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Interactive comment on "CHROTRAN 1.0: A mathematical and computational model for in situ heavy metal remediation in heterogeneous aquifers" *by* Scott K. Hansen et al.

M. Walther (Referee)

marc.walther@ufz.de

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Comments on "CHROTRAN 1.0: A mathematical and computational model for in situ heavy metal remediation in heterogeneous aquifers" submitted to GMD by Scott K. Hansen, Sachin Pandey, Satish Karra, and Velimir V. Vesselinov

The manuscript describes the principles of a newly developed numerical model to simulate heavy metal contamination remediation involving biological fate (together with clogging) in saturated porous media; two example setups are provided to show the model's functionality. The approach is based on the open-source simulation toolbox PFLOTRAN and builds upon its functionality by extending the reactive module for the

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purpose of simulating the fate of heavy metals.

The structure of the manuscript is logically, providing an initial literature review, followed by a description of the used approach for the model development, before example calculations are presented. The manuscript is written in a clear and concise language; figures are used sparcely, tables summarize required model parameters; an appendix gives a short overview on the file structure for the newly developed features.

My view of the work is twofold. On the one hand, I highly support the publishing of new developments together with a proper benchmarking; this may at the first place not be acknowledged as a scientific advancement, but it very much provides the basis for the latter in many follow-up applications. This is furthermore highlighted by the fact that more and more approaches become increasingly complex which requires a proper documentation for a sustainable development of these approaches. In this light, I strongly support the publishing of this manuscript. On the other hand, I think that there is one major issue with the approach the manuscript presents. Heavy metal remediation is usually governed by the redox potential, which furthermore will change during the reaction and within biomass (biofilm). In the whole manuscript, I could not find any discussion or reasoning why you do not want to consider redox potential in your approach, which is so substantial for the whole reaction system. Having said this, I would like to raise the question whether the approach is sufficient for the broad applicability it claims to have (see page 3, line 30 ff). Also, the two examples only confirm the expected behaviour and cannot be used as benchmarks for the new processes. Therefore, I would like to encourage the authors to give reason 1) why it is ok to neglect redox potential, 2) why their approach is still capable to fulfil the expectations, and 3) provide appropriate benchmarks to ensure correct functioning of the new implementations.

I furthermore listed a number of specific comments below.

I hope that I could help to improve the manuscript and would be available for a second review, if the authors wish so.

General

Please sort the variables by their occurence in the equation.

For all variables explained, I suggest to use dimensions (LENGTH, TIME etc), not units (meter, seconds etc), whenever appropriate.

Introduction

The introduction nicely lists some published approaches for modeling heavy metal fate in saturated porous media. I understand that your literature study concluded that there was no sufficient model to fulfill the requirements listed in page 4, line 3 (btw: these achievement should rather be given in a summary at the end). I am wondering if you had any incentive to implement such a complex modeling approach (in other words: what was your motivation to develop such a new model)?

Page 3, Line 3: "t" is Time?

Page 3, Line 3: I am wondering, whether the dimensions of the equation are correct (please correct me, if this is a wrong intension). The two left-hand side terms should have [MASS/VOLUME/TIME], but the right-hand side seems to have [MASS/VOLUME]. Can you explain this please?

Model description

P5, L11: What is L_b?

P5, L11ff: many explained units seem to be concentrations, please state this in the bold names.

P5, L26: - "...is the current porosity at LOCATION x"? - I assume, you define the porosity with 0 < theta < 1 relative to the total pore volume (ie. 1 - volume of solid phase)? - Why is it not D = D_i / theta(x,t) + D_m / (1 - theta(x,t))?

P6, L4ff: q is not defined (you probably can write something like "with the water mass

fluxes related to head via Darcy flux q")

P6, L7ff: - theta is already defined on P5. - please revise the list of variables to use "and" and commas appropriately.

P6, L8: I suggest to move the note on additional capabilities of CHROTRAN to P5, L3, where you already give a small hint on additional features. Here, it seems not necessary to repeat this.

P6, L23: I would like to discuss your statement, that you do not want to include the dispersive flux. I would argue that the distribution of the different components of the reactive system, ie. an aqueous contaminant, an electron donor, a biocide, is majorly governed by advection and hydrodynamic dispersion. With three (or more) governing components, the reactions should especially depend on the mixing of the fluid (and thus the solutes). However, you say that you do not want to consider mixing due to dispersion. Also, in biochemical applications, bacterial growth is usually limited by nutrient availability; growth of biomass often happens at the fringe of the biomass area (not talking about a biofilm here), while the inner areas will have a limited nutrient supply (as outer biomass has already used up all available nutrients). This, again is governed by (transverse) dispersivity and the mixing of the required constituents for biomass growth. Can you please elaborate on this? Besides the discussion on the relevance of dispersion, you sometimes speak of the "advection-dispersion operator" (eg P8, L12), which is somewhat misleading as you do not want to consider dispersion.

P7, L12ff: I like fact that you describe the relevant biochemical processes (L11 says "chemical" processes). The mentioned assumptions, which you often state to be "common" or you assume to follow Monod or linear kinetics, however, should be backed up by a few references who did this in a similar way.

P7, L27: A question of understanding: If biomass decays, e.g. through lysis, will this release the heavy metals again, or will other biomass be able to use this as nutrients?

P9, L1, Eq 11 ff: Maybe, I missed it, but what is S?

P9, L10ff: Please add some references for the testing cases, benchmarks, and applications which PFLOTRAN is used for. Furthermore, I understand that your new implementation may be hard to test against other software that do not have the capability to run these setups. However, I think that you could have chosen examples that have the option to either neglect the new processes or to include them; for the former, you could run alternative models and test them against your implementation; for the latter, differences should be visible that should be validated against mass balances for consistence.

P10, L3: Where can I find the CHROTRAN repository? (Please add a reference to P12, L20.)

P11, L4: What does the unit "M" stand for?

Figure 2: - If t=400d, flow velocities at the well are very small (practically zero?) due to bioclogging. At this point, you start to inject a biocide. I have to questions: 1) As hydr. conductivity is very low, the distribution of the biocide should majorly be governed by diffusion. I am astonished that this relatively large area ($\sim$5x5m^2) is remediated so fast. Can you explain this? 2) For all t>400d, the shape of the "remediated area" (where the biocide is injected) shows the shape of a diamond; why isn't this shape similar to the shape of the biomass? Is this a numerical artifact?

Summary and conclusions

P11, L26: You did not show the three-dimensional capabilities of your code.

P12, L4: You also did not show the HPC capabilities of your implementation.

Source Code

I could find the source code on github, but could not find any pull requests or commits that build upon the original PFLOTRAN code. Therefore, I could not check any of

the new developments you implemented. I highly recommend, especially for further development of your code, to provide a repository that uses as an initial commit an unchanged PFLOTRAN version and then shows your additions as several, logically combined commits.

Appendix

P12, L26: Please indicate the PFLOTRAN version you used as a base. Do you think you could easily rebase your code to a future release of PFLOTRAN?

P13, L28: please add reference to VisIt and ParaView. See this for the latter: https://www.paraview.org/publications/

Typos, Grammar etc

Page 3, Line 4: Please remove the comma in "where C, is the U(VI) concentration". Later, C is also reused for other heavy metal concentrations, please mention that.

P10, L10: Please change meter to square meter.

P10, L12: epsilon, the initial concentration should have a unit.

P12, L24: "complier" -> "compiler"

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