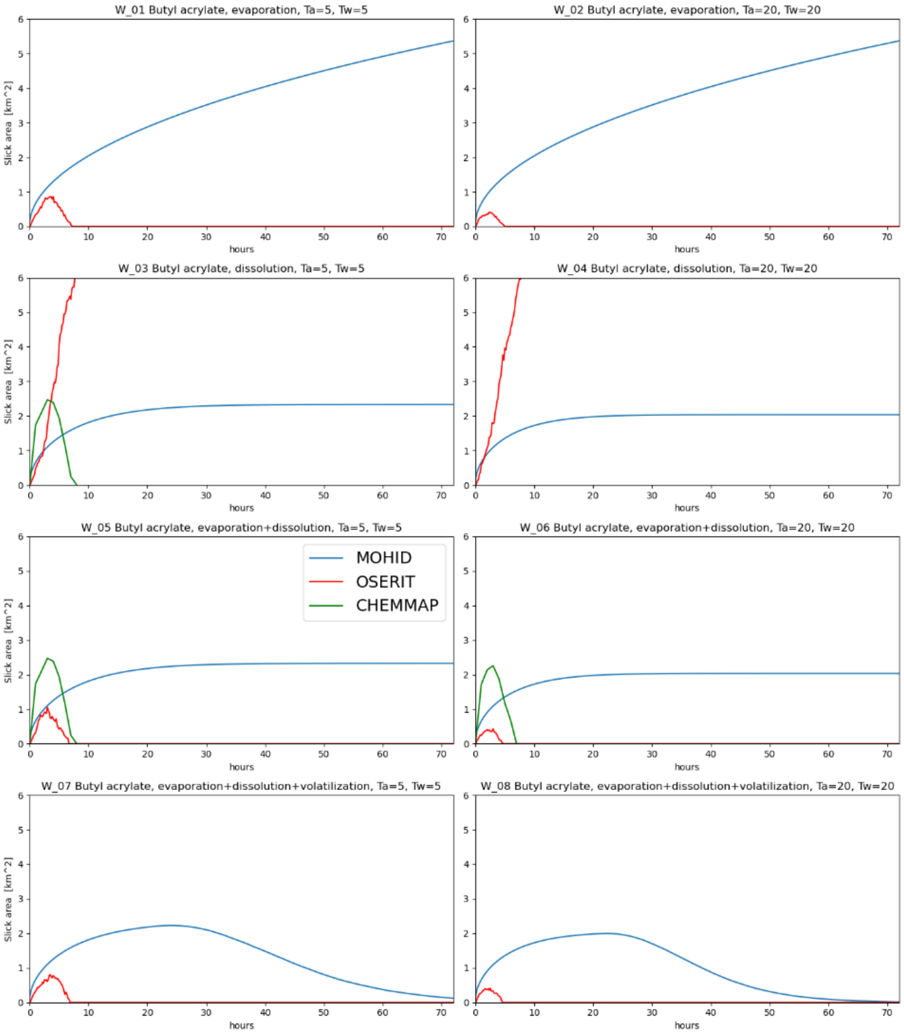

Figure 61 : Area for the slick in the simulations in square kilometers of MOHID (blue), OSERIT (red) and CHEMMAP (green) for the weathering cases. CHEMMAP is only there for the case 3, 5 and 6

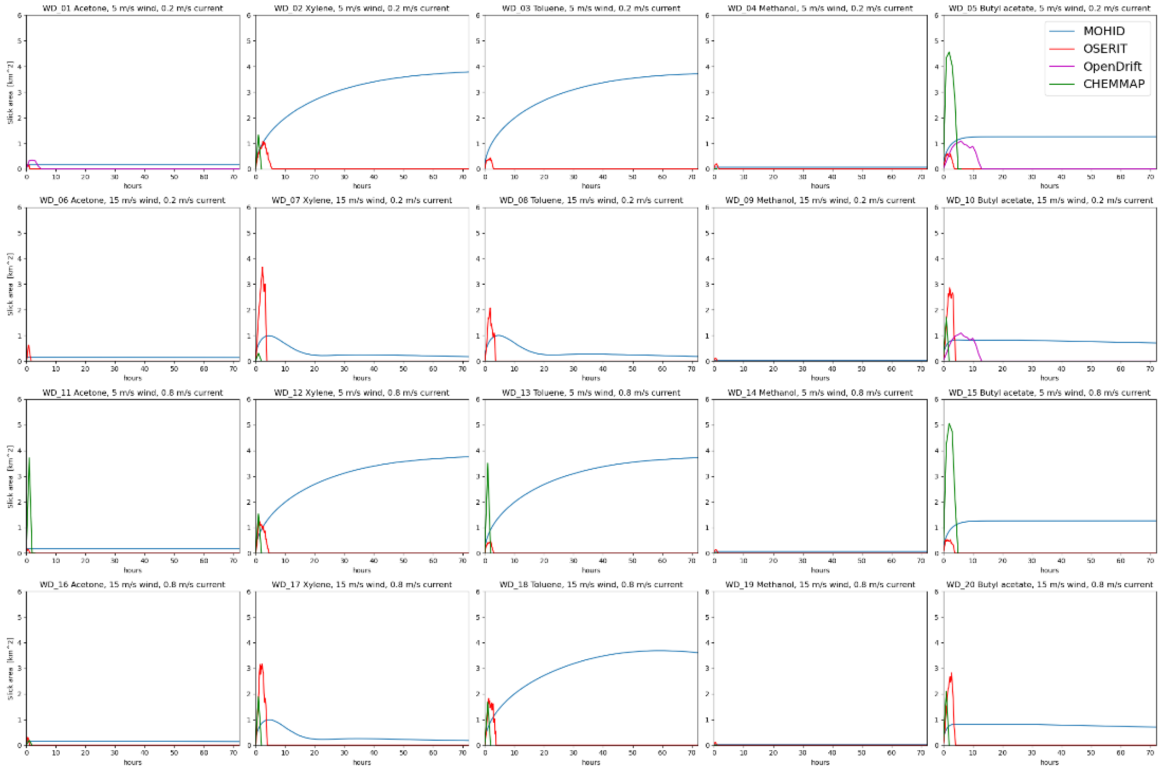

Figure 62 : Area for the slick in the simulations in square kilometers of MOHID (blue), OSERIT (red), OpendDrift (purple) and CHEMMAP (green) for the weathering drift cases

7.4. Drift

As showed in the followings plots, the particles drift in a comparable manner in all models. However, the primary difference lies in the behavior of dissolved particles in MOHID. In the other models, these particles near the surface only follow the current, whereas in MOHID, the wind also has an impact on them. Additionally, the particles in the air drift less far away in MOHID compared to the other models because the domain limits their movement to 2° of longitude.

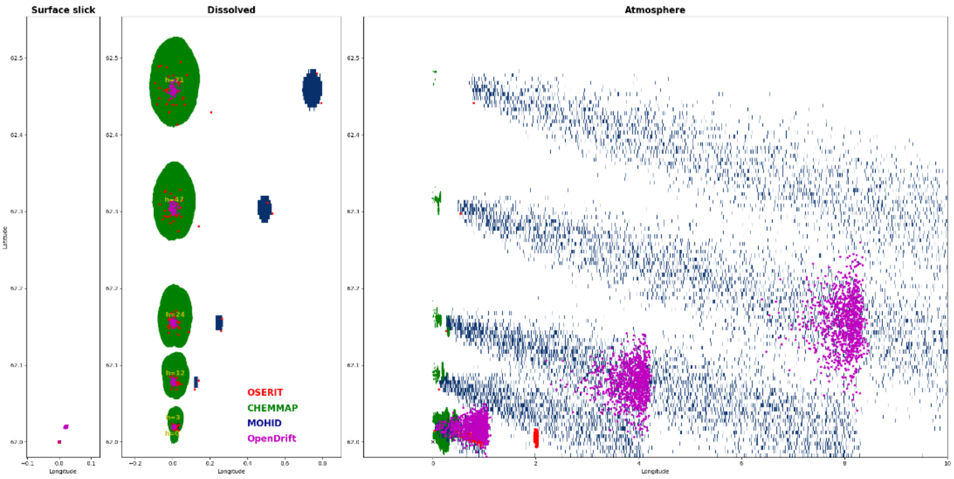

Figure 63 : Drift comparison of OSERIT (red), CHEMMAP (green), MOHID (blue) and OpenDrift (purple) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 1

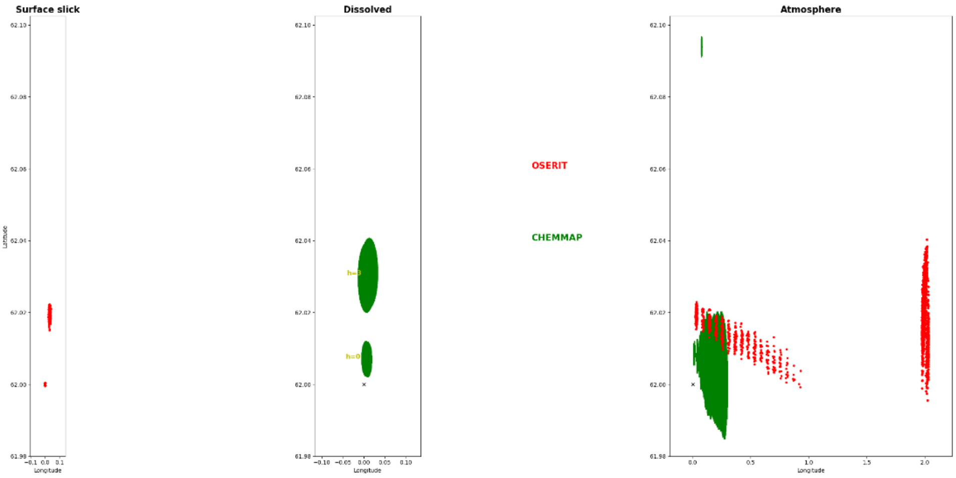

Figure 64 : Drift comparison of OSERIT (red)and CHEMMAP (green) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 2

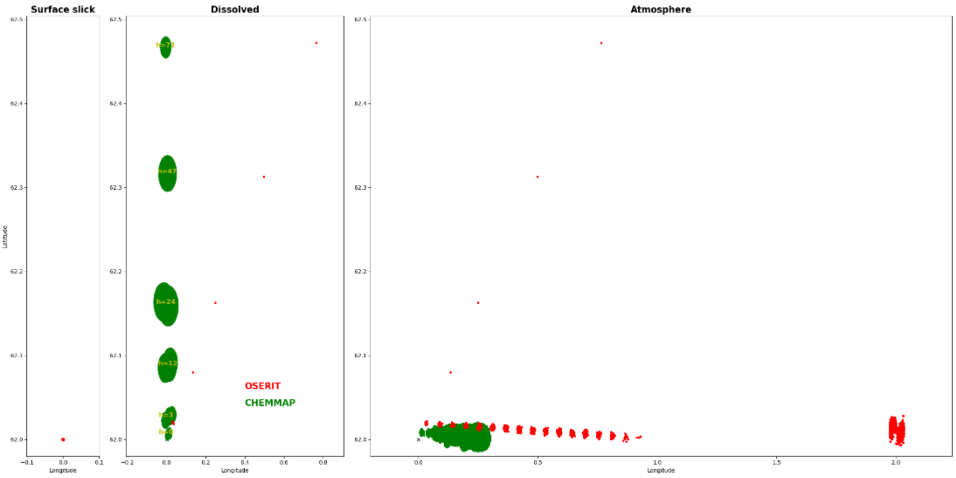

Figure 65 : Drift comparison of OSERIT (red) and CHEMMAP (green) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 3

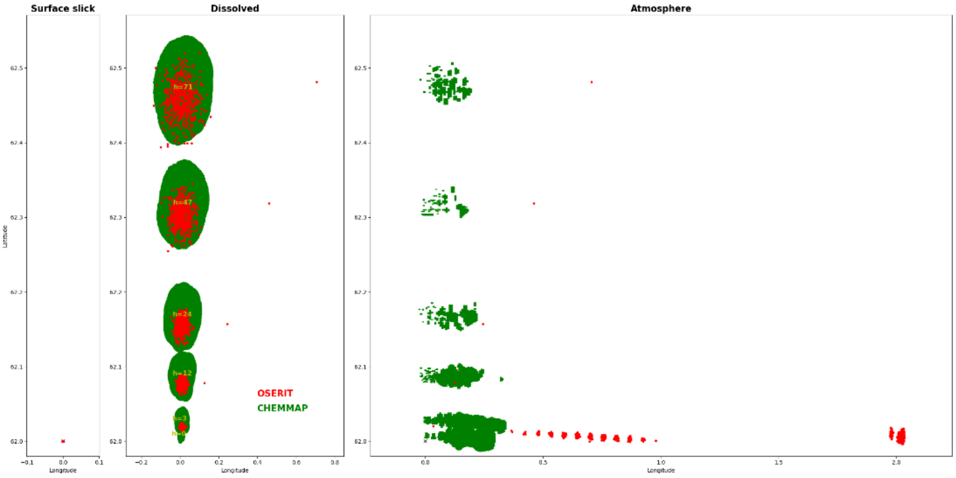

Figure 66 : Drift comparison of OSERIT (red) and CHEMMAP (green) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 4

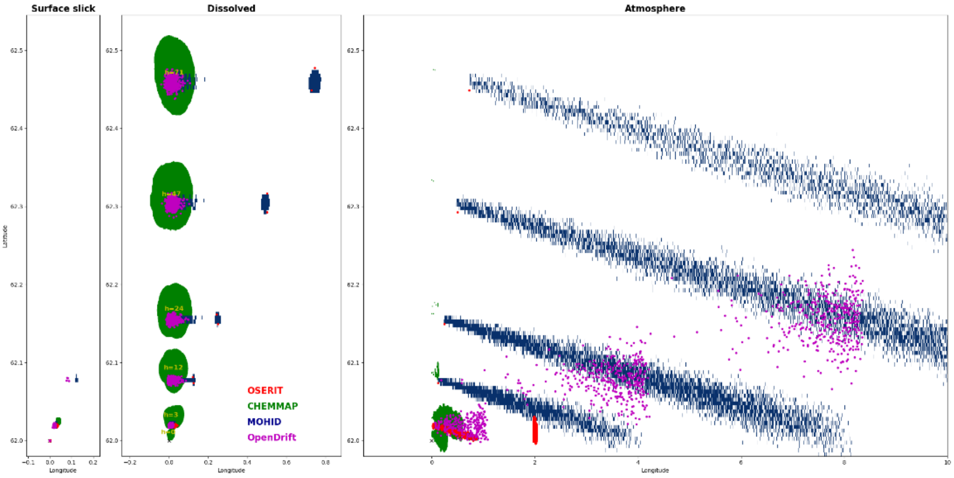

Figure 67 : Drift comparison of OSERIT (red), CHEMMAP (green), MOHID (blue) and OpenDrift (purple) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 5

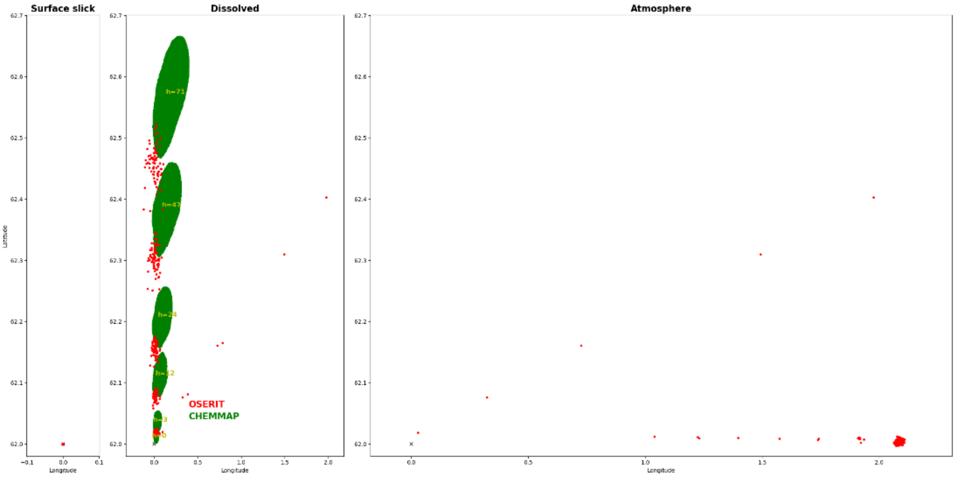

Figure 68 : Drift comparison of OSERIT (red) and CHEMMAP (green) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 6

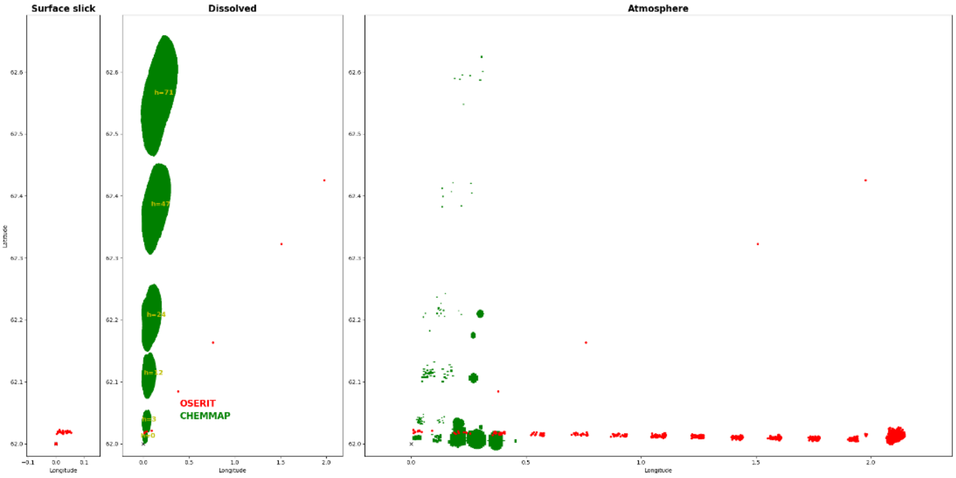

Figure 69 : Drift comparison of OSERIT (red) and CHEMMAP (green) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 7

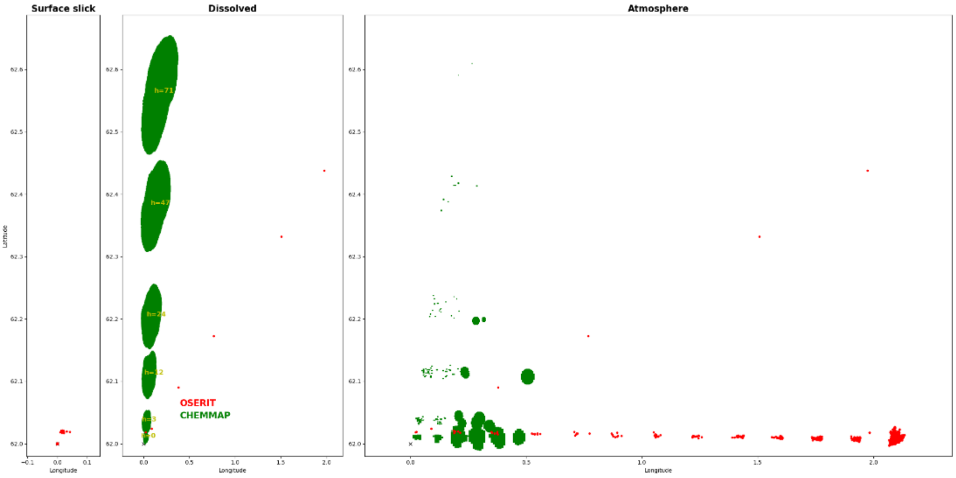

Figure 70 : Drift comparison of OSERIT (red) and CHEMMAP (green) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 8

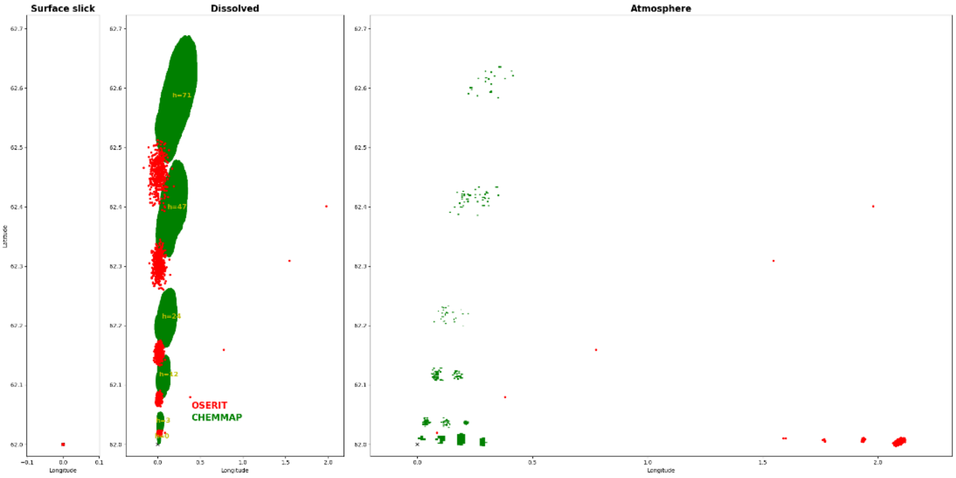

Figure 71 : Drift comparison of OSERIT (red) and CHEMMAP (green) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 9

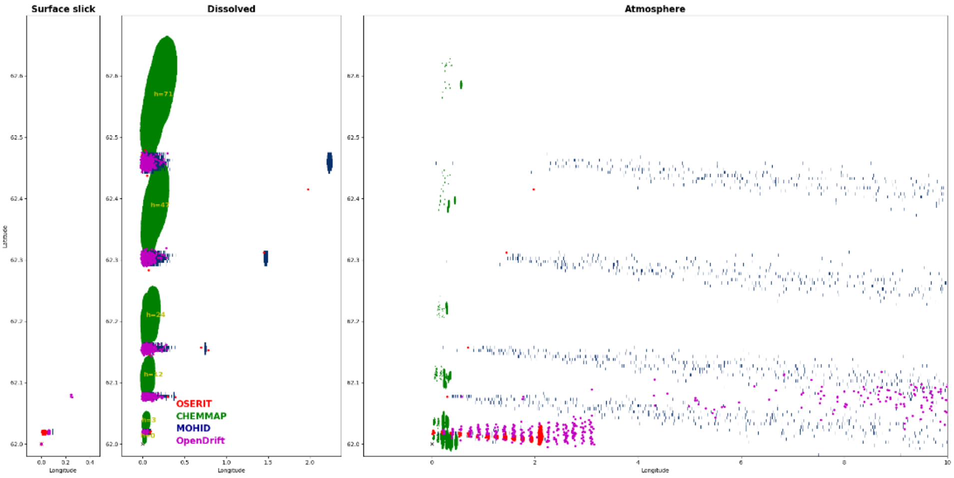

Figure 72 : Drift comparison of OSERIT (red), CHEMMAP (green), MOHID (blue) and OpenDrift (purple) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 10

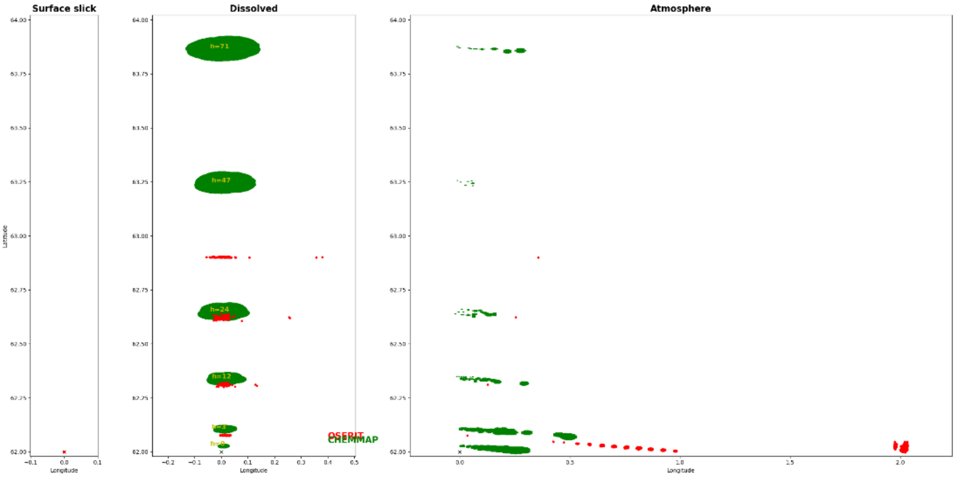

Figure 73 : Drift comparison of OSERIT (red) and CHEMMAP (green) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 11

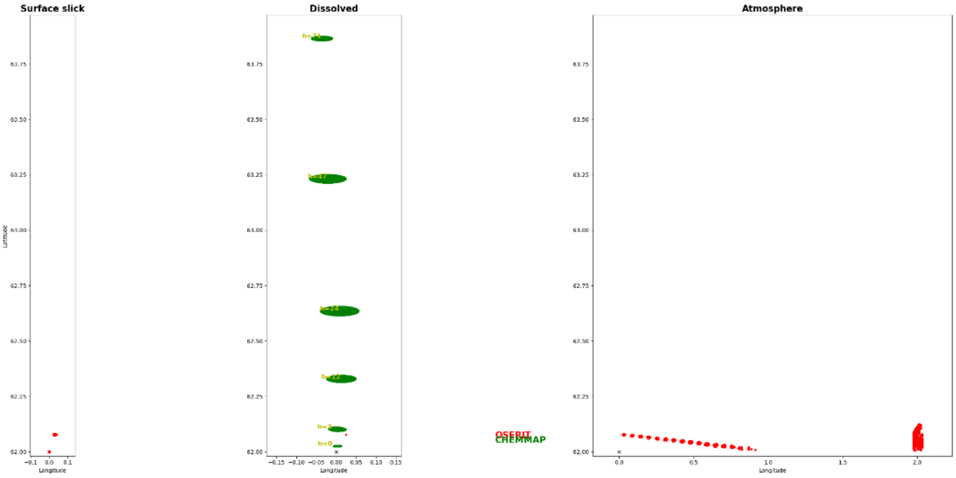

Figure 74 : Drift comparison of OSERIT (red) and CHEMMAP (green) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 12

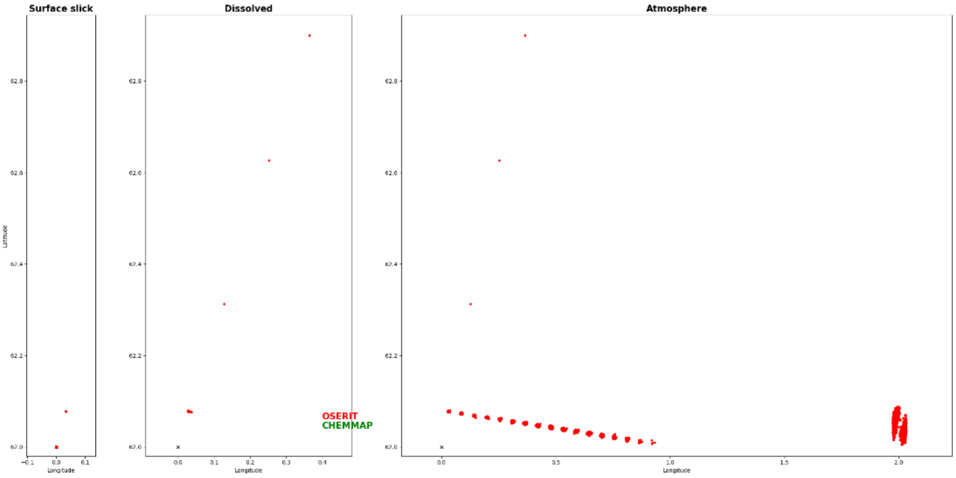

Figure 75 : Drift comparison of OSERIT (red) and CHEMMAP (green) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 13

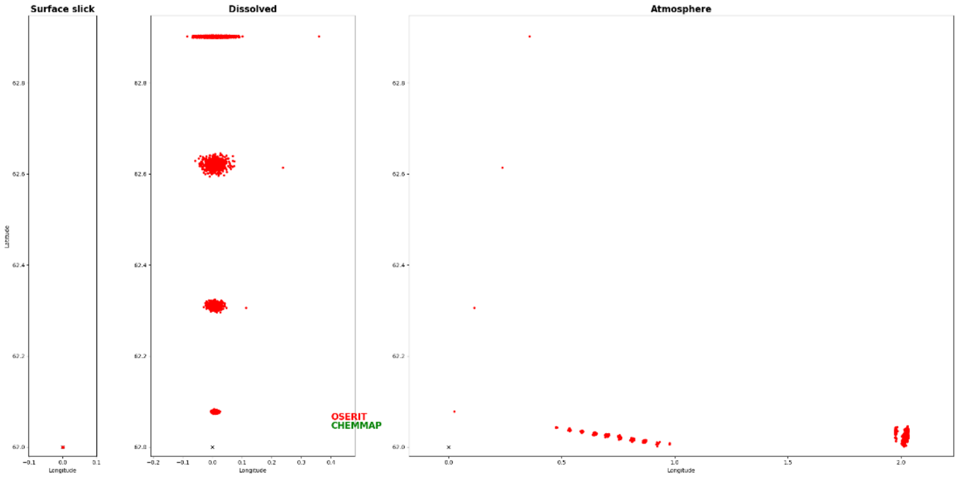

Figure 76 : Drift comparison of OSERIT (red) and CHEMMAP (green) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 14

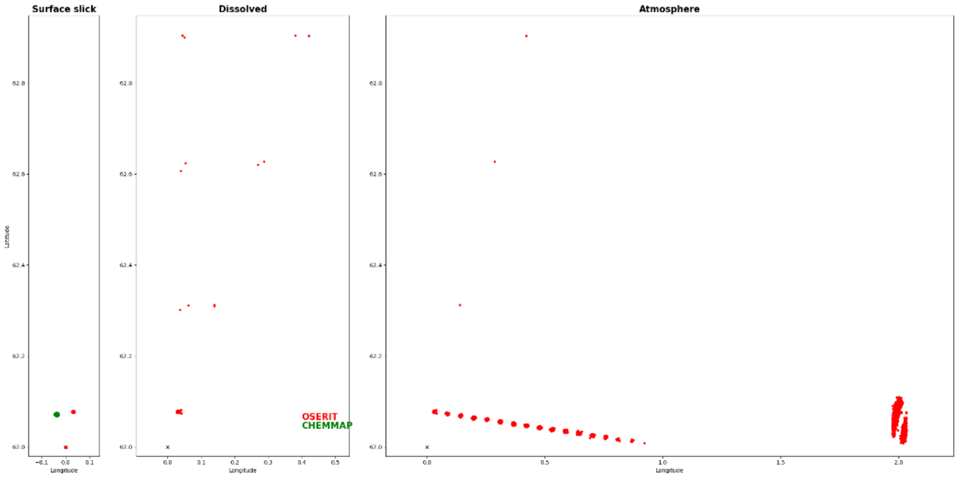

Figure 77 : Drift comparison of OSERIT (red) and CHEMMAP (green) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot

are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 15

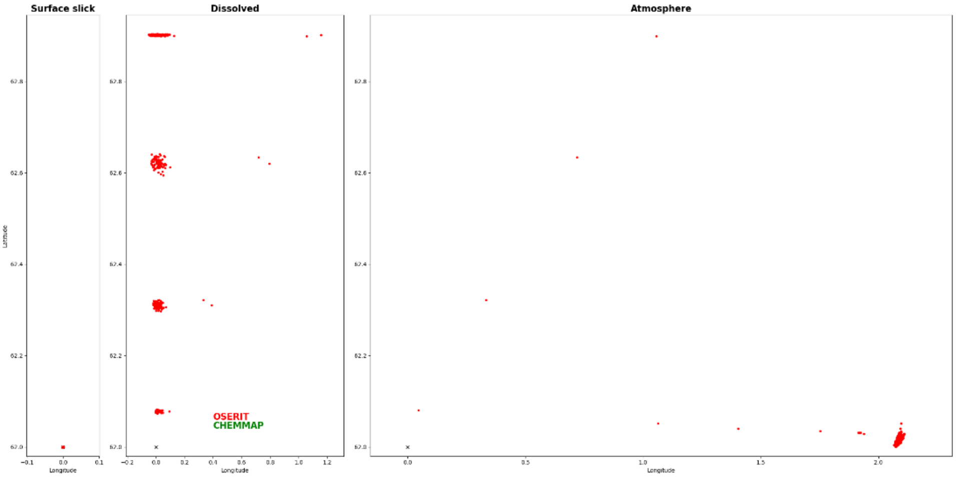

Figure 78 : Drift comparison of OSERIT (red) and CHEMMAP (green) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 16

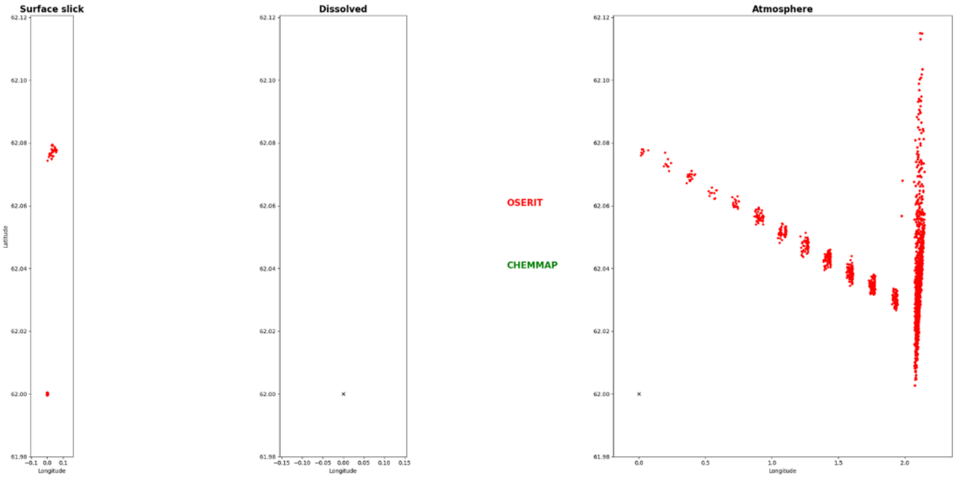

Figure 79 : Drift comparison of OSERIT (red) and CHEMMAP (green) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 17

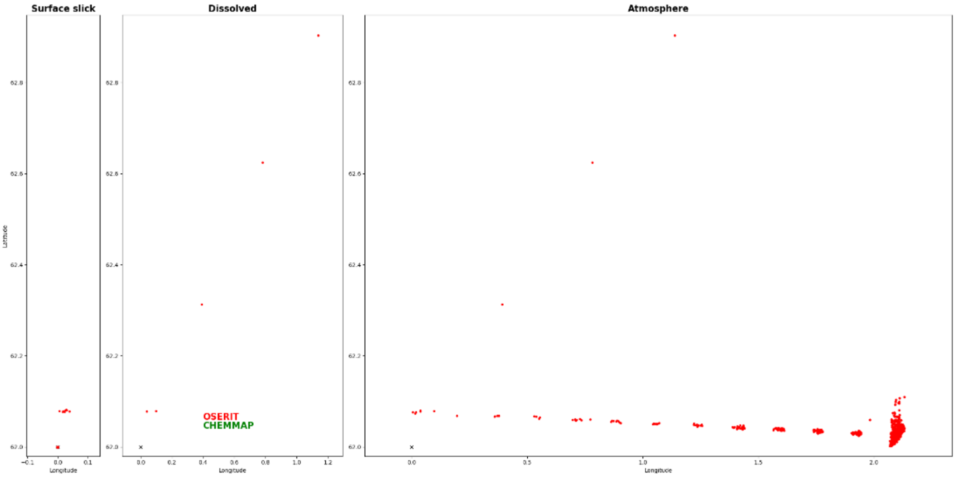

Figure 80 : Drift comparison of OSERIT (red) and CHEMMAP (green) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 18

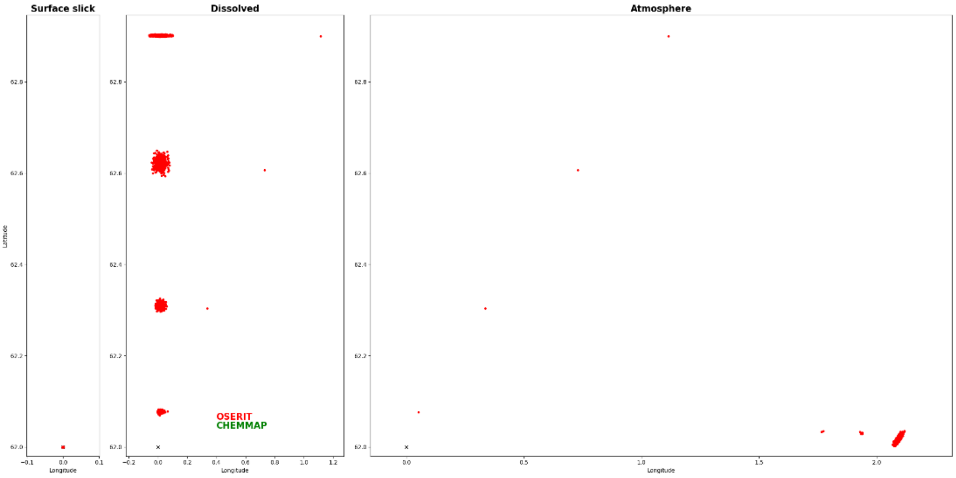

Figure 81 : Drift comparison of OSERIT (red) and CHEMMAP (green) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 19

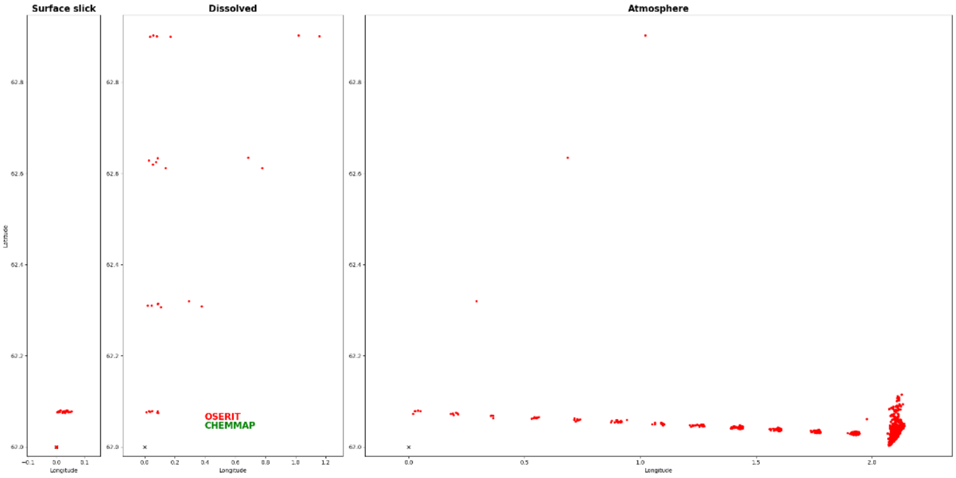

Figure 82 : Drift comparison of OSERIT (red) and CHEMMAP (green) for the surface slick (left), the dissolved phase (center) and the evaporated fraction (right). The current is going from North to South and the wind going from West to East. The plot are represented at the start and after 3, 12, 24, 47 and 71 hours. This is for the weathering drift case 20