

Review of

# A model for marine sedimentary carbonate diagenesis and paleoclimate proxy signal tracking: IMP v0.9

submitted to *Geoscientific Model Development*  
by Y. Kanzaki et al.

## 1 General comments

Yoshiki Kanzaki and co-authors present the “Implicit model of Multiple Particles (and diagenesis)” (IMP). IMP is an early diagenesis model, build along the lines of the classical model of Archer (1991), which is extended to explicitly include the vertical distributions of all the solids considered. Three different solids are currently considered in IMP: carbonate, organic matter and clay (or any other inert material). Carbonate can be considered in multiple classes. IMP was developed to systematically explore the distortion of proxy signals (e.g.,  $\delta^{13}\text{C}$ ,  $\delta^{18}\text{O}$ ,...) by bioturbation and chemical erosion. Different bioturbation models are considered: biodiffusion, homogeneous mixing, automaton based parametrisation derived from (e)LABS.

The paper fits well into the scope of *Geoscientific Model Development*. I found the study very interesting. The paper is generally well readable, although one stumbles here and there upon sentences whose meaning is not clear or whose syntax is not correct her. It would also gain a lot from a more precise language usage. These – minor – shortcomings should nevertheless be straightforward to fix.

There are other shortcomings that are far more important. The paper has been submitted as a *Model Description Paper*. The model description part is, however, of very uneven quality: while some parts are pleasantly detailed others are lacking even the most important information. It is, e.g., not explained how the  $\text{O}_2$  penetration depth  $z_{\text{ox}}$  is calculated.

The limitations of the diagenesis model are not discussed, not even mentioned. Sulfate reduction is the only sub-oxic/anoxic OM oxidation pathway, thus skipping the energetically more favourable  $\text{NO}_3^-$  reduction, Mn(IV) and Fe(III) reduction pathways. No secondary redox reactions are considered. Some discussion on the implications of these simplifications would be of order.

Similarly, the strengths and disadvantages of the different bioturbation model formulations are not discussed (the biodiffusive approach leads to block tridiagonal Jacobians, that can be inverted by an efficient block oriented Thomas algorithm, whereas the LABS derived transition matrix is likely to be full, without any special structure) and thus contributing to a Jacobian that will be computationally costly to invert.

Finally, the experiment descriptions also leave too many questions open. Here, especially the species-dependent mixing experiment is poorly documented. The current text makes it impossible to understand how exactly the model has been set-up for this experiment.

I am convinced that this manuscript can make an interesting contribution to *Geoscientific Model Development*, provided it undergoes a major revision, to provide a better description of what is done, how it is done and why it is done that way.

## 2 Specific comments

### 2.1 Model Basics and Structure

**Page 8, Eq. (23):** Equation (23) is only valid for intraphase biodiffusion; for interphase bioturbation, there is an extra term related to the porosity gradient (see, e.g. Munhoven, 2021)

**Grid:** The grid description is unfortunately not clear. It starts with a language problem: “[...] discretized into  $N = 100$  irregular grids where the grid size increases [...]” does not make sense. Reading this as “[...] discretized into  $N = 100$  irregular grid intervals where the interval size increases [...]”, and using the information provided in Table 2 (mapping function and control parameter value) to generate the underlying distribution (with 101 grid points delimiting 100 grid intervals), and paying attention to avoid catastrophic numerical cancellation in the factor  $(\beta - 1)$ , with  $\beta = 1 + 5 \cdot 10^{-11}$ , one obtains a very odd result: the deepest grid interval takes more than 81% of the total extent (405.8 cm), the second deepest 2.86% (14.3 cm) and the third one 1.68% (8.41 cm). So, provided the reported information on the grid generation is accurate, I would consider the bottom of the grid as essentially useless. The resulting extreme numerical diffusion might possibly deteriorate the quality of all the results. The extreme jump in the grid interval lengths by a factor of almost 30 from the second deepest

to the deepest interval (compared to less than 2 from the third to the second deepest layer) will lead to tremendous numerical diffusion, which might significantly influence the results further up in the sediment column. Although the adopted mapping function from the normalized regular to the finally used irregular grid is continuous (and continuously differentiable) – a condition that irregular grid mappings have to fulfil to ensure that consistency and convergence order of the numerical discretization schemes remain unchanged – the difference in the grid interval lengths acts, from a practical point of view more, like a discontinuity, which might ruin the convergence properties of the algorithm.

One might furthermore wonder why the model grid has to extend to a depth of 5 m. The useful (“undisturbed” information is tapped at a much shallower depth, just below the mixed layer (i.e., typically at 10–20 cm depth). With a calcite/clay input mass ratio of about 9:1, at most of the order of 10 cm of sub-mixed-layer sediment can possibly be unburied during a chemical erosion event and the information stored in the gridded part of the sediment column deeper than, say 20–30 cm is actually not required here..

I finally also wonder whether the recorded “undisturbed” signal would be consistent with the signal recorded in the main sediment column, even if there were no numerical diffusion – numerical diffusion was put forward as a reason for tapping the useful information right below the mixed layer: even in the absence of numerical diffusion, the signal in the main column may be altered by sub-mixed-layer chemical reactions. Furthermore, if chemically altered material later becomes subject to chemical erosion (i.e., returns to the mixed-layer), its composition can be expected to be different from that in the “undisturbed” record. How important might the resulting inconsistencies be?

**Page 10, lines 267–273:** Why not move this transition matrix representation of the biodiffusive model of bioturbation to Sect. 2.2.2 (“Bioturbation”)? In that place it would contribute to emphasize the overarching nature of the transition matrix approach. A priori, it was not clear in my mind that biodiffusion could also be part of the transition matrix approach (albeit in discretized form).

**Section 2.5.1 (pages 10–11):** This is obviously the central part of this manuscript. I find it quite short in that respect. The advantages/disadvantages (potentials/shortcomings) of the different methods could be stated in more

detail. I would also like to challenge the authors on several assertions made here. I do not see why method 3 is less flexible than methods 1 and 2. To me, methods 2 and 3 are mathematically speaking absolutely identical. The only difference I can see is in the way the input data have to be processed. That processing can, however, be considered to be carried out outside the model itself.

**Page 12, lines 332–345:** The discussion about how time tracking could be implemented is, as far as I can see, not entirely correct. Obviously, method 1 would be extremely costly to adopt for time, but it clearly is the one that would offer the best time resolution. Method 1 essentially discretizes the complete age-dimension carried by one sedimentary component (e.g., calcite) as an ever-growing number of  $\text{CaCO}_3$  variants, each one representing one age-class. It is difficult to comprehend how method 2 could possibly conserve more accurate information with only two variables, compared to method 1. For any given time-step, the input data for method 1 are given by one single class, and those for method 2 by one interpolated value between the end members. To me, one appears as accurate as the other, for any given single time-step. For the next time step, another single class is created and added for method 1, while another interpolated value between the end members is added for method 2, and so forth. After  $n$  time steps with method 1, one can clearly distinguish between the fates of each single class of material brought in during the  $n$  steps; with method 2, this is not possible, as the  $n$  interpolates have been added, with little chance to deconvolve the resulting information. So, to me, method 1 is the accurate one, not method 2.

**Page 14, lines 410–412:**

“This difference can be explained by a burial velocity enhancement caused by high organic matter preservation in the oxic-only model, which is not considered by Archer (1991).”

This is probably correct, but why not check it instead of speculating? This can be easily done by setting  $V_{\text{OM}}$  to 0.

## 2.2 Experiments and Results

**Throughout:** there seems to be a mismatch between “time step” and “instants in time” Actually, no information about the step lengths (time steps) adopted for the integration of Eq. (1) in time.

**Page 14, lines 398–400:**

“Absence of significant void spaces or expansions in solid sediment has been adopted as a convergence diagnostic by the sediment diagenesis model of Archer et al. (2002), [...]”

This sentence could possibly be misunderstood, as this is actually not the only diagnostic used by Archer et al. (2002). Their convergence diagnostic is first “[...] based on conservation of mass to within 2% for all solid phase and dissolved constituents (appropriate balances between rain, reaction, diffusion, and burial rates).” (Archer et al., 2002, p. 17-4, par. [19]). They continue writing that the sum of the solid phase concentrations *also* provides a convergence diagnostic.

Conserving mass to within a few % only – a side-effect of requiring letting the sum of the solids’ volume fractions float within a few % (line 255, page 9) – might be sufficient for steady-state calculations. In transient simulation experiments, I would anticipate that deviations of the order of a few % could cause considerable model drift in transient simulation experiments. It would be better not to leave any loose ends and therefore to enforce strict static volume conservation.

The statement at line 400 (“The results of the second experiment thus confirm [...]”) is a non sequitur. The results do not confirm the applicability of the model for time-dependent simulation experiments: they only do not infirm it.

**Page 15, lines 437ff:** Although I understand that multiplying the transition matrix by 1/10 might facilitate the calculation, it also reduces the mixing intensity by a factor 10, and thus describes a completely different setting. Are the results for the so reduced mixing intensity accepted as final in case the calculations converge, or are they used as a starting point for a continuation method, wherein the mixing intensity is then gradually increased to approach the original matrix? I think that the results obtained with the matrix divided by 10 cannot be used for a comparison with others where no such reduction was adopted.

**Section 3.2.3, pages 17–18** This experiment needs to be better documented. Critical information is missing here: what bioturbation model has been used to get these results? In the text, we read about different bioturbation depths for small and large particles, with reference to Bard (2001). The

bioturbation model of Bard (2001) is, mathematically speaking, rather convoluted and it is not clear to me how it might be transposed to the transition matrix framework adopted here. At first sight, it is possibly a homogeneous mixing model, but I am not entirely even sure that it is possible to transpose it at all into the transition matrix framework of IMP. In that model, the bioturbation depth is the main control parameter. How that bioturbation depth has been used as a control parameter here – if it has, which is unclear as well – is not explained. Please make this description more complete and if necessary also provide additional theoretical foundations

It should also be noticed that some theoretical homework is of order when it comes to different mixing rates for small and large particles. The solids' advection rate is actually always defined as the movement rate of the bulk solids (Meysman et al., 2005, see, e.g.). Accordingly, the advective rate may not be equal to  $w$  in Eq. (1) – this is already not the case when interphase biodiffusion is adopted as a bioturbation model. In case a biodiffusion model is used, it should be noticed that Eq. (23) is not applicable (this is mentioned as a sufficient condition at lines 214–216 for Eq. (23) to hold, but it is also necessary).

### 3 Technical and minor corrections

**Abstract:** Please include the meaning of the model name acronym somewhere in the abstract.

**Page 3, lines 65–66:** “The reason for this is that published sediment mixing models are generally unable to realize diagenetic reaction” – not sure what is meant here (should “are generally unable to realize” possibly read “do generally not take into account”?)

**Page 3, line 81:** “Following presentation” should read “Following the presentation” (or “After the presentation” ?)

**Page 4, line 91:** Is it possible to “share” *distinct* characteristics?

**Page 6, line 160:** “mocsy” should read “mocsy 2.0”

**Pages 6 and 7:** The notation  $dz_i$  for the thickness of layer  $i$  is not recommendable, as there are later ratios of such thicknesses are used (e.g., page 7, Eqs. (13) and (14)), which could be confused with derivatives and thus lead to unnecessary misunderstandings. I suggest to replace  $dz_i$  by  $\delta_i$  or  $\Delta_i$ , perhaps  $h_i$ .

**Page 7, line 181:** Is  $A$  the horizontal cross-sectional area?

**Page 7, lines 195–196:** Very cumbersome and syntactically incorrect sentence. I suggest to reformulate it as "Equation (15) is a finite difference version of Eq. (17) ..."

**Page 8, lines 212 and 213:** I suggest to replace  $D_b$  by  $D_{\theta,b}$  or something the like in these two instances to emphasize that different biodiffusion coefficient values may be used for different particle classes (different classes of particles are later supposed to be transported in different ways by bioturbation) The special case for a single  $D_b$  for all solids then comes more naturally at line 214.

**Page 9, lines 236–237:** This sentence may be misleading, as "specified at the beginning of each time integration" could be wrongly interpreted as saying that an time-explicit approach is used in IMP

**Page 9, lines 253:** How is "significantly different" translated quantitatively?

**Page 10, lines 277ff:** Which version of LABS was used here in the end? Reed et al. (2007)? Or was it eLABS (Kanzaki et al., 2019)? Please specify.

**Page 10, Equation system (24):** First of all, this way of defining  $(K_{\theta,ij})$  is difficult to understand. At first it looks like some kind of implicit definition. Is there not more clear way to write this?

Second there seem to be two errors:

- " $2 \leq j = i + 1 = n_{ml}$ " should probably read  
" $2 \leq j = i + 1 \leq n_{ml}$ "
- " $1 \leq j = i - 1 = n_{ml} - 1$ " should probably read  
" $1 \leq j = i - 1 \leq n_{ml} - 1$ "

**Page 11, line 309:** “[...] and accompanied generation of alkalinity, [...]”:  
not sure what this could mean. With  $\text{Ca}^{14}\text{CO}_3/\text{CaCO}_3$  ratios of the order  
of  $10^{-14}$ , alkalinity changes by  $\text{Ca}^{14}\text{CO}_3$  decay should really be on the neg-  
ligible side of life.

**Page 11, lines 294 and 298:** “ $2^p$ ” should read “ $2n_p$ ” as each proxy re-  
quires two end-members.

**Page 13, lines 364–365:** “5 time steps” should most probably read “five  
instants in time”. By the way, which time step was chosen for the integra-  
tion? A variable one? a constant one – how long?

**Page 13, lines 377ff:** It would be fair to state that these are replications of  
experiments from Archer (1991).

**Page 14, line 392–393:** Strange sentence. – please reformulate.

**Page 14, line 410:** “than Archer (1991) model” would more correctly read  
“than the model of Archer (1991)”

**Page 14, line 434:** “provability” should probably read “probability”

**Page 14, line 413:** “in  $\text{CaCO}_3$  rain” should read “of the  $\text{CaCO}_3$  rain”

**Page 15, line 439:** “are now shown” should read “are not shown”, I guess.

**Page 16, line 455:** would “at depths” not better read “from depths”?

**Page 16, lines 470 and 472:** Text imprecise: chemical erosion requires  
dissolution, but dissolution does not necessarily lead to chemical erosion.  
Please reformulate.

**Page 17, line 490:** “When dissolution is imposed [...]”? Would “When  
dissolution is intensified [...]” not be more correct?

**Page 17, lines 503–504:** “Simulated proxy signals are considerably shorter in apparent duration as described in the above paragraph.” – not sure what this means.

**Page 18, line 520:** “the more” should read “the better”

**Page 18, line 521:** “accumulation rate differs between” would better read “accumulation rates are different for”

**Page 18, line 539:** “The source codes of IMP model” should read “The IMP source codes” (delete “model”)

**Page 18, line 540:** “specific version used of the model” should read “specific model version used”

**Page 22, lines 636–637:** This URL points to the secondary JSTOR archive copy of the reference. It better had to be replaced by the DOI of the original paper (available in open access): DOI:10.5670/oceanog.2009.100

**Page 24, line 710:** The DOI of the MATLAB version 1.1 of CO2SYS is not resolving any more. The current URL is [https://cdiac.ess-dive.lbl.gov/ftp/co2sys/CO2SYS\\_calc\\_MATLAB\\_v1.1](https://cdiac.ess-dive.lbl.gov/ftp/co2sys/CO2SYS_calc_MATLAB_v1.1).

**Page 39, Table 1:**

- I guess, “Number of sediment grids” means “Number of sediment grid points” as there is most probably only one grid.
- For the density of OM, a value of  $1.2 \text{ g/cm}^3$  is reported with reference to Mayer et al. (2004). I have not been able to find that value of  $1.2 \text{ g/cm}^3$  in Mayer et al. (2004). Considering the  $\rho_{\text{OM}}$  values reported for marine samples in Table 1 of that reference, I find a higher value of  $1.45 \pm 0.23 \text{ g/cm}^3$ . Please clarify.

It would be good to specify more clearly that  $\text{OM} \equiv \text{CH}_2\text{O}$ . Only in this case some of the ratios such as the  $\text{OM}:\text{CaCO}_3$  ratio  $r$  make sense, as one mole of OM then represents one mole of OC. Readers used to Redfield composition might be confused else.

**Figures 2, 7, 8, 10:** It is recommended not to use green and red/orange colours tones in parallel on a graph (see <https://www.geoscientific-model-development.net/submission.html> - “Figures & Tables”, point 7)

## References

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Guy Munhoven