Response to Referee 1

"SedTrace 1.0: a Julia-based framework for generating and running reactive-transport models of marine sediment diagenesis specializing in trace elements and isotopes", by Jianghui Du

The author provided a Julia based code for generating diagenetic reactive transport codes. The goal of the model development is well described and the code realizes the flexibility to enable various usages targeting at different sediment environments with different tracers of interest. The model's validity has been well examined and example simulations demonstrate the capacity of the model well. Accordingly, I think the paper is well-suited for publication in GMD. Followings are my comments on specifics that I hope the author may find of some use to improve the manuscript.

Reply: Thanks for your comments and suggestions!

Potential internal inconsistency. pH calculation in Sect. 4.2 does not seem to take into account detailed aqueous speciation (e.g., no accounts of Fe + CO3, Fe + HCO3, Fe +HS in Eqs. 27, 28, etc.). However, those are included in aqueous speciation calculation in Sect. 4.3. As long as concs. of included aqueous species with EIs or other tracked aqueous species are insignificant compared to total concs. of EIs/other tracked species, pH calculation as well as mass balance must not be significantly affected, but we can think of a situation where some ion pairs matter relative to EIs/other tracked species, e.g., ferruginous oceans in the Precambrian or deep depths of sediments where porewater chemistry is in equilibrium with some soluble solid phases. This may be my misunderstanding but potential problem here is model's internal inconsistency between aqueous speciation and pH modeling, and potential violation of charge balance in porewater. If this is the case, it should be clarified.

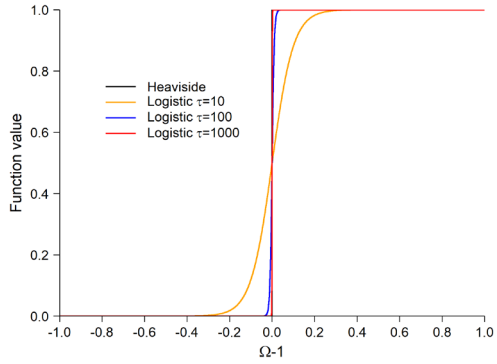
Reply: In SedTrace v1 the major ion speciation is fixed following that of modern seawater, and trace element speciation is assumed to have no impact on major ion speciation (such as HCO3 and CO3) because of low concentration. Thus, the current version of SedTrace is not suitable for cases when seawater/pore water composition is dramatically different from the modern seawater. In the revision, we will clarify this point.

Numerical diffusion. Especially related to Sect. 4.4. It is well known that numerical diffusion affects proxy record and thus different models have attempted to deal with it together with diagenetic reactions (e.g., Kanzaki et al., 2021; Munhoven, 2021). It probably does not affect steady state age-profiles, but the author should make it clear how the model deals with numerical diffusion and its effects on proxy reading or comparison with observations.

Reply: In advection dominated regime transient simulation will perform worse than steady-state simulation because of numerical diffusion using the finite volume complete flux (FVCF) scheme; regardless, even with numerical diffusion the FVCF scheme will ensure at least first-order convergence (ten Thije Boonkkamp and Anthonissen, 2010; ten Thije Boonkkamp and Anthonissen, 2011). As such, SedTrace v1 is best suited for steady-state simulations. That's why currently we do not include any examples of transient simulations of paleo-proxies. We will clarify this limitation of SedTrace in the manuscript.

L419-425. The author should show a plot of Logistic and Heaviside functions as a function of omega so that it is easy for the reader to compare the two functions and evaluate the approximation here as I have not seen this approximation elsewhere. Also, Eq. 24 does not look the same as that in L428. Please make sure they are consistent. Also, it would be better to show how this approximation affect the results where omega calculation can affect sediment profiles (e.g., Fig. 4).

Reply: Yes, there's a typo in Eq. 24. It should be $\tanh(\tau(\Omega-1))/2+1/2$. Thanks for pointing this out. Approximating Heaviside or other discontinuous functions by differentiable functions is common in other fields like engineering and deep learning (Iliev et al., 2017). In the following figure, we show the Heaviside function together with its Logistic approximation. As the parameter τ increases, the approximation becomes better.



We have compared the Santa Barbara Basin model results using the Heaviside function vs. the Logistic approximation (τ=1000) and found the differences are negligible. For example, the relative difference of modeled CaCO3 concentration, mainly controlled by dissolution/precipitation reactions, is at most 10^{-7}. The Logistic approximation is optional and the user can disable it by setting `AllowDiscontinuity = true` in `ModelConfig` when generating code. We will clarify this point in the revision.

Technical comments:

Code. I have tried to install and use the code to test example simulations in this paper (from examples directories) but ended up not being able to (failed with windows Cygwin and virtual Ubuntu in windows). This could be only because of me not used so much to Julia but it might be better to indicate under what environments the code has been tested so far and is supposed to work. This does not have to be in the text but anywhere else like Supplement or docs in code repository.

Reply: SedTrace was developed and tested on Windows 10. And using the GitHub action workflow we have tested it on the latest Ubuntu and macOS (non-Apple silicon chips) platforms. However, it has not been tested on Windows-Cygwin or -Linux virtual machines which we have no access. We did notice in the recent testing that a dependent package has had a breaking change after the release of SedTrace v1.0, causing code failure in certain cases. We have fixed this issue and released SedTrace v1.2 with improved version control system. We will continuously maintain and update SedTrace. And code issues can be reported to the Github page. We will clarify this in the code repository.

L106. Why does it have to be in mathematica notebook, which is not open to everyone? It would be better to give some final form of derivation in the main text or even supplement (or any form available to the reader) rather than saying that the reader can check them if they can use mathematica.

Reply: We have converted it to a PDF file now.

L106. maybe --> may be

Reply: Corrected.

L831. Sensitivity --> sensitive

Reply: Corrected.

L1097. It would be easier to read results if the author also provides delta values (1000 x ln alpha) in per mil.

Reply: Will do.