Comments

Introduction

The authors of "ARTEMIS version 1.0: A Reactive Transport Enhanced Rock Weathering Model with Coupled Soil Carbon and Nutrient Dynamics" present an extensive modeling effort aimed at simulating the dynamics and impact of enhanced rock weathering (EW) on agricultural land. With PHREEQC as the core model platform, they couple soil geochemistry with organic matter-, plant- and nutrient dynamics (based on SWAT) to track weathering geochemistry and CO2 exchange with the atmosphere. Specific attention goes to fertilizers, with different types implemented and made available for the user. ARTEMIS is set-up to allow flexible user interaction in different agricultural contexts. This is a welcome addition to different EW-models currently being developed and used, and will be an additional tool available to the EW community.

Manuscript organization

While the authors extensively describe all aspects of their setup, the manuscript would benefit from a clearer structure. Scientific motivation of model choices, mathematical model description, model implementation and description of the user interface are currently intertwined, which make the manuscript difficult to digest. Readability, clarity and transparency would improve significantly if these are separately treated. Implementation specific syntax is also intermingled with symbols in the mathematical model description sometimes without clarification (see e.g. remarks on table 4). Examples of unclear structure are given in detailed comments below.

Scientific comments

1. Inconsistent treatment of CO2 production from respiration

My major conceptual problem with the presented model is the inconsistent treatment of CO2-production from microbial respiration. On the one hand, respiration of SOM, manure and residues, and ureolysis are explicitely and dynamically modeled, and the produced CO2 is transferred to the pore water in the typical way that kinetics are stoichiometrically coupled to pore water concentrations in PHREEQC. (The essential parts of the code is found on L:1734; L1766 and L1789 of getphreeqcrun.m where the stoichiometric coupling is defined – for ureolysis on L4048).

But at a second location, i.e. the plant section of the model, heterotrophic respiration is calculated in a different manner. As we read in section 2.8 of the manuscript, total soil respiration (i.e. root respiration + microbial respiration) is computed from plant growth, with specific equations differing for generic crop (equation 40), sorghum (sum of equation 46 and 45) and oil palm (equation 48). Implicit in all equations is that soil microbial respiration is taken as a fixed fraction of root respiration. This is indeed often used as a rule of thumb when no information on microbial respiration is available. **But the main issue here off course is that microbial respiration in this model is computed twice: once in the SOM module, and once (approximately) in the plant module**.

The second issue here is that the authors take a completely different approach to compute the impact on CO2 in the plant module. Instead of dynamically simulating CO2 input, they assume steady state and make use of the analytical solution of the CO2 profile (equation 50). These concentrations are then forced in the model domain by assuming instantaneous equilibrium between the gas and the liquid phase (EQUILIBRIUM_PHASES in PhreeqC). This, at a given alkalinity, completely determines the DIC content of the pore water, and thus any additions made in the parts of the code relating to SOM, manure and residue respiration, and ureolysis, are nullified. In other words: **in this setup, the kinetic coupling of respiration and ureolysis has no direct effect on CO2**.

It is possible that the authors have overlooked this partially because respiration and ureolysis not only produces CO2, but also ammonium. The latter increases the alkalinity of the solution, and thus there is an indirect effect of the kinetic coupling on the DIC of the porewater: increasing alkalinity lead to higher DIC at the same pCO2.

There are several ways the authors could correct this: the most consistent with their current approach, in my view, would be to use heterotrophic respiration from the SOM module (incl. Manure, residus and ureolysis) and add that to the root respiration from the plant module to compute total respiration. This total respiration could then be used in the steady state computation of vertical profile. The ammonium release could still be coupled in the same way as the authors already did.

2. Use of older concepts in SOM dynamics

Scientifically, the treatment of SOM relies on an older concepts of SOM dynamics. This is worrying given the many recent papers on the impact of EW on SOM decomposition and stabilisation (e.g. Steinwidder et al 2024; Boito et al 2025 just to mention a few), and the importance of accounting for both inorganic and organic C when evaluating CDR rates. A good representation of SOM dynamics should build on the current understanding of SOM, i.e. in terms of aggregate and MAOM formations, rather than on the outdated concepts of active and passive pools (many papers over the last decade, check e.g. the work of Francesca Cotrufo and Jocelyn Lavallee). I understand model-choices are often pragmatic, but at minimum a thorough discussion of the implications for model prediction accuracy is warranted.

3. Incorrect equations, and not always clear where ARTEMIS deviates from SWAT

I found a some errors in the equations. Although the authors have used SWAT as an inspiration for nutrient cycling, SOM dynamics and plant growth, the ARTEMIS implementation is different from the SWAT implementation; but the equations and description in the manuscript do not reflect this. See detailed comments below.

In general it is unclear from the text to which extent the treatment of plant growth, nutrient cycling and SOM dynamics in ARTEMIS deviates from the treatment in SWAT – many of the equations in this manuscript seem verbatim copies from the SWAT manual. Since this is a very long paper, I would also suggest to move the equations that are copied from the SWAT manual as much as possible to an appendix. As such you can keep the model description light and focused on model principles, and keep reader attention focused on why SWAT is chosen, where ARTEMIS deviates from SWAT, and on the coupling between the geochemical model and the SOM/nutrient/plant model. And in any case, it should be made clear when equations are quoted from the SWAT manual, and which equations are new or ARTEMIS specific.

4. Secondary phases

The treatment of secondary phases is very limited, in particular an explanation is missing about which secondary phases are allowed to precipitate, and why they were chosen or omitted, and wether this choice was part of the calibration effort or not.

Complex code base; machine specific code; missing files

ARTEMIS is more than a single model, and can bee seen as a platform for applying the embedded model to different contexts. However, the elaborate code was honestly, sometimes intractable. It took me a while to figure out that the main model loop is to be found between L1842 and L2162 of getphreeqc.m. The code contains quite some comments that reflect the developing insight of the coder, and a lot of legacy code that is commented out.

This is a hybrid continuous-discrete time model; a master loop operates on a daily time step, and the inputs of the model (temperatures, soil moisture, etc) are defined at that time step. Within that master loop PHREEQC is called to dynamically simulate the kinetics of weathering, plant and SOM dynamics, and 1D transport. This should be more clearly expa\lained in the manuscript. A tabel of the quantities that are updated by the master loop (using the xxx_MODIFY syntax of PHREEQC or otherwise) would be helpful.

The complexity of the code makes it impossible to fully check the model code (I have only delved in the treatment of CO2, see above). However I found some machine specific code that will not run on other computers (one example on L453 of getphreeqcrun.m we find dbdir='/home/lyla/phreeqcdbincludefiles/'). Also some files that are referenced in the code are not distributed (e.g. file basaltRATESPHASES4 at L287 of getphreeqcrun); it is not clear if this is an obsolete reference or not.

Detailed comments

Section 2.1 See comment on manuscript organisation. Already in the very beginning, the paper quickly goes into technical and unnecessary detail about user options about how cation exchange is treated and parameterized.

L104-108 p5 At the end of the section about inorganic dissolution and precipitation, limitations and recommendations with regards to to organic matter cycling are included. These would be better placed in the discussion section.

L119-130 → discussion section

L190-204 → discussion section

L260 → major pathways to acidification, but no mention of respiration?

L272 → Decomposition helps reverse acidification because it releases nutrients back to the soil??

L294-296 → Model motivation

L297-299 → Discussion section

L300 – 357 detailed comments on SOM treatment:

- As it decomposes, SOM transforms to increasingly recalcitrant forms which decompose more slowly → this is an outdated view of SOM dynamics. See general remark.

- The choice for the SWAT model is not motivated. Why did the authors believe the SWAT model is up to the task? What are the strengths and weaknesses of the SWAT model? This is also not discussed later on.

- Further, I believe this description is just the repetition of the most important parts of the SWAT model treatment of SOM dynamics, and N- and P-release. But from the way it is written, this is not entirely clear. Please introduce the section as such (e.g. "SOM dynamics was implemented as in the SWAT model; we repeat the most important equations below") , and motivate why these specific equations of the SWAT model are mentioned. Please also consider whether these equations can be put in an appendix.

- More importantly: the key equations 8 and 12 are incorrectly written down.

The right hand sides (RHS) of both equations are the daily total amounts of nitrogen transferred respectively from the passive to the active pool, and from the active pool to the nitrate pool. This is consistent with the SWAT manual (p180-190), and with lines 215 and 227 of the nminrl.f code (https://bitbucket.org/blacklandgrasslandmodels/swat_development/src/master/).

Since SWAT runs at a 1 day time step, this is in fact the rate, integrated over 1 day, or the difference between the pools over a time step. So the new value of the state values is the old value, **increased/decreased** with these integrated rate. See also L222 and 240 of the abovementioned SWAT model file.

Or for equation 8: N_hums,new = **N_hums,old +** RHS_8

An similarly for equation 12: N_huma,new = **N_huma,old +** RHS_12

If the authors want to write down the SWAT equations, that's what they should have written. However …

- This is NOT what is implemented in Artemis. The stable and active humic species are implemented as KINETIC species in PHREEQC. (see the file ./phreeqcdbincludefiles/SWATRATESPHASEStunable where this part of the model is and not as a discrete, 1 day time step model as SWAT and as implied by the manuscript description. This means that the authors have used the RHS of eq 8 and 12 in a differential equation, and let phreeqc explicitely integrate this using the internal variable time step integrator. So to be consistent with the implementation, the correct equations 8 and 12 should be:

d_N_hums/dt = RHS_8

d_N_huma/dt. = RHS_12

- Similar remark for equation 13 I'm not going to work it out here but please do correct.

- I haven't checked equation 14 – please check all equations and correct when necessary.

- Implementing a model with a fixed daily time step, in a variable time step scheme typically means recalibration is needed, what is I believe what the authors have done, but should describe explicitely.

- Table 4: Please add a column to this table with the symbols used in the manuscript. This table contains code specific paramter names, which are different from symbols in the manuscript. I assume e.g. that the first parameter kNhumsday corresponds to the parameter beta_act in equation 12, and the second humactfract corresponds to f_active in equation 8? Please be consistent and complete.

L337 “By default, ARTEMIS releases CO_3^{2-} stoichiometrically along with ammonium from the active humus pool.”. See general comment on treatment of CO2.

L356-357 → Implementation specifics

L375 Please mention that this is the nitrification rate.

L379-382 → Implementation specifics

L359-391 description of nitrification, denitrification and volatilization of ammonia: it comes across as unnatural to first describe the temperature and moisture dependence and only later the rate laws themselves. Please reverse. Also, it would be helpful to describe in words “nitrification+volatilization, and denitrification are modeled as first order rate laws, with rate modulation factors for moisture and temperature dependence” or something along those lines.

L379-382 → implementation specifics

L397 “t is time (elapsed hours)” → does it matter that time is measured in hours here? In other locations, rates are given as “per day”, and isn’t phreeqc internally running in seconds? Please consider using a single unit of time throughout.

Table 6 UANx is a fertilizer that contains Urea. In the model code (file ./phreeqcdbincludefiles/plantRATESS L491-544 I find a rate law implementation for ureolysis with urease. This is not described in the manuscript, and therefore it is not clear whether Urea stays unaltered in solution upon dissolution of fertilizer pellets, or whether it is hydrolized using the implemented rate law.

L404 As with SOM dynamics and nutrient cycling, I miss a synthetic description of model principles in the section about Plant dynamics. The authors mention “nutrient uptake is demand based” and then in the second sentence immediately go to user specifics. On how to describe general model principles, the SWAT manual can serve as inspiration: “The plant growth component of SWAT is a simplified version of the EPIC plant growth model. As in EPIC, phenological plant development is based on daily accumulated heat units, potential biomass is based on a method developed by Monteith, a harvest index is used to calculate yield, and plant growth can be inhibited by temperature, water, nitrogen or phosphorus stress.”.

L475-721 Hydrology and CO2: I second the community comment and the other reviewer’s comments on the treatment of hydrology and CO2 transport. General remarks about readability, manuscript structure and explicit differentiation SWAT code also hold here.

L525 I like the joke on this line.

L700 “However, note that CO_3^{2-} is by default released during decomposition of organic matter (Sections 2.3.2 and 2.3.3), such that heterotrophic respiration is partially dynamic.”. See general comment on CO2 treatment. I believe that what the authors here mean is that the alkalinity addition by respiration changes the carbonate system, and thus changes the DIC in the porewater even at constant pCO_2.

L713-717 → discussion section