Geoscientific Model Development Discussions

Geosci. Model Dev. Discuss., author comment AC2
https://doi.org/10.5194/gmd-2022-212-AC2, 2022

Reply on RC1

Manuel Aghito et al.

Author comment on "ChemicalDrift 1.0: an open-source Lagrangian chemical fate and transport model for organic aquatic pollutants" by Manuel Aghito et al., Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2022-212-AC2, 2022

We thank the reviewer for the useful comments. While we need to wait for feedback from all reviewers before we can give a complete and detailed answer and update the manuscript accordingly, we would like to quickly address some of the important issues pointed out.

Hope this will help understanding our choices, and we will of course try to motivate them better in the manuscript if we were not clear.

Review of "ChemicalDrift 1.0: an open-source Lagrangian chemical fate and transport model for organic aquatic pollutants" by Aghito et al.

In this manuscript, the authors present a new modelling framework for organic pollutants, built on the OpenDrift framework. They apply the framework to three different examples, in the Baltic, North and Adriatic Seas.

The manuscript is generally well-written and easy to follow and navigate through. The figures are clear, and the inclusion of a code snippets gives a nice impression of the ease-of-use for the users in using the model. I can imagine that this manuscript is a good reference for new users of the model.

However, I do have a few very serious concerns that avoid me from recommending this manuscript for publication in GMD:

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1. There is essentially no validation of the code. How confident are the authors that the code works as intended? They mention functional testing in the abstract, but I could not find that in the manuscript body. Also, is there any unit testing?

Yes, “functional testing” was used improperly, we meant “testing of the model functionalities”, we can rephrase. Unit testing is extensively used in OpenDrift, and thus also covers the components of the new module chemicaldrift.py, except for the chemistry calculations.

Regarding validation, our strategy is to describe the model in this manuscript, which does provide some simple verification of the equations, and provide extensive evaluation in follow-up papers, where we will provide simulations on regional and European scale. This approach is also suggested in the GMD guidelines for Model description papers, quoted “Where evaluation is very extensive, a separate paper focussed solely on this aspect may be submitted” (https://www.geoscientific-model-development.net/about/manuscript_types.html#item1) and would also fit very well with the main author publication plan for the PhD degree.

The general drift and mixing parameterisations in OpenDrift are addressed and validated in many papers using OpenDrift (see https://opendrift.github.io/references.html).

The modeled processes (partitioning, degradation, and volatilization) are implemented based on formulations used in other chemical fate models, like for example the Aquatox tool by the US Environmental Protection Agency, or provided by reference textbooks like Schwarzenbach, Gschwend, Imboden - Environmental Organic Chemistry, so it is expected that these processes are calculated correctly.

The novelty is the integration of aquatic chemistry within OpenDrift, which allows to model the chemical processes at various scales and with seamless update of important parameters like temperature, salinity, mixed layer depth, SPM concentration, and to study the combined effect of ocean physics and chemistry.

We provide some simple verification that the chemical equations work as expected with the given examples, like in Fig.8, showing the expected effect of temperature and salinity on the chemical partitioning, or in Figs. 3-7, showing that chemical mass is reduced exponentially due to degradation and volatilization, and comparing the fate of two different chemicals, which is also consistent with our expectations since benzo(a)pyrene is much less volatile and has higher affinity to particles than naphthalene.

A comprehensive evaluation of the overall model is indeed very challenging. Concentrations of pollutants in the water column in marine environments are often lower than instruments limits of detection and cannot be measured. We can’t validate if we don’t have sufficient data. Moreover, chemicals in the environment are not released by a single point source like for example would be the case in a petroleum accident, so also the task of collecting all possible contamination sources (directly released to the sea by e.g. ships or oil platforms, or discharged from rivers, water treatment plants, factories, or deposited from the atmosphere) is very difficult in itself.

Nevertheless, ecotoxicological studies show that chemicals like PAHs and heavy metals can be harmful to marine species at very low concentrations, so it is important to develop tools for predicting the concentrations.

It would be a very long shot if we were attempting to provide a validation and then claiming that the model would be applicable in general, with different environmental conditions, input data obtained from different sources, and different scales.

It is more reasonable to perform parameter tuning, model calibration, and model evaluation in specific case studies. This is planned in ongoing activities and will be addressed in follow-up papers.

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2. The authors also do not present any performance assessment. How does the code scale with number of elements? Can it work in parallel (OpenMP, MPI?) mode? What is the memory footprint of the additional codes, compared to the rest of OpenDrift? How is IO dealt with?

Trajectory calculations are difficult to parallelize in general, but many sub-components (bottlenecks) of OpenDrift are parallelized using e.g. multiprocessing module.

We have actually worked with parallelization with ChemicalDrift after the submission of the manuscript. This has been implemented using Python multiprocessing library, splitting a simulation in 64 subprocesses, each applied to chemicals discharged in separate longitude intervals, and this gave a strong reduction of the simulation time. We can simulate for example open loop scrubbers emissions of a selected chemical for a whole year (2018) and for the whole European region, using approximately 900000 Lagrangian elements, in less than 2 hours on our HPC.

The IO is inherited from OpenDrift, and is based on export to CF-compliant netCDF files, and generic import (readers), see https://doi.org/10.5194/gmd-11-1405-2018, 2018.

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3. In the examples, there is no assessment of the sensitivity of the results to choices like integration time-step, number of modeled elements, input/output-frequency etc; making it difficult for the reader to gauge how robust the results are to the user parameters.

Sensitivity analysis is of course very important and needs to be performed. This should include physical parameters, chemical parameters, and numerical parameters like time-step and number of model elements. Given the large number of parameters and the broad range of variability and uncertainties of these, sensitivity analysis is also expected to provide different conclusions in different case studies. To give an example, while in one case study we might have accurate measurements of KOC and fOC, we know that in general these parameters are subject to huge variations in the environment. Hence, our plan has been to address sensitivity analysis as a step of model verification in follow-up papers focussing on specific case studies.

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4. The code builds heavily on OpenDrift itself, and is in some way an obvious further extension of the Radionuclides extension. Most of the new code is simply an implementation of physical equations, presented without much numerical or computational consideration.

We focussed on describing the novelty, which is the integration of the chemistry of organic compounds in the OpenDrift framework. This is not in OpenDrift, and not in Radionuclides. All equations described in the manuscript correspond to new code implemented in ChemicalDrift.

The numerical framework is indeed largely inherited from OpenDrift, hence the focus of this manuscript is on the chemical processes, and not the numerical implementation.

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5. Because of the four points above, I seriously doubt that this manuscript falls within the scope of GMD. The way it is presented, it feels more like an application of OpenDrift to a few very specific chemical processes within the context of a European project; rather than a versatile and potentially widely useable community code. Perhaps another journal (e.g. on marine pollution) might be more relevant for this work?

The chemical processes handled within ChemicalDrift are general, and not limited to the specific EMERGE project, although it provided funding for the development. The model can easily be used in many other applications where risk assessment of contamination of organic pollutants is useful: discharges from shipping in general, fish farms, produced waters for oil platforms, discharges from rivers, water treatment plants, deep sea mining. The integration within OpenDrift, which provides a very flexible and simple interface, will facilitate the use of ChemicalDrift in other applications.

Moreover, ChemicalDrift can easily be extended to other types of chemicals, like for example ionizable compounds, and heavy metals, and updates made after the submission of the manuscript are already available on the github repository.

The examples given in the paper are only preliminary demonstrations, presented without any quantitative analysis, for the scope of describing the model. The examples are based on EMERGE data since this is the project we have been working on. We think that follow-up papers presenting and analyzing simulation results might indeed be more suited to another journal with more focus on environmental chemistry.