Geoscientific Model Development Discussions

Geosci. Model Dev. Discuss., referee comment RC1
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Comment on gmd-2022-212

Anonymous Referee #1

Referee 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-RC1, 2022

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:

- 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?
- 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?
- 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.
- 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.
- 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?

Furthermore, I also have some minor comments and suggestions:

- lines 8, 18, 221, 423 and other locations: At places, words like 'powerful', 'valuable', etc make it sound more like a sales-pitch than a self-critical scientific assessment. I suggest to be very careful with this self-congratulatory framing.
- line 26: Can it be assumed that all readers know what a Lagrangian model is? Also, OpenDrift could be explained in more depth
- line 66: what is a 'severe' oil spill? Why would it not work for non-severe oil spills?
- line 67: this wording suggests that the only difference between OilDrift and ChemicalDrift is the concentrations that can be tracked; but I think there are many more differences? Perhaps rephrase?
- line 73: mention here already that (re-)deposition is not taken into account?
- line 74: I don't think this statement is meant to imply that only findings from open-access literature is used (so ignoring closed-access literature)? Perhaps rephrase?
- line 85. Fig 1 caption and further: I am a bit confused whether the terms 'compartment' and 'phase' refer to the same concept, or something different. If they are the same, I suggest using only one of the terms throughout
- line 168: 'neglected' is not the right word here. Vertical velocity is a diagnostic variable in most ocean models
- line 172-174: How good is this assumption here? What is the typical error made when using this assumption in realistic scenarios?
- line 175-179: what is the physical interpretation and motivation behind this parameterization?
- line 226: k should be type-set in mathmode?
- Table 3: I'm a bit surprised that the authors use the interpolated CMEMS data here. Why not the non-interpolated original version of PHY on the MOi servers at e.g. https://www.mercator-ocean.eu/en/solutions-expertise/accessing-digital-data/product-details/?offer=4217979b-2662-329a-907c-602fdc69c3a3&system=d35404e4-40d3-59d6-3608-581c9495d86a (which also includes vertical velocity)
- line 355: while helpful for visualisation, I fear that such a representation of element 'mass' by size might be a bit misleading to some readers, who may not appreciate that elements don't actually have an actual 'size'
- line 363: 'is demonstrated'
- line 367: The statement about the Lagrangian framework here is a bit misleading. It would be perfectly possibly to run two separate tracers in an Eulerian framework and that way also separate the sources. The Lagrangian framework does have advantages, but the way it's formulated now is not one of them