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Geoscientific Model Development Discussions

Interactive comment on "HR3DHG version 1: modelling the spatio-temporal dynamics of mercury in the Augusta Bay (southern Italy)" *by* Giovanni Denaro et al.

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Dear Authors, dear Editor, First of all, my apologies to the Editor and to the Authors for delay. The manuscript "HR3DHG version 1: modelling the spatio-temporal dynamics of mercury in the Augusta Bay (southern Italy)", the supplement and the code of the HR3DHG model are quite complex and it took a while to read and examine them thoroughly. Nonetheless, I found them all very interesting. The detailed description of the model (in the supplement) facilitates understanding of the modelled processes and the parameters used in the equations. HR3DHG is most probably the most complex and the most promising Hg model in coastal environment at the time, and as such an ex-

tremely useful tool for the entire Hg-modelling community. Linking a 3D hydrodynamic model, coupling more than one nutrient-phytoplankton models in a Hg model, and simultaneous simulation of several species in the sediment and the water compartments, represent an important novelty in Hg modelling. Furthermore, the abundant set of collected data in the Augusta Bay, and of the parameters from literature (Tables S1-S3) are a valuable addition to the Hg-modelling community. The results of the performed research show relatively good agreement with experimental values. Based on the results, the authors were able to explain the spatio-temporal behaviour of Hg species in the water and the sediment compartments of the Augusta Bay.

My major concerns with this manuscript are the following:

A. General:

Introduction: I am missing a more comprehensive overview of Hg modelling performed on the scale of the Mediterranean Sea and its parts. The authors do not report any of the 2D and 3D models developed and applied before this study. These models, although not as complex as the presented HR3DHG, were also supported by a hydrodynamic model and performed quite well at the scale of the entire Mediterranean and at smaller scale (Gulf of Trieste, Adriatic Sea) with regard to both transport and transformations of two or three Hg species. My suggestion to the authors would be to investigate the article by Zhu et al. (https://doi.org/10.1016/j.scitotenv.2018.04.397) and the references therein, and to include the previously developed multi-dimensional models into the section Introduction. The same comment is valid for the chapter Discussion: 2D and 3D models were used before the HR3DHG model.

Sensitivity analysis confirms high significance of circulation (Line 501). Is therefore the constant-density approach correct? Non-stratified conditions are acceptable in winter months, while the temperature stratification in the summer may significantly influence the circulation and the fluxes through the picnocline. Whether to use stratified or non-stratified conditions depends on temporal resolution applied: with seasonal (or finer

temporal resolution) stratified conditions should be taken into account.

To proceed with the same concern: the temporal and spatial dynamics of the simulations are unclear. Several questions arose during reading:

a) How were data from various seasons (Fig 1) taken into account (for calibration/validation)? Particularly when the constant water-density was accounted for in the model.

b) What is the temporal resolution of hydrodynamics (real-time = hourly, or any other resolution) used in transport simulations, and how often was the velocity field changed in a long-term simulation? Was a perpetual year used or did the conditions change (using any of the possible IPCC scenarios for changing climate conditions or anything similar)? A 250-year simulation would require an explanation of the applied parameters.

c) When adapting hydrodynamics from the shyfem model to the HR3DHG grid, were the velocities interpolated to the HG grid or integrated over the cells of the HG grid? When using real-time hydrodynamics, the correct transport can only be achieved by integration.

d) A table with temporal dynamics of each of the variables and (environmental) parameters would be useful. I.e. how often are the input parameters changed (annually/seasonally/weekly) and in which way the results were obtained (re-initialisation with experimental data/a single long simulation for 250 years?)

Another question is the agreement of simulated and experimental results:

a) The complexity of the model requires thorough verification, calibration and validation. In order to confirm an “excellent agreement of the model with experimental data”, validation of the model should have been performed with calibrated parameters. Was such a procedure done and if yes, on which temporal scale? The latest available experimental data are from 2017, and the modelling results for 2017 can be reproduced from

the initial 2005, 2011 or 2012 experimental data. How different would be the modelling results for 2017 using the same set of calibrated parameters? In any case, it is very difficult to justify results of a 250-year long simulation even without the climate and other environmental changes that may occur in such a long time interval. b) Several statistical methods for evaluation of model efficiency (Nash-Sutcliffe, Kling-Gupta, rmse) can be applied in order to quantify the agreement with experimental data. The results of these tests would give a better impression on the model performance than qualitative description by using excellent/good/poor based on visual agreement between figures.

Mass balance (Table S9 and Conclusions lines 544-545):

a) In the section Conclusions (line 544) the authors discuss the mass balance, which has never been established and presented. A mass balance should consist of quantities of the species under consideration (inventories) and fluxes, and in most cases, (see the references in Zhu et al.) such balances are presented in graphical form.

b) What is the inventory of (at least HgT) in the domain and in each of the compartments (water/sediment)? How do the fluxes affect the inventory? All that is evident from the numbers in the Table S9 is the constant decrease of the fluxes. Is the presented mass balance obtained solely from the results of the model or is it supported by experimental results? Furthermore, is the annual balance closed or open? With steadily decreasing fluxes and the deposition remaining more or less unchanged (term AD in Table S9), the inputs and the outputs should balance once in the future. When?

B. Details (manuscript):

Line 73: Rajar et al. (doi:10.1016/j.marchem.2006.10.001) and Zagar et al. (DOI 10.1007/s11356-013-2055-5) established two (annual) Hg mass balances in the Mediterranean Sea. There, the atmospheric deposition and the rivers’ contributions were found to be significantly more important than any of the point sources. In order to support the statement that “the Augusta Bay has a key role in Mediterranean Hg inventory” this role should be quantified and compared to the previously published

values.

Lines 120-121: The sentence explaining why the results were unaffected by the chosen initial condition is not clear.

Line 149: What is the temporal resolution of hydrodynamics? I.e., how many different velocity fields were used for computing transport?

Lines 320-340: Were the results of the calibration procedure constant or variable (in time) input parameters? If temporally constant, for which period (set of measurements). Were the same constant coefficients used for another time interval between measurements? If variable, on what temporal scale?

Figure 6: Shows a decreasing trend for all fluxes. The Hg inventory in the Bay is most probably decreasing as well (unfortunately the mass balance is not established in a way to either confirm or contradict this hypothesis). Were these results obtained by accounting for computed or measured deposition? There is a high discrepancy (factor 2.5) between these two values. As reported by several previous modelling/mass balance studies (Zhu et al., and the references therein), deposition is a very important source of Hg in the Mediterranean. Including deposition into the performed sensitivity analysis would be very useful for clarification of this question.

C. Details (Supplement):

References to Figs in the supplement should be noted as eg. Fig S5, not Fig 5.

In several equations the annual flux is debated. Were fluxes calculated also on seasonal (or finer) temporal scale?

Equations S8 and S21: Where is the dry deposition, as the first term in line 59 and the most right-hand term in S21 only have the wet part, connected to precipitation P?

Equations S23 (and S37): if tortuosity is not taken into account in neither Dw-in (or Dw-or) nor δw, please explain whether and how this is compensated in the equation.

Tables S4, S10: The presented concentrations are given for 2011 and 2017. Any other comparison possible?

Several of these questions are, in my opinion, crucial for understanding the performed simulations and for justification of the agreement between the model and the experimental results.

I will be pleased to read and discuss the improved manuscript!

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