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Humanitarian Aid &
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Enhancing HNS preparedness through training and exercising

HNS Model intercomparison: MOHID & CHEMMAP

Task C: Tools for Modelling Impact

Action C.1.5.2: Model comparison – other models

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1. Summary

This document presents a simplistic exercise of model intercomparison in case of an event of a chemical spill in water. MARINER chemical spill model (MOHID) is compared with CHEMMAP model in one predefined virtual scenario with typical and constant environmental conditions. A Floater-Evaporator-Dissolver substance was considered, once is more diverse in terms of fate and behaviour.

MOHID model results are in agreement with what is expected having in mind the physical-chemical properties of the substance used, although significant differences were identified when compared with CHEMMAP model, mainly in terms of the kinetics of the processes. However, those differences may be associated to the used physical-chemical properties of the substance (e.g., the vapour pressure), or even to a different configuration of the models (e.g. wind speed).

In the future, further virtual scenarios should be considered, in order to allow a more complete and valid evaluation of the different responses of the models and sensitivity analysis.

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2. Methodology

This exercise was defined assuming the following constant conditions:

- Models compared: MOHID (operated by Bentley) vs. CHEMMAP (operated by CEDRE)
- Chemical Substance = Butyl acrylate (F-E-D)
- Wind conditions:
    - wind speed = 3 m/s
    - wind direction = from north
    - Wave conditions = no waves
    - release type = point
- suspended sediments concentration = 0 mg/l
- water salinity = 36ppt
- water temperature = 16º C
- air temperature = 20ºC
- simulation length: 72h
- spill amount = 1 000 m^3
- spill duration = instantaneous
- release depth = 0m (surface area = 0m^2)
- spill location and time:
    - 1-1-2017;
    - Latitude = 40.00;
    - Longitude = -10

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3. Results

3.1. MOHID

The MOHID model results demonstrated a progressive transfer of mass to the atmosphere (evaporation from the surface and volatilization from the water column).

The dissolved fraction was all volatilized as well, and approximately after 2 days, all the chemical was removed from the water. After one day, almost no chemical can be found in the surface. Approximately 1.7% of chemical is degraded at the end of the first day.

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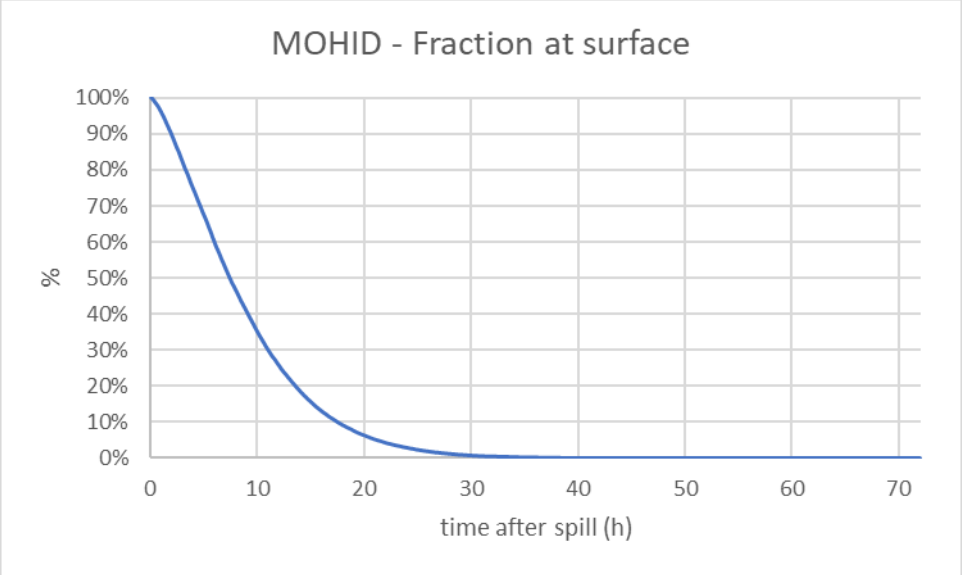

Figure 1 – evolution of the chemical mass fraction at the water surface (MOHID model)

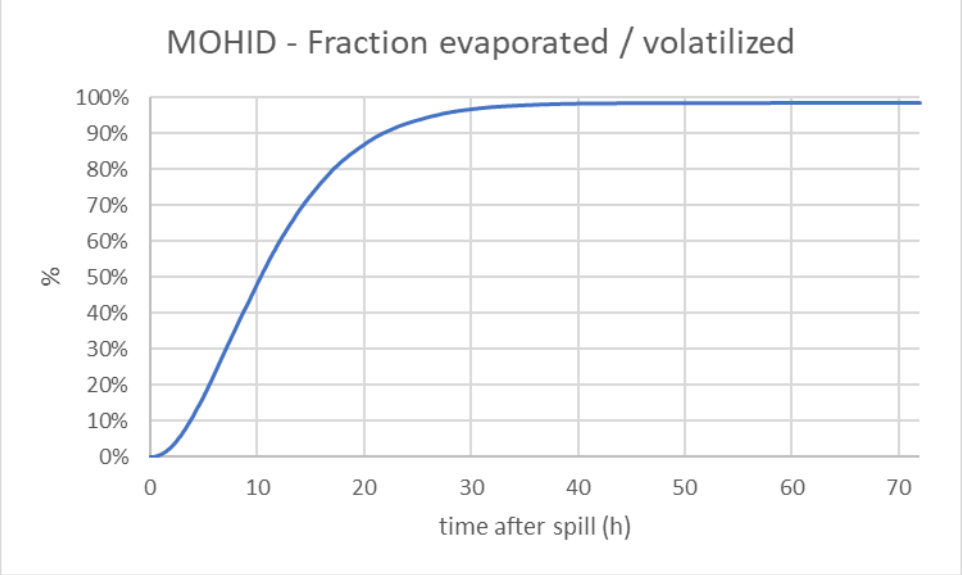

Figure 2 - evolution of the chemical mass fraction transferred to the atmosphere (MOHID model)

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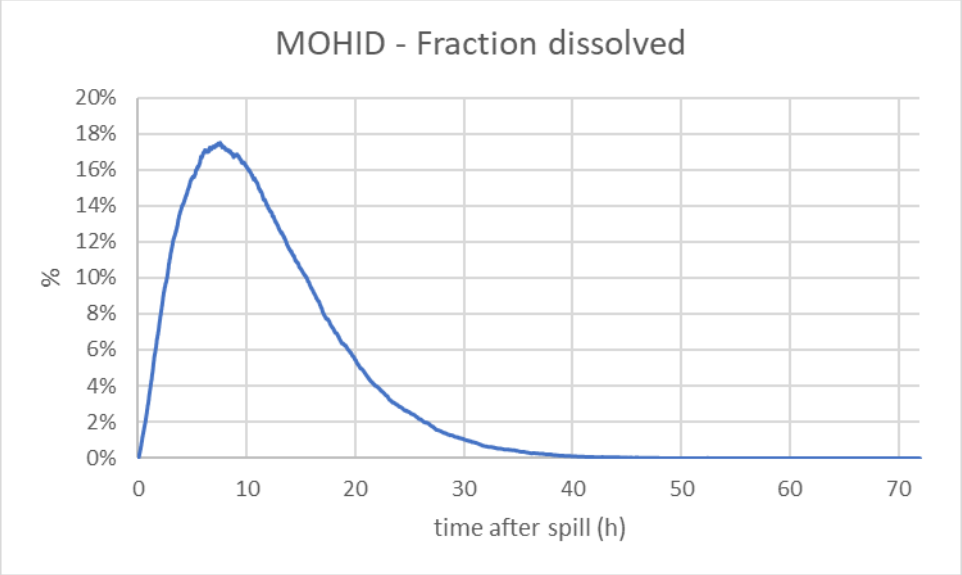

Figure 3 - evolution of the chemical mass fraction dissolved in the water column (MOHID model)

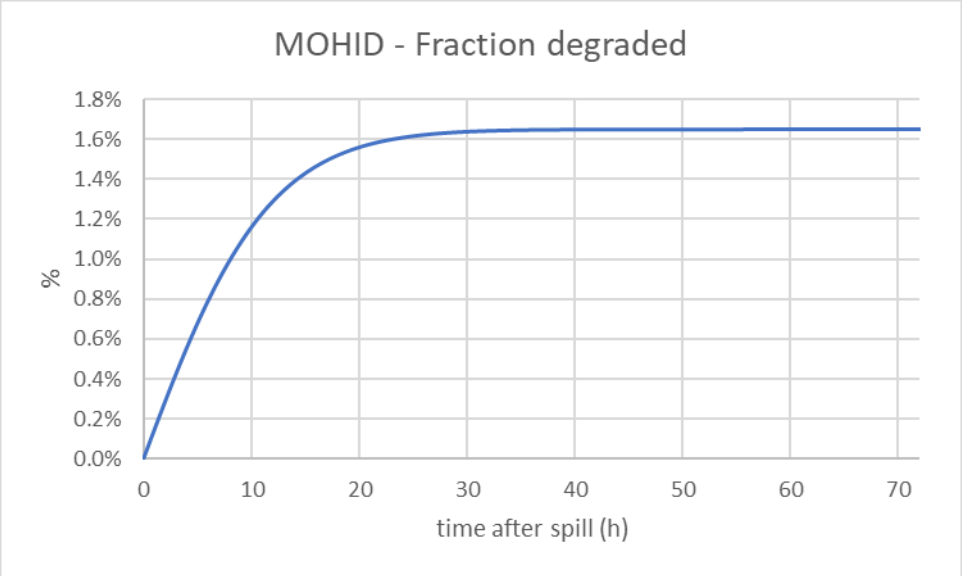

Figure 4 - evolution of the chemical mass fraction degraded (MOHID model)

3.2. CHEMMAP

In the case of CHEMMAP model, the variation of mass balance is very high in the beginning of the spill simulation – most of the chemical tends to be removed from the surface, evaporating in the first couple of hours, and with the dissolution process happening in the same time scale as well. Along time, the dissolved fraction is also reduced, either by volatilization or degradation.

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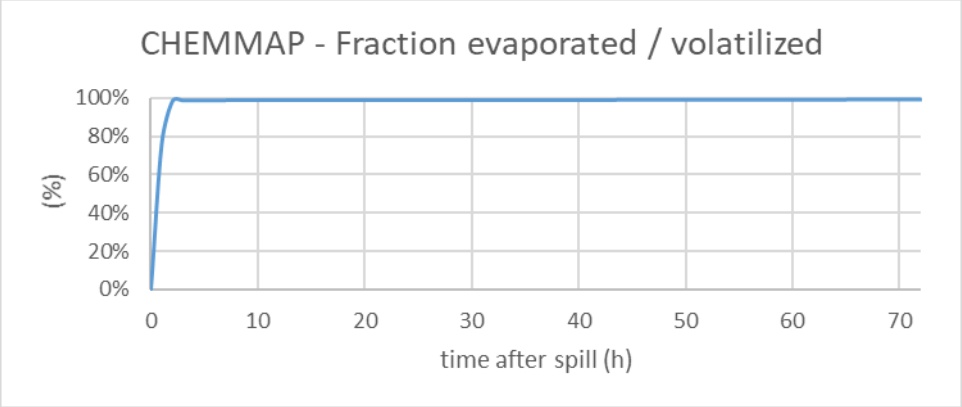

Figure 5 – evolution of the chemical mass fraction at the water surface (CHEMMAP model)

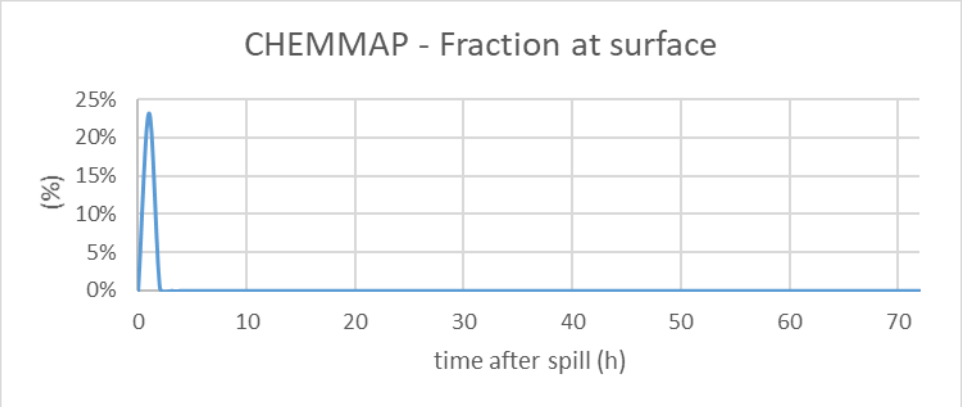

Figure 6 evolution of the chemical mass fraction transferred to the atmosphere (CHEMMAP model)

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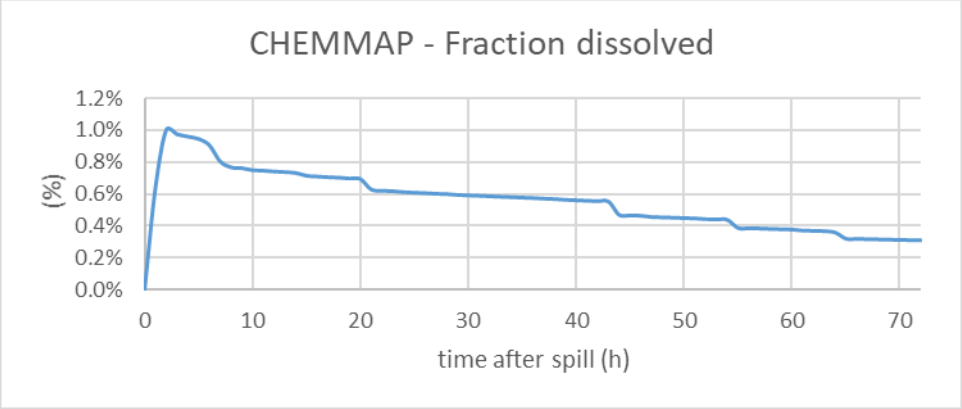

Figure 7 - evolution of the chemical mass fraction dissolved in the water column (CHEMMAP model)

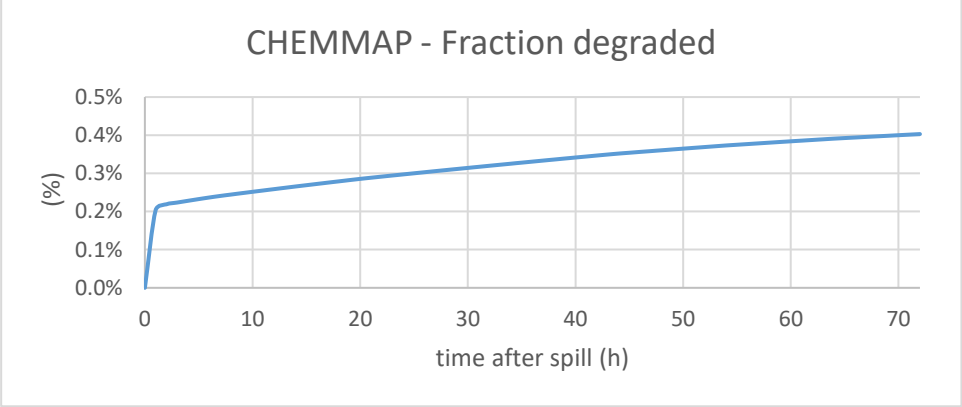

Figure 8 - evolution of the chemical mass fraction degraded (CHEMMAP model)

4. Discussion

The comparison of MOHID model vs. CHEMMAP allows to visualize a much faster evaporation in CHEMMAP, which results in a faster chemical surface removal, and less dissolution and degradation. The mass transfer to the atmosphere in CHEMMAP is mostly due to the evaporation from the surface, and in MOHID is due to the volatilization of the in the water column.

Nevertheless, the identified differences might be associated to different physical-chemical properties considered for the chemical substance (e.g., vapour pressure), or any unidentified difference in the environmental conditions (e.g. wind speed). These potential differences should be identified in the future. Different vapour pressure or wind speed significantly influence the chemical behaviour.

More modelling scenarios (more substances, and different environmental conditions) should also be analysed, to facilitate a proper characterization of the differences between the models.

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