

General comments

The study showed that incorporating CSIA reduced uncertainty in PiBEACH model for estimating S-metolachlor concentration in soil. The study is interesting, with a good conclusion and abstract. However, the structure of the article requires MAJOR improvements. Some are mentioned below, but the authors' additional effort is also welcome.

Specific comments

Ln 11: What do you mean by “the calibration of pesticide dissipation”? Which parameters are related to pesticide dissipation?

Ln 16 This is confusing; previously, you mentioned “calibration of pesticide dissipation.” Typically, you calibrate the parameters of the model. Now you are mentioning “predict daily pesticide dissipation.” In this case, you are saying that pesticide dissipation is like an output of the model PiBEACH. Can you explain this? It is very important to understand your research.

Ln 23, In the phrase “the incorporation of CSIA data into conceptual distributed hydrological models,” you should mention that only for PiBEACH, you did not test more conceptual hydrological models (perhaps the results are different). For this article, it could be beneficial to incorporate one more model.

Ln 41. In the phrase *“In addition, existing models frequently fail to accurately quantify the contribution of concomitant pesticide dissipation processes for accurate estimation of off-site pesticide transport (Gassmann et al., 2021).”*

Previously, you provided information on the contribution of processes for the pesticide dissipation process, such as degradation, sorption, and volatilization. I think this term (pesticide dissipation) requires a small paragraph for a definition first because, in the phrase of Ln41, it is not clear what you mean by “the contribution of concomitant pesticide dissipation processes.....” Commonly, hydrological models simulate (quantify) “concentrations” over time or “transport”; for example, you can see SWAP-PEARL, HYDRUS, or MACRO models. Therefore, the models do not quantify pesticide dissipation processes as an output; they are mechanisms **IN** the model. When I read about pesticide dissipation, the first thing that came to mind was DT50 (degradation). Therefore, I suggest including a small explanation of the term, changing it, or citing an author explaining the concept.

Ln 45 In the phrase “data limitations to constrain model parameters,” Please include at the end of this paragraph “by calibration”. So, the final phrase should read “data

limitations to constrain model parameters by calibration.” Remember that several pesticide parameters can be obtained by laboratory analysis.

Ln 55-57 I think this phrase is key for your purpose. Maybe after this phrase, you should provide your opinion and mention that this is one of the research goals, increasing the understanding of your research.

Ln 72 Is the incorporation of CSIA an “alternative” or “complementary” approach?

Ln 138 It mentioned soil samples from 13 marked plots. I GUESS you mean the black dots in Figure 1. We still do not know which samples were obtained from weekly measurements (green dots in Fig. 1). The methodology needs to be organized better.

Ln 149 I suggest including the total number of observations you have for calibration. You have three types of observations to include in an objective function. Concentrations of S-metolachlor in the topsoil, CSIA, and runoff discharge. It is important to know that number because you are calibrating 25 parameters (which is a lot!) In my experience, you should not calibrate more than five, which still is a lot. Otherwise, you get problems with parameter uncertainties.

Ln 170. OK, PiBEACH needs meteorological records, among other things, but it did not provide details of how those measurements were taken or analyzed in laboratory conditions.

Ln 158 If you mean Supplemental information by “SI”, you should put the definition of the acronym one time.

Ln 178 Can you please mention the mixing topsoil layer length in this phrase? The mixing layer is generally a challenging topic and, in my opinion, an unsolved problem for hydrological models.

Ln 201 The Model only accepts that number of layers. Or is that set by the user?

Ln 220 In Eq.1, you mentioned that the balance is solved for each layer with soil depth Z . But the runoff term should not be included in deeper layers. This raises the question of whether you obtain a unique theta per cell or a theta for each layer (5 layers in the profile per cell). It would help if you clarified this, especially for HYDRUS, MACRO, openLISEM, or SWAP-PEARL users.

Ln 230: You mentioned the balance at each cell I was given by Eq. 2. My question is, does this model solve the mass balance per layer (5 in your case), or does it generate a mesh with smaller cells? (Connected with the previous question)

Ln 246. Where is the mixing layer depth used in Eq. 4? I think you should change J by $q_{x,y}$ in this equation.

Ln 296 It is not better to include h_{ref} than θ_{ref} . The water content depends highly on texture; $0.2 \text{ cm}^3 \text{ cm}^{-3}$ of water content could be either high or low. Instead, the h does not have that inconvenient.

Ln 305 OpenLISEM cannot simulate preferential flow yet, to my knowledge. So, this phrase required modification.

Ln 350 Which threshold did you use to reduce parameters from 43 to 25. Basically, how did you define a parameter as highly sensitive? Additionally, you should mention which outputs were analyzed during sensitivity analysis, i.e., did you include sensitivities to isotope output?

Ln 370 Where did you previously mention “daily discharge at the outlet”? You mentioned weekly runoff. The observations are unclear, and you need to structure the methodology better.

Ln 373 OK, you explain that in addition to incorporating CSIA data in the objective function, you will analyze the spatial distribution of this observation. For better understanding, you should use Fig 1 at this point.

Ln 393 If the graph (Fig 3C), the “y” axis is in DT50, please use DT50 instead of k_{eg} during the discussion. Additionally, I do not know how this graph and analysis (Fig 3C) provide useful information for the research. All that you mentioned in the graph and discussion can be easily obtained from Eq. 8, derived from another hydrological model, so basically, it is something simple and well-known.

Ln 400 The graph should be improved (.svg). Additionally, you mention the error bars linked to soil bulk density. I think this is important and should be mentioned in the methodology (please improve the organization of methods).

Ln 404 Please indicate if metolachlor concentrations are in liquid or total concentrations (also, this should be explained in the methodology).

Ln 420 OK WIC calibration reduced uncertainty, but what happens with the other 24 parameters? In the case of NIC or WIC calibration, do they maintain the uncertainty bounds? Or perhaps it changes, and how? This is important to analyze because that uncertainty may be translated to other parameters. Additionally, is there some field (laboratory) information on the common parameter values for this compound? especially DT50. I agree that DT50 could be one order of magnitude different from the expected one. Still, it is welcome to have the laboratory reference to see if calibration

did not modify parameters to “unexplainable” values. That also holds for the 24 remaining parameters that you calibrate. That kind of analysis is expected from this kind of research.

Ln 439. OK, it would be nice to see if there are significant differences in the comparison variance. The plot situation showed a smaller reduction in the SD. The “plot” may not be recommended, but you need ANDEVA or something like that for that affirmation.

Ln 444 “Modeling results”: Do you mean calibration results? Ec was calibrated? In this case, did you compare it with previous studies on that parameter? Something like that should be expected for DT50 and perhaps other calibrated parameters. (Similar comment that above)

Ln 457 Why did you mention that degradation obtained with the model was like observations? In which part of the methodology did you explain that compound degradation was performed under laboratory conditions or other? You need to improve the structure of the article.

Ln461 Here, we explain how the BAM% was obtained, but this is a methodological part.

Technical comments

L10. to the limited availability of field data **capable of distinguishing** between. Please change by “distinguishing”.

L17. incorporating changes **of** the carbon isotopic signatures. Please change “of” by “in”.

L36. leaching, volatilization, off-site transport, Please included **“and”** before off-site.

L46. each of which generally **accounting** for several physico-chemical. Please modify by accounts.

L59. in topsoil and at the catchment outlet **is** currently. Please change “is” by “are”.

L70. it may also generate unknow and. Please change “unknow” by “unknown”.

And some more that you can check.