Comments on manuscript gmd-2021-211,

″RADIv1: a non-steady-state early diagenetic model for ocean sediments in Julia and MATLAB/GNU Octave″
by Olivier Sulpis et al.

General comments:

Sulpis et al. presented a new diagenesis model RADI with some examples of its application. The model adopts recently published rate laws for dissolution of calcite and allows for DBL parameterization. The model will be useful to the community especially because it is written in MATLAB and Julia. The manuscript is concisely written and easily understood. However, I have a couple of points of concern regarding the description of model and its performance evaluation and applicability.

1. Model's overall structure

The overall structure of the model is not described in detail. I could find only a few sentences, e.g., L130-132: 'equations composing RADI are based on CANDI, the method-of-lines code by Boudreau (1996b). Unlike the model of Boudreau (1996b), RADI does not solve a set of reactive-transport differential equations but instead computes the concentrations of a set of solids and solutes at each time step following a time vector set by the user.'

Equations provided by the authors, however, indicate that they seem to use some time-forward finite difference method, e.g., L387: 'backward-difference discretization prevails', and thus they seem to have governing differential equations from which difference equations are derived. If so, what is the difference from CANDI with respect to the general model structure including adopted numerical method?

It is somewhat disturbing to read that the model does not solve reactive-transport differential equations (L130-132), and correspondingly the authors did not provide any governing equations. A general reactive-transport equation (e.g., Boudreau, 1996, 1997) formulates the mass conservation law dictating that mass loss/gain via transport and reactions, and mass change within each sediment layer are balanced for each species. Thus, any model (including RADI) should end up in solving reactive-transport equations although the numerical approach can vary with models. Again, however, the numerical method and its difference (if any) from those of other models (including CANDI) are not clearly described in the text.

2. Model evaluation experiments

In steady-state experiments, the authors used Muds to be compared with RADI (Sections 3.1 and 3.2). However, the comparison does not make any sense to me if RADI is tuned but Muds is not, to specific sites considered in this paper.

Also, the diagenetic influence of the updated rate law for $CaCO_3$ dissolution was discussed by comparing Muds and RADI (Section 3.4). This does not make any sense to me, either, given that ΣCO_2 and TAlk production profiles from OM degradation can be different between the two models. If the authors want to discuss the effect of adopting the new rate law for calcite, they should compare two RADI simulations adopting the new and previous rate laws with individually tuned rate constants under otherwise the same boundary conditions.

3. Model's applicability

The authors argued that RADI can be used for simulations imposing an intense ocean acidification event such as PETM (Section 4.4), but one may doubt it. Under an intense dissolution event (such as PETM), chemical erosion can happen where burial velocity can become negative at certain sediment depths. However, the burial velocity calculation scheme of RADI does not seem to allow this (Eq. (14), Section 2.3 and Fig. 1). Indeed, given that burial calculation does not seem to reflect any mass/volume changes in solid species caused by reactions, the transient simulation of RADI should be limited to the cases where the effect of solid mass/volume changes on burial rate is minor, e.g., short term experiments with minor changes in solid phase concentrations such as those in Sections 4.1-4.3. To enable the application to cases involving a significant $CaCO_3$ dissolution, RADI has to adopt a different burial velocity calculation scheme, such as that adopted by Munhoven (2021, GMD, 14, 3603).

Specific comments:

Fig. 1. Sediment layer/point numbers within the model domain and depths assigned to sediment layers/points seem to be confused. For example, in Fig. 1 Z looks like the total number of sediment points/layers meanwhile it is defined as the total sediment thickness in Table 1 and text. The same goes to dz.

L131-132. Quite vague description of the model. It is unclear how the model is different from or similar to CANDI (please also see general comment 1).

L141. Is the threshold for dz/dt for stability of the numerical solution dependent on w?

L354. Is 30% d^{-1} the most used rate constant with the reaction order of 4.5? I thought 100% d^{-1} is more often adopted in the literature (e.g., Archer, 1991, 1996; Archer et al., 1996).

Eqs. (11)-(14). What is the difference between x and w? Also, in Eq. (13) porewater volume fraction should be used instead of solid volume fraction. How do you calculate w_∞ and u_∞? I guess the authors assume $w_\infty = u_\infty = x_\infty$?

Section 3.1. It does not make any sense to compare 2 models if the 2 models are not tuned to the observations in the same way (only RADI is tuned and Muds is not tuned?). If the rate constants

and/or rate laws are different between the two models, I would expect different boundary conditions for 2 different tuned models.

L528-530. Is the assumption to calculate DBL thickness by Sulpis et al. (2018) consistent with RADI's assumption? In other words, isn't the calculation of DBL thickness by Sulpis et al. (2018) affected by including $CaCO_3$ dissolution by OM-derived CO_2?

L549. The good reproduction of NO_3 profile seems to be achieved at the cost of bad OM profile reproduction, for which Muds does seem to do a better job. I think the same goes to the O_2 profile difference between the two models.

Fig. 4. Calcite concentration does not seem to increase at the bottom, which looks weird given the oversaturation of calcite at the bottom and assuming that RADI allows for precipitation.

Section 3.2. The issues raised for Section 3.1 can apply to Section 3.2.

L649. I guess the authors can definitely tell by repeating the same tuning experiments with RADI adopting the rate law used by Muds. (Please also see general comment 2.) Could you attribute some of differences in ΣCO_2 and TAlk profiles to the difference in OM diagenesis schemes between the models?

Fig. 8. How can it be possible that O_2 and CO_2 fluctuate while OM and $CaCO_3$ do not? Is the magnitude of fluctuation of OM and $CaCO_3$ too small to see in the figure?

Section 4.3. Why changes in OM degradation and $CaCO_3$ dissolution are significant while no changes are recognized in Section 4.2? Is this only because imposed DBL changes are larger in Section 4.3? Or is the response of sedimentary system to DBL change dependent on the time rate of DBL change imposed?

Technical corrections:

L71. 'Cappellen' should be 'Van Cappellen'.

Table 1 and throughout. Although the authors stated that variables are written in italic and model notations are in monospaced font (L93), this rule is not completely followed.