

***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.**

Anonymous Referee #2

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Review of gmd-2017-51

The manuscript “CHROTRAN 1.0: A mathematical and computational model for in situ heavy metal remediation in heterogeneous aquifers” by Hansen et al. (gmd-2017-51) presents a conceptual modeling approach for the reaction-transport simulation of chromium in groundwater. The conceptual approach considering, transport sorption, biotic and abiotic reduction of Cr(VI), growth and decay of microbial biomass, and clogging of the pore space due to biomass accumulation is implemented into the 3D reactive transport environment PFLOTTRAN. The performance of the approach is demonstrated using two generic case studies.

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The manuscript is well written and the presented approach appears in general technically sound making use of well-established concepts. Some of the assumptions regarding the considered processes and their kinetic description would need a better explanation/justification but my largest concern regarding this manuscript is whether it indeed presents a new model or whether it presents 'just' an application of PFLOTRAN for the simulation of Cr(VI). Given that the shown model applications are two generic scenarios without any in-depth discussion of the results and their potential meaning, it is not possible to validate the applicability of the presented conceptual approach (i.e. set of equations) to real-world scenarios. If – as I appears to me – the novel aspect of the manuscript is restricted to the conceptual approach it would not justify publication of the manuscript.

Specific comments:

P3, L28: Is the only short-coming of the existing models for Cr(VI) reduction the fact that they consider 1D transport only? If so, why is there a need for an alternative description of the reactive processes?

P4, L21: No, there are several other codes which would be capable of simulating the presented processes (perhaps not always the clogging, but certainly all the reactive processes). See e.g., Schäfer et al., 1998, Journal of Contaminant Hydrology 31: 167; Mayer et al., 2002, Water Resources Research 38: 1174; Prommer et al., 2003, Ground Water 41: 247; Centler et al., 2010, Computational Geosciences 36: 397. All these models would be sufficiently flexible to allow describing the presented processes using the set of equations shown further down in the manuscript.

P5,L5-8: While I support this line of approach I am wondering why it would need an 'new' model for its simulation. What is presented in the following is the abiotic and biotic redox transformation of two (partially) mobile species. This is handled by quite a number of reaction-transport models for groundwater settings and it actually does not matter if the electron donor or the electron acceptor is considered as contaminant.

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P5, L11: It appears quite strange/confusing introducing B with the unit mol/L but then interpreting 1 mol as 1 g ... Why not stating that the unit of B is up to the user and eventually requires the units of the parameter S_D to be defined consistently.

P5, L26: This implies that the reactivity of the sorbed and the dissolved donor is the same. If this would be the general case, many researchers studying reductions of bioavailability due to sorption would waste their time. Some words of discussion/justification would be needed here.

P6,L12/Eq.6: In the literature one can find a large number of possible relations between changes of porosity and changes of hydraulic conductivity due to (bio)clogging. However, to my knowledge a linear relation has not been proposed, yet. Give reference/justification for this assumption.

P8, L8/Eq.9 and P9, L1/Eq.11: Why is there no dependency of microbial growth on the contaminant/electron acceptor? This implies that everywhere some other (more favorable) electron acceptor must be available at non-limiting concentrations. If this would be the case why should there be a consumption of the heavy metal? Also, why is the bio-reduction rate not controlled by the presence of the electron donor? The equation implies that as long as there is sufficient biomass there would be a bio-reduction activity even if there is no further supply of the electron donor. This does not appear meaningful to me.

P9, L7/Eq. 15: Is there a process-related justification of the existence of B_min or has this been introduced for technical/numerical reasons?

P9, L12: No, there are other codes which could be used for this purpose (see comment above for P4, L21). However, I agree that benchmarking is not needed here. PFLOTRAN is well established and any benchmark would not allow determining if the presented concept is meaningful.

P9, L14: Are any of these validations available in the literature? If not this statement

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might of course be true but any evidence for this is lacking.

P 10, L8: Clarify, are the parameters shown in Tables 1 and 2 those also shown in Figures A1 and A2. I support showing these figures to visualize how the case specific input has to be provided but for communicating parameter values a table is more appropriate. Also: where do these parameter values come from, literature, own experiments/studies, educated guess or . . . ? What is the initial porosity (especially for the clogging case shown further down)?

P 11, L2: Is a constant head injection a reasonable assumption? Usually wells impose a certain flow rate. As there is no shear force related biomass removal considered I assume that the model would not predict reasonable effects for a fixed injection rate well.

P 11, L20: If the biomass seems to inhibit any injection through the well, the dithionite injection would not lead to any effects as long as the biomass is not decreasing due to natural decay allowing at least some injection to take place. Right?

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