Response to Reviewers and Comments (ARTEMIS Version 1.0)

General response

Many thanks to Carl Steefel and the two anonymous reviewers for their comments and recommendations. These comments were helpful not only for the manuscript itself, but for Version 1.1 and future model development. We especially appreciate the time taken to read and critique a long, technical manuscript, and in the case of anonymous reviewer 2, to actually delve into parts of the code as well.

There were several key points/recommendations made by all three:

1. **<u>The model should solve the Richards equation rather than relying on the simplistic hydrology (bucket model) implemented in Version 1.0.</u> A newly upgraded version (1.1) of the ARTEMIS model now solves the Richards equation. The revised manuscript will feature model runs with the new hydrology, along with figures showing how the hydrological variables, weathering rates and alkalinity export differs from the simplistic bucket model. The new code and a revised user guide will also be uploaded to zenodo (Version 1.0 being frozen) and referenced in the revised manuscript.**
2. **<u>The manuscript is too long and reads like a user manual.</u> Much of the text in the Methods section related to running the code is being relegated to the new user guide for Version 1.1 of ARTEMIS.**
3. **<u>Compare ARTEMIS with existing geochemical models.</u> We have a new table of models used for recent or widely-cited ERW and related publications in progress. These include CrunchTope (Stolze et al 2024), TOUGHREACT (Deng et al 2023), T&C SMEW (Zhang et al 2025), SCEPTER (Baek et al 2023,Kanzaki et al 2022,2025), the Sheffield integrated ERW model (Beerling et al 2025) and the PHREEQC modelling from Kelland et al 2020. We also include MIN3P (Mayer et al 2012) and WITCH (Godderis et al 2006) as these arise in our updated discussion of biological processes and forcings.**

4. **Show how ARTEMIS responds to processes. The revised manuscript will include new figures showing effects of respiration (autotrophic and heterotrophic), nutrient uptake, fertilisers, organic matter decomposition, surface and roughness fractals, nitrogen cycling and the new soil moisture from the Richards equation. This may end up in the Appendix.**
5. **Gas diffusion should be explicitly modelled. We agree that this should be done, not only for CO2 and O2 but also for NH3, N2O and NO2. Their emissions, which affect air quality and overall greenhouse gas balance, could also be modelled given much of the nitrogen cycle is already represented. We consider that our present approach, where we calculate the layer CO2 gas concentrations before the model run, will suffice for the time being. We already include a figure showing the time-series of these concentrations (Figure C1 of the submitted manuscript), but will also include a new figure showing CO2(g) curves with depth.**

Specific line-by-line responses:

Anonymous Referee 2 (RC2)

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.

Thanks; that was what we were aiming for.

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.

Much material in the Methods has been relegated to the Version 1.1 user guide. We will reorganise the remaining material so that the motivation, description, implementation are less intertwined and easier to digest in our revised manuscript.

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.

Thanks for pointing this out. The production of CO2 during decomposition is indeed microbial, yet one of the drivers of this model is total soil respiration which will include heterotrophic (microbial) respiration. There are several ways to approach this double-accounting. First, we can switch off the CO2 production during decomposition, and this can easily be done with a keyword argument to the model (getphreeqcrun.m). The alternatives are to try to remove the heterotrophic respiration component from the given total soil respiration, so that the model is forced only with autotrophic respiration. Ideally, root respiration should be represented kinetically as a function of the biomass. As there is not enough time to develop the alternative approaches now, our new model runs will have no CO2 production during decomposition. We are aiming to improve the representation of gas phases in future, and will revisit the respiration at that time.

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.

That is correct; the CO2 is currently reset every day based on the analytic profile, as respiration is not represented explicitly. (It also means that double-accounting for heterotrophic respiration as discussed above is currently counteracted every day.) The idea was that respiration would keep the CO2 concentrations topped up, but there are better approaches that will be explored alongside addition of gas diffusion and emissions.

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.

Yes, ammonium is produced during decomposition (and ureolysis), and this component of the nitrogen cycle was a key reason for trying to represent decomposition and ureolysis in ARTEMIS. And yes, CO2 production during decomposition should have been switched off given we were forcing the model with total (heterotrophic+autotrophic) soil respiration from the Community Land Model, rather than the modules available to create soil respiration e.g. for sorghum. We did indeed overlook these issues and there will be no such double-accounting in the revised version.

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.

Thanks, this is a good approach in combination with gas diffusion and will be implemented in the next model version. Heterotropic respiration will be removed from the modules currently available to calculate it in the preprocessor (e.g. for sorghum and oil palm). Note however that these modules are not used in cases where total soil respiration is a forcing, as in our current set of model runs. In that case, one would need to remove the heterotrophic respiration from the total respiration. When using another model to generate a respiration forcing, one would need to be careful to use autotrophic respiration only. In any case, the aim for the next model version is to represent root respiration kinetically, as discussed above.

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.
The SWAT-based SOM module was developed in 2020 and was envisioned as a placeholder pending implementation of decomposition schemes in major land models (e.g. Century in the Community Land Model). It was indeed a pragmatic choice at the time. However, those land models, and widely-used soil carbon models such as RothC, still have organic carbon pools that also predate current views of POM/MAOM. Although we have already acknowledged that ARTEMIS does not represent MAOM-ERW interactions, we agree that the limitations of the SOM module deserves more attention and will update the text of our revised manuscript accordingly. Most of the other ERW models in our new Table have fewer carbon pools than ARTEMIS, and also do not reflect the more recent concepts of POM and MAOM. The exception in our table is T&C-SMEW, which has dissolved, POM and MAOM pools. We note that ERW interactions with MAOM are being actively investigated experimentally; we do not know of any model that represents ERW effect on MAOM, for example.

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.
We agree; see the specific points about the equations 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.
Yes, some of these equations are like those presented by Neitsch et al (2011) for the SWAT model. We will move some of that material to an appendix in our revised manuscript, or relegate to the updated user manual.

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.
Secondary phases were chosen for pragmatic reasons; they were not part of the calibration effort. Carl Steefel raised the matter of secondary phases as well, as they undergo various transitions on timescales which may or may not be relevant for ERW. PHREEQC tends to precipitate only the phase with the most favourable thermodynamic parameters, so phase-phase transitions are difficult to represent realistically. For example, gibbsite was chosen as the representative Al sink because the amorphous Al(OH)3 which precipitates first converts to gibbsite on timescales (days to weeks) which are very short compared to the timescales of interest for ERW (years to decades). We will add text to clarify the reasons for our choice of secondary phases in our revised manuscript.

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.
Thanks for taking the time to look at the code and apologies for the clutter. It is being reorganised, with preliminary code related to settings and metadata relegated to nested functions and legacy code removed. The development effort took place over several years, with different versions for different experiments all contributing to the code uploaded to zenodo. The version 1.0 software already on zenodo is frozen, so these changes will be reflected in version 1.1, which also includes other model updates including implementation of the Richards equation.

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.
This is a good idea; a detailed version is possibly best placed in the user guide which already contains some diagrams and information (but not a diagram showing the loop structure) in a chapter called "Navigating the software". In the revised manuscript, we will restrict ourselves to a simpler version.

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.
Thanks for identifying that hardcoded path; it has been replaced in version 1.1 of ARTEMIS. A new environment variable $ARTEMIS has also been created to avoid these kinds of issues. Thanks for noticing that the file basaltRATESPHASES4 was missing. It had been

accidentally removed along with some earlier versions, but has now been reinstated in the phreeqcdbincludefiles subdirectory. It differs from basaltRATESPHASES5 in that the latter has a corrected formula for the Tawau andesitic basalt. These changes will be part of Version 1.1, as Version 1.0 is frozen on zenodo.

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.
User option material is being moved to the User Guide for Version 1.1 of ARTEMIS, and out of the revised manuscript.

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
We will move these sections of text as suggested in our revised manuscript.

L260 → major pathways to acidification, but no mention of respiration?
We will add a remark about respiration in the revised manuscript, which applies to all ecosystems. The pathways listed here are specific to agriculture.

L272 → Decomposition helps reverse acidification because it releases nutrients back to the soil??
We will reword this text as it is release of base cations from organic matter that counteracts acidification.

L294-296 → Model motivation
The revised manuscript will be reorganised as suggested.

L297-299 → Discussion section

The revised manuscript will be reorganised as suggested.

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.

yes, this approach does not reflect the current view of particulate and mineral-associated organic matter. This is true of other models in our new table as well. We will discuss this in our revised manuscript.

- 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.

In the earlier stages of ARTEMIS development, SWAT offered a denitrification approach that did not depend on variables that ARTEMIS lacked, such as oxygen. Because SWAT is widely used it seemed like a good choice at the time. The three-pool organic matter and other N-cycle kinetics were added at the same time. We will discuss the strengths and weaknesses of the SWAT carbon pools and kinetics in the revised manuscript.

- 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.

We will relegate some of those equations to the user guide, and cite Neisch et al (2012) in the revised manuscript.

- 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
Thanks, this is a good point; PHREEQC does indeed treat these as differential equations, and this has been corrected in the revised manuscript as suggested.

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

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

- 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.

Thanks for pointing this out; we will describe these steps in the revised manuscript.

- 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.

Thanks, we will update that table, which may be better placed in the new user guide.

L337 “By default, ARTEMIS releases CO2−3 stoichiometrically along with ammonium from the active humus pool.”. See general comment on treatment of CO2.

CO2 will no longer be released by default in Version 1.1, as heterotrophic respiration is likely to be included in the total respiration where that is used as a forcing. The daily resetting of the gas concentrations is also incompatible with this setting.

L356-357 → Implementation specifics

This material will be relegated to the new user guide.

L375 Please mention that this is the nitrification rate.

Agreed.

L379-382 → Implementation specifics

This material will be relegated to the new user guide.

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.

Agreed, this will be reversed as suggested.

L379-382 → implementation specifics

This material will be relegated to the new user guide.

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.

thanks for pointing this out. Yes, PHREEQC does internally operate in seconds. The pellet dissolution parameters (Table 7 of the submitted manuscript) are given per hour from the original publication, so the equation reflected those time units. Within the BASIC code in the RATES block, these units are converted accordingly. We will clarify these points in the revised manuscript.

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.

Urea decomposes according to the Ureolysis rate law. We will revisit this text and clarify this point.

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.”.

Thanks, we will reword that text as suggested.

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.

As stated in our general response to the common points raised by both reviewers and the community comment, the Richards equation is implemented in Version 1.1; gas diffusion and advection is planned for subsequent development. The revised manuscript is being cleaned up as suggested.

L525 I like the joke on this line.

Ooops! TiCAT was likely a global change which should not have been applied to the word "sophisticated"!! Thanks for pointing it out. We are glad it provided some amusement but the mistake has been corrected.

L700 “However, note that CO2−3 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 alkalinityaddition by respiration changes the carbonate system, and thus changes the DIC in the porewater even at constant pCO2.

Because the layer pCO2 is reset to predetermined values every day, however, CO2 from decomposition cannot alter layer pCO2 too greatly. Nevertheless, release of CO2 should not automatically take place when the total respiration is a forcing, and indeed should not take place at all until gas diffusion has been implemented.

L713-717 → discussion section

This material will be moved as suggested.