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RESEARCH ARTICLE

REVISED Machine learning-based identification of key biotic and abiotic drivers of mineral weathering rate in a complex enhanced weathering experiment

[version 3; peer review: 2 approved, 1 approved with reservations]

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Abstract

Background

The optimization of enhanced mineral weathering as a carbon dioxide removal technology requires a comprehensive understanding of what drives mineral weathering. These drivers can be abiotic and biotic and can interact with each other. Therefore, in this study, an extensive 8-week column experiment was set up to investigate 30 potential drivers of mineral weathering simultaneously.

Methods

The setup included various combinations of rock types and surface areas, irrigation settings, biochar and organic amendments, along

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with various biota and biotic products such as earthworms, fungi, bacteria and enzymes; each varying in type or species and quantity. The resulting changes in dissolved, solid, and total inorganic carbon (ΔTIC), and total alkalinity were calculated as indicators of carbon dioxide removal through mineral weathering. Three machine learning models, Least Absolute Shrinkage and Selection Operator (LASSO), Random Forest and eXtreme Gradient Boosting (XGB) regression, were used to predict these indicators. Dominant drivers of the best performing model were investigated using SHapley Additive exPlanations (SHAP).

Results

SHAP analysis revealed that each CDR indicator was influenced by different factors. However, key drivers were consistently abiotic, though biota also made a significant contribution to the predictions. The most representative CDR indicator, ΔTIC, was predominantly driven by steel slag addition and mixed rock grain sizes but was also substantially impacted by earthworms and microbes.

Conclusions

These findings provide valuable insights into the complex interplay of numerous abiotic and biotic factors that affect mineral weathering, highlighting the potential of machine learning to unravel complex relationships in biogeochemical systems.

Plain language summary

The increasing concentration of carbon dioxide (CO_2) in the atmosphere, driven by human activities, is the primary cause of global warming. To limit global temperature rise to below 2°C, CO_2 emissions need to decline to net zero, and excess CO_2 must be removed using carbon dioxide removal (CDR) technologies. Many existing carbon capture technologies are energy-intensive and compete for resources such as land, making them challenging to scale. As a result, alternative methods like enhanced weathering are gaining attention due to their potential for CO_2 removal without these drawbacks.

Natural mineral weathering is a process where carbonic acid, formed from CO_2 and water, reacts with minerals, breaking them down and capturing carbon in the form of dissolved bicarbonate ions or carbonate minerals. This natural process slowly reduces atmospheric CO_2 over long time scales. The process can be enhanced, amongst others by grinding minerals to increase their surface area, which leads to an increase in CO_2 removal, but potentially also yields co-benefits, such as improving soil health. Besides grinding minerals, biota could possibly further enhance weathering, for example by producing organic acids, enzymes and siderophores, or by physically mixing soil and rocks. However, the impact of these biota on mineral weathering

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and the interactions between multiple drivers of mineral weathering are complex and not yet fully understood.

To explore these drivers, an extensive column experiment was conducted with 200 columns per round, running across 10 rounds. Each column contained unique combinations of minerals, organic amendments, and biota, including bacteria, fungi and earthworms, and was irrigated with different flow rates and frequencies. The impact on CDR was assessed using indicators such as changes in dissolved inorganic carbon, solid inorganic carbon, total inorganic carbon, and total alkalinity.

Given the complexity of the dataset, machine learning (ML) was used to predict the CDR indicators. To address the "black box" nature of the used ML models, they were combined with explainability methods, which identified the most influential drivers of mineral weathering. These drivers were mainly abiotic, but several biota also had a substantial impact on the predictions.

This study demonstrates how combining large-scale experiments with ML and explainability techniques can provide valuable insights into optimizing enhanced weathering strategies for CDR.

Keywords
enhanced mineral weathering, carbon sequestration, machine learning, explainable AI

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REVISED **Amendments from Version 2**

We rephrased a sentence in the penultimate paragraph of the Introduction. In the Methods, we elaborated the Data preprocessing section. In the Extended Data, we added SHAP interaction plots of the dependence of the SHAP values of irrigation flow rate, the number of earthworms and the inoculum densities of A. pullulans and of B. subtilis, with the surface area of steel slag (Figure C6). In addition, a number in Table A6 was corrected.

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Introduction

The increasing concentration of carbon dioxide (CO_2) in the atmosphere due to human activities is the main driver of climate warming (IPCC, 2018). To limit global warming to below 2°C, CO_2 emissions must decline to net zero as quickly as possible and excess CO_2 must be removed from the atmosphere using carbon dioxide removal (CDR) technologies (IPCC, 2018). In response, scientists across various fields are exploring and optimizing CDR technologies. One such CDR technology is enhanced weathering (EW), which accelerates the naturally occurring process of mineral weathering (Hartmann *et al.*, 2013; Köhler *et al.*, 2010). In mineral weathering, dissolved carbonic acid (which is in equilibrium with gaseous CO_2) reacts with minerals to form water-soluble bicarbonate ions, increasing dissolved inorganic carbon (DIC), part of which may not be degassed back to the atmosphere for millennia (Berner, 2004; Hartmann *et al.*, 2013; Köhler *et al.*, 2010). During the mineral weathering process, disintegrating rocks also release cations and silica (Beerling *et al.*, 2018; White & Buss, 2014), and part of the formed DIC and cations (e.g., Ca^{2+}) may react and precipitate carbonate minerals, forming solid inorganic carbon (SIC) and releasing part of the CO_2 originally sequestered (Hartmann *et al.*, 2013).

Natural weathering rates can be vastly accelerated by, amongst others, grinding minerals to increase reactive surface areas, which gave rise to the term EW. EW could exploit significant quantities of waste rock streams (Renforth, 2019) and may have agricultural co-benefits (Beerling *et al.*, 2018). Moreover, EW does not compete for land with other CDR technologies such as soil organic carbon sequestration, reforestation or bio-energy production with carbon capture and storage (BECCS) and may thus be combined with these CDR technologies (Horton *et al.*, 2021; Janssens *et al.*, 2022). However, care must always be taken to ensure that the added minerals will not increase heavy metal availabilities beyond risk-bearing thresholds (Dupla *et al.*, 2023; Gastmans *et al.*, 2016; Vienne *et al.*, 2022).

To date, efforts to accelerate mineral weathering have predominantly focused on a suite of abiotic variables, such as mineral type and grain size. The potential impacts of biotic factors are often overlooked (Vicca *et al.*, 2022), despite the fact that studies have shown that biota can potentially boost weathering. For example, fungal and bacterial species can actively facilitate the weathering of silicate minerals (Berner, 2004; Finlay *et al.*, 2020). One mechanism by which biota accelerate mineral weathering is their respiration, increasing the CO_2 pressure of the system. Consequently, due to Henry's law, concentrations of the weathering agent carbonic acid increase and CDR is stimulated (Dontsova *et al.*, 2020; Gerrits *et al.*, 2020; Perez-Fodich & Derry, 2019; Vicca *et al.*, 2022). Besides CO_2 pressure, a manifold of biotic factors, such as enzymes and siderophores (chelators) could further stimulate weathering (Vicca *et al.*, 2022; Wild *et al.*, 2022). To date, the complexity of biota-weathering relationships is far from resolved (Milici *et al.*, 2024), and Deng *et al.* (2023) recommended future research aimed at improving understanding of the roles of biotic-abiotic interactions in controlling EW efficiency.

In soils, quantification of EW is exceptionally difficult, among others because the increases in DIC and total alkalinity (TA) following mineral weathering can be undone by secondary mineral precipitation, which may remove DIC and TA from the soil solution (Amann *et al.*, 2022; Kelland *et al.*, 2020; Niron *et al.*, 2024). In real-world situations, e.g., in agricultural experiments, this is aggravated by the fact that soils are extremely heterogeneous in almost every aspect, often rendering soil samples poorly representative for the total soil. For this reason, EW experiments are often conducted in controlled environments, such as column experiments, to ease the quantification by homogenizing many of the variables potentially affecting EW rates. Given the myriad of abiotic and biotic drivers at play, along with their broad potential ranges, it is virtually impossible to test every conceivable combination of experimental settings in a repeated multifactorial experiment. Therefore, experiments that aim to simultaneously test the many possible drivers and their interactions inevitably result in complex datasets that make traditional statistical methods ineffective. The mostly unreplicated driver combinations in such complex experiments, as well as relatively small amounts of data compared to the number and possible ranges of possible drivers, open the door to a machine learning (ML) approach.

Most EW studies focused on the effects of only one driver or at best a combination of two or three drivers. This leaves the interaction effects of multiple drivers on EW largely unknown. Here, to simultaneously test the impacts of 30 potential biotic and abiotic drivers of EW, each with multiple different added amounts or size classes, an extensive column experiment was set up with unique combinations of rock powders, organic amendments, biota and biotic products (Calogiuri *et al.*, 2023). These column inputs were chosen to explore several research questions. For example, steel slags are known to weather faster than basalt, but may lead to unlivable conditions for biota due to potential rapid increases in pH and heavy metals. Therefore, various rock types were assessed individually and in mixtures. Second, studies have shown that finer grain sizes increase weathering rates due to increased reactive surface area (Basak *et al.*, 2021; Vanderkloot & Ryan, 2023). However, fine grain sizes may block or retard water infiltration, leading to pore water oversaturation and precipitation of newly formed minerals that may even inhibit further weathering (Amann *et al.*, 2022). In our experiment, grain sizes were therefore varied and often mixed. Additionally, as biochar may scavenge base cations from solution and theoretically shift the equilibrium of mineral weathering

(Amann & Hartmann, 2019), biochar was added to some of the applied mixtures. To test the impact of biota on the weathering rate, species of bacteria and fungi that were previously shown to induce mineral weathering, amongst others through production of enzymes and siderophores and through formation of biofilms on rock surfaces (Corbett *et al.*, 2024; Gerrits *et al.*, 2020; Gostinčar *et al.*, 2014; He *et al.*, 2021; Kim *et al.*, 2005; Niron *et al.*, 2024; Nwoko *et al.*, 2021), were added to the mixtures. Also earthworms were added, primarily for their soil mixing activity, removing precipitated secondary minerals from the silicate surfaces, and to stimulate microbial activity (Vicca *et al.*, 2022). To support the activity of the microbes and earthworms and fuel their respiration, different types of organic amendments were added. Moreover, we tested the effect of adding nitrogen and phosphorus on EW via a potential effect on microbial activity. Last, the addition of enzymes and organic acids was assessed. The columns were then irrigated at different frequencies and throughput rates. Due to the open column setup, CO_2 and thus CDR could not be directly measured. Instead, the impact of the inputs on CDR through mineral weathering was assessed based on measurements of SIC, DIC and TA, and on the inorganic carbon (IC) and TA initially present in the system. These are commonly used indicators of silicate weathering (Clarkson *et al.*, 2024). The change in DIC leaching and in SIC sum up to the total inorganic carbon (TIC) sequestration. TA can provide further insight into differences in weathering dynamics between treatments.

The resulting data was thereafter analysed using an ML approach that combined predictive modeling and model explainability, as has previously been done for other high-dimensional setups, e.g., in pharma industry (Bannigan *et al.*, 2023; Luo *et al.*, 2024), health industry (Raihan *et al.*, 2023) and to study water- and air quality (Bacanin *et al.*, 2024; Park *et al.*, 2022; Wang *et al.*, 2021). We selected three predictive ML models; least absolute shrinkage and selection operator regularization (Lasso), Random Forest (RF), and eXtreme Gradient Boosting (XGB), which are popular tools in literature and which we chose for the following desirable characteristics; Lasso performs linear regression combined with feature selection by penalizing less important variables, which is particularly useful in high-dimensional settings where many predictors may be irrelevant (Santosa & Symes, 1986; Tibshirani, 1996). This feature selection is achieved through L1 regularization, i.e., by adding a penalization term to the L1-norm of the coefficients in the regression model. This results in a sparse solution where some coefficients are exactly zero (Tibshirani, 1996). Consequently, Lasso excludes unimportant predictors, which simplifies the model and enhances the accuracy. Weathering reactions, such as those promoted in enhanced weathering experiments, are driven by thermodynamics and are, in absence of biotic interactions, highly linear such that their kinetics can be modelled well (Curtis, 1976; Heřmanská *et al.*, 2022; Heřmanská *et al.*, 2023). Model outputs may be transformed to yield linear relationships or normal distributions, enabling parametric statistical approaches to elucidate results from experiments or variability in time series. However, *in situ*, microbes will respond to the altered environmental conditions and availability of elements in soils, among others by altering their respiration, exudation of organic acids, or taking up reaction products. These microbial responses thus elicit a suite of feedbacks that the current generation of geochemical models cannot reproduce, rendering some geochemical reactions unpredictable and highly non-linear. Under these real-world conditions where reaction kinetics cannot be reproduced by existing models, machine learning that can cope with non-linear relationships may enable the attribution of observed changes in weathering reactions to potential drivers.

RF and XGB allow modeling nonlinear relations and employ ensemble tree learning to improve the prediction accuracy (Chen & Guestrin, 2016; Ho, 1995). RF achieves this through bootstrapping decision trees and the final prediction is obtained by averaging the outputs of all the trees, effectively reducing overfitting and increasing model robustness (Ho, 1995). As a result, RF is increasingly used for ecological applications, e.g., Xie *et al.* (2021); Shi *et al.* (2021). XGB is an advanced boosting technique that refines its predictions by iteratively training new trees to correct the errors of the previous trees, often leading to superior performance (Chen & Guestrin, 2016). Furthermore, XGB includes mechanisms for regularization, which helps prevent overfitting by controlling the complexity of the model, making it both a flexible and robust choice for predictive modeling in ecological and environmental studies. Although XGB often outperforms RF, application of XGB in ecology (e.g., Huang *et al.* (2019); Park *et al.* (2022); Valavi *et al.* (2022)) is less prevalent. Other ML models have shown little added value compared to XGB on small, tabular datasets; with e.g., neural networks underperforming on such datasets and proving harder to explain (Shwartz-Ziv & Armon, 2022), and support vector machines often being more complicated to tune and not as accurate.

The main drawback of RF and XGB is that they, like most ML models, are black box models, meaning that they are not inherently interpretable (Lucas, 2020). This drawback can be largely overcome by combining the black box ML models with explainability techniques such as Shapley Additive exPlanations (SHAP) (Lundberg *et al.*, 2017) or Local Interpretable Model-agnostic Explanations (LIME) (Ribeiro *et al.*, 2016). These techniques provide information on the importance of the input features to the predictions and have previously been used in ecology to study, amongst others, species distribution models (Ryo *et al.*, 2021), water ecosystems (Kruk *et al.*, 2021), water quality (Park *et al.*, 2022; Wang *et al.*, 2021), tree species richness (Brugere *et al.*, 2023) and plant phenology (Mortier *et al.*, 2024). We used SHAP values to enhance the interpretability of the black-box models, as they are model-agnostic, can account for interactions between features and are often used in ecology (Brugere *et al.*, 2023; Kruk *et al.*, 2021; Mortier *et al.*, 2024).

Notwithstanding that DIC resembles TA in most organic-poor systems, in organic-rich systems, TA has an inorganic and organic component (Song *et al.*, 2020). Moreover, in a purely abiotic system, DIC and SIC are in equilibrium (yet controlled by kinetic rate constants of carbonate precipitation and

dissolution), implying that a driver that accelerates or decelerates SIC formation would induce opposite changes in DIC and SIC, relative to comparable columns without the driver. However, biota can influence these kinetic rates, e.g., by exuding acids or the enzyme carbonic anhydrase, or by kickstarting precipitation due to cells functioning as carbonate nucleation sites. Therefore, we hypothesise that the prediction of change in amount of SIC (ΔSIC), change in amount of DIC (ΔDIC) and change in amount of TA (ΔTA) will be driven by different features.

This study aims to uncover how mineral weathering results in CDR by combining insights in the key drivers of four different mineral weathering indicators. First, this paper summarizes the extensive column experiment designed to test the effects of 30 potential abiotic and biotic drivers on EW. Next, the weathering process is evaluated by calculating four different indicators of mineral weathering rate, i.e., ΔDIC, ΔSIC, change in amount of TIC (ΔTIC) and ΔTA. To address the challenges posed by the complexity and dimensionality of the dataset, we first employed a range of regression models, including Lasso, RF, and XGB, to predict the CDR indicators based on the input materials of the columns. Finally, by integrating these ML models with explainability through SHAP values, we gained deeper insights into the underlying mechanisms of mineral weathering, making this approach a powerful tool for optimizing enhanced weathering strategies.

Methods

Column experiments

In order to elucidate the influence of abiotic and biotic factors on EW, ten rounds of column experiments were conducted in a climate chamber set at 25°C and 30% relative humidity. Each round consisted of 200 columns, each of which comprised a cylinder (7 cm diameter x 15 cm height) filled with a mixture of a wide range of combinations of abiotic and biotic inputs. Full details of the experimental setup are provided in Calogiuri *et al.* (2023). In summary, each mixture contained 360–400g of rock powder, consisting of 1–3 different rock types with different possible grain sizes (Table A11 in Extended Data (Janssens *et al.*, 2025)). Here, the rock types were a peridotite rock with about 90% olivine content, a steel slag, and two rocks in the field of basalt and basanite/tephrite according to the TAS diagram (see Figure A1 in Extended Data). The rocks and slags used are detailed in Tables A3–A7 in Extended Data.

To this mixture, different amounts of biochar, organic amendments, living or dead earthworms, bacteria, fungi, enzymes, and additional N (in the form of urea or NH_4Cl) and P (in the form of KH_2PO_4) could be added. The biochar was produced from natural wood (Verora, Germany; see Table A8 for its properties). The organic amendments were wheat straw (Pets Place, the Netherlands), co-digestate of pig manure and biowaste (Groene Mineralen Centrale, the Netherlands) or a mixture dominated by alfalfa with additions of wheat and grape molasse (hereinafter referred to as 'alfalfa mixture' for simplicity; Pets Place, the Netherlands). The elemental compositions of the biochar and organic amendment are listed in Table A9 in Extended Data.

The earthworm species were Allolobophora chlorotica (A. chlorotica) and/or Aporrectodea caliginosa (A. caliginosa)), and were collected from the park De Blauwe Bergen in Wageningen, the Netherlands (51°58'51.8"N 5°39'38.0"E) at the start of each round of experiments. To prevent the earthworms from escaping, a mesh was placed on top of the columns. The bacteria were *Bacillus subtilis str.* Marburg (DSM 10^T) (*B. subtilis*) and/or Cupriavidus metallidurans str. CH34 (DSM 2839^T) (*C. metallidurans*), both sourced from Leibniz Institute DSMZ, Germany. The fungi were *Knufia petricola str.* A95 (Wollenzien & de Hoog) Gorbushina and Gueidan 2013 (CBS 123872) (*K. petricola*), sourced from Westerdijk Institute, the Netherlands, *Aureobasidium pullulans str.* 316 (de Bary & Löwenthal) Arnaud (DSM 3497) (*A. pullulans*) and/or *Suillus variegatus* (Sw.) Kuntze (DSM 1752) (*S. variegatus*), both sourced from Leibniz Institute DSMZ, Germany. Last, the enzymes were laccase, urease and/or carbonic anhydrase.

In some of the treatments, the microbes were premixed with the organo-mineral mixture; inoculation was done at the start only or also after four weeks; and in some treatments autoclaving was performed to kill the any/all pre-existing microbes in the rocks and organic amendments (126–135°C for 4 hours) to maximize the colonization potential of the added microbial species. For eight weeks, natural ground water was applied via a downflow irrigation system, with different water throughput rates and frequencies (see Tables S1–S2 in Extended Data for its properties). A complete overview of the inputs and their added amounts is listed in Table 1. To collect the leachates, each column was placed above a jerrycan cooled at 4°C to minimize microbial growth and dissolved organic carbon consumption (Kirschbaum, 1995).

At the end of each round of experiments, samples were taken from both the solid mixture in the column and the leachate, from which several quantities were measured to study the CDR due to mineral weathering. To obtain a representative sample from the solid mixture, the mixture was homogenized and samples were taken using the coning and quartering method (Campos & Campos, 2017). After performing loss of ignition (LOI) on the solid sample (for three hours at 550°C; Koorneef *et al.*, 2023), its concentration of carbon, i.e., SIC concentration (mass%), was measured (using C analysis, Flash 2000 CN Soil Analyser, Interscience, Antwerp, Belgium). In the leachate sample, the concentrations of TA (μmol l^{-1}) and DIC (mg l^{-1}) were measured (using Automated Gran titration, Titrando (600 series), Metrohm, Hamburg, Germany; and FormacsHT TOC analyser, Skalar, Antwerp, Belgium). The uncertainty of the DIC measurements is given with around 20% and that of TA with 2%.

Since (bi)carbonates and alkalinity were already present in some of the input materials (minerals, organic amendments), their SIC concentration was measured to be able to isolate the IC in the solid mixture resulting from mineral weathering. To assess the amount of DIC and TA resulting from processes other than mineral weathering, such as weathering and DIC release of trace carbonates in organic feedstocks, control experiments were conducted in parallel. In these control

Table 1. Model features with their added amounts.

Model features	Description	Amounts
Irrigation		
irrigation flow rate	Irrigation flow rate	50, 100, 150 ml day^{-1}
irrigation frequency	Irrigation frequency	1, 2, 5 times day^{-1}
Rocks		
basalt SA	Total surface area of basalt rocks (see Extended data - Eq. B.18 (Janssens *et al*., 2025))	$\in$ [0,4231] m^2
basanite/tephrite SA	Total surface area of basanite/tephrite rocks (see Extended data - Eq. B.18 (Janssens *et al*., 2025))	$\in$ [0,759] m^2
peridotite SA	Total surface area of peridotite rocks (see Extended data - Eq. B.18 (Janssens *et al*., 2025))	$\in$ [0,2820] m^2
steel slag SA	Total surface area of steel slags (see Extended data - Eq. B.18 (Janssens *et al*., 2025))	$\in$ [0,5299] m^2
mixed grain size	Whether multiple grain sizes were mixed or not	true/false
rock+biochar mass	Total mass of the rocks and biochar addition	400, 440 g
Biochar		
biochar mass	Mass of biochar from natural wood	0, 4, 10, 20, 40 *g*
Organic amendments		
straw mass	Addition of wheat straw	0, 10 g
digestate mass	Addition of co-digestate of pig manure and biowaste	0, 10 g
alfalfa mixture mass	Addition of a mixture dominated by alfalfa with additions of wheat and grape molasse	0, 10 g
Earthworms		
# earthworms	Number of initially live earthworms	$\in$ [0, 12]
chlorotica ratio	Ratio of initially live *Allolobophora chlorotica* earthworms w.r.t. total number of initially live earthworms (see Extended data - Eq. B.19 (Janssens *et al*., 2025))	$\in$ [0,1]
# † earthworms	Number of initially dead earthworms	$\in$ [0, 12]
† *chlorotica* ratio	Ratio of initially dead *Allolobophora chlorotica* earthworms w.r.t. total number of initially dead earthworms (see Extended data - Eq. B.20 (Janssens *et al*., 2025))	$\in$ [0, 1]
Fungi		
# *K. petricola*	Inoculum density of *Knufia petricola str*. A95 (Wollenzien & de Hoog) Gorbushina and Gueidan 2013 (CBS 123872)	$\in$ [0,5.4*e*8] cells
# *A. pullulans*	Inoculum density of *Aureobasidium pullulans str. 316 (de Bary & Löwenthal) Arnaud (DSM 3497)*	$\in$ [0,5.4*e*8] cells
# *S. variegatus*	Inoculum density of *Suillus variegatus (Sw.) Kuntze (DSM 1752)*	$\in$ [0,4.3*e*8] cells
Bacteria		
# *B. subtilis*	Inoculum density of *Bacillus subtilis str. Marburg (DSM 10T)*	$\in$ [0,4.7*e*11] cells
# *C. metallidurans*	Inoculum density of *Cupriavidus metallidurans str*. CH34 (DSM 2839T)	$\in$ [0,4.0*e*11] cells
premixed	Whether the microbes were premixed with the organo-mineral mixture	true/false
sterilized	Whether the rocks and organic amendments were autoclaved before adding biota	true/false

Model features	Description	Amounts
halftime inoculation	Whether the bacteria and fungi were added after 4 weeks	true/false
Enzymes		
# laccase	Laccase concentration	∈ [0,300] U
# carbonic anhydrase	Carbonic anhydrase concentration	∈ [0,3998] U
# urease	Urease concentration	∈ [0,370] U
Extra additions		
# P	Extra phosphorus addition	0, 0.3 mmol
# NH_4Cl	Extra ammonium chloride addition	0, 0.3 mmol $week^{-1}$
# urea	Extra urea addition	0, 0.15 mmol $week^{-1}$

experiments, DIC and TA leaching from columns containing only 400g sand, as well as columns filled with 400g sand and each type of organic amendments, was quantified (see Tables A10–A11 in Extended Data). Further details regarding the design and construction protocol of the column experiments can be found in Calogiuri *et al.* (2023).

Data preprocessing

To examine CDR and the underlying mineral weathering process, we focused on four targets; Δ*SIC*, Δ*DIC*, the sum of the two, coined Δ*TIC*, and Δ*TA*; all expressed in *mmol* (per column over the 8-week experiment). Their derivations can be found in Extended Data, section B.1. In short, Δ*SIC* (*mmol*) was calculated from the measured *SIC* concentration (*mass%*) at the end of each experiment and the mass of the solid bed (*g*), and was corrected for the weight loss due to LOI and for the *SIC* that was initially present in the abiotic components and organic amendments. The two targets measured in the leachate, Δ*DIC* and Δ*TA* (*mmol*), were calculated using the irrigated volume (*l*) and, respectively, the measured *DIC* ($mg\ l^{-1}$) and *TA* ($\mu mol\ l^{-1}$) concentrations in the leachate. To obtain the amounts stemming from mineral weathering, the concentrations originating from the initial carbonates in the rocks and organic amendments, which were approximated using the measurements of the control experiments, were subtracted. Last, Δ*TIC* was obtained by summing Δ*SIC* and Δ*DIC*.

Next, the dataset was preprocessed. Columns with missing target data due to measurement errors were omitted, as well as columns where an experimental error occurred, such as flooding or loss of leachates. Experimental treatment combinations that were repeated were compared and outlying repeats were discarded if the standard deviation of the set of repeats was large with respect to the spread of the data (larger than 75% of the interquartile range). In rounds 1 to 3, additional samples for chemical analyses were taken from the leachate after three weeks, which affected the measurements after eight weeks. Therefore, data of rounds 1 to 3 were omitted for the prediction of Δ TA, Δ DIC and Δ TIC. Because the leachate sampling happened in the leachate container, it did not impact the column with solid matter above, whose data were still used. As we realized early in the project that the leachate data from the first three rounds could not be used in this analysis, many input combinations covered in these first three rounds were repeated in later rounds. As a result, this information was not lost for the ΔDIC, ΔTA and ΔTIC models. While the ΔSIC data contained more replicates, these were properly dealt with in the cross validation (CV) approach (see next section, 'Predictive models') to avoid bias in our analyses. Therefore, we believe that excluding the first three rounds did not introduce biases in this study. This resulted in 749 datapoints for Δ*DIC*, 1202 for Δ*SIC*, 725 for Δ*TIC* and 593 for Δ*TA*. Next, the input features were defined (Table 1); e.g., the mix of rock powders was translated to features that represented the total surface area (SA) of each rock type (see section B.2 in Extended Data) and whether or not rock powders with different grain sizes were mixed. This resulted in a mix of boolean and numerical features, which were standardized (Table 1).

Predictive models

To uncover the optimal conditions for enhanced mineral weathering, ML was used to predict the CDR indicators; ΔDIC, ΔSIC, ΔTIC and ΔTA. To this end, three different regression models, Lasso, RF and XGB, were fitted to the data using Python (version 3.10), and its scikit-learn (Pedregosa *et al.*, 2011) and XGBoost (Chen & Guestrin, 2016) libraries.

While ML models are often trained and evaluated using cross validation (CV), doing this to both optimize the model's hyperparameters and evaluate the model can lead to an optimistically biased estimate of the model performance (Stone, 1974). Therefore, in this study, the selection of the optimal hyperparameters, model training and performance evaluation were done using a nested 10×10 CV approach. This approach comprised two levels of CV: a 10-fold CV inner loop for hyperparameter tuning and model training, and a 10-fold CV outer loop for validation. First, in the outer loop, the data was split into 10 training and test sets using 10-fold CV. This entailed splitting the data into 10 folds. To avoid instability of the models due to unbalanced splits, the splitting was done using stratified sampling, with the extra constraint that the absolute value of the coefficient of determination (R^2) of the naive prediction (i.e., predicting the mean target value), which should be zero for balanced datasets, was smaller than

0.02. This is done in order to avoid that evaluation metrics are too strongly impacted by outlying values (i.e., very large or very small target values). The restriction based on the naive R^2 makes sure that the train and test split have a similar spread in target values. Next, nine folds were grouped together to form the training set, while the remaining fold served as the test set. Subsequently, this training set underwent a second 10-fold CV in the inner CV loop; being further divided into 10 folds using stratified sampling, that were combined into 10 training and validation sets. These inner-loop training and validation sets were then used for hyperparameter tuning using a grid search, wherein the hyperparameters that led to the best mean absolute error (MAE) on the validation set were selected. The grid search iteratively explored all possible combinations of the varied hyperparameters (listed in Table C1 in Extended Data). This resulted in one model with optimal hyperparameters, which was then evaluated using the remaining test set in the outer CV loop, thereby concluding the first iteration of the outer loop. This process was repeated 10 times, each time with another training and test set, resulting in ten trained models and ten sets of performance metrics. Finally, model performance was assessed by averaging the performance metrics of these ten models. Besides the MAE, we evaluated the performance of the models using the R^2 and the mean squared error (MSE).

SHAP value analysis

The models described above allow predicting the four target variables, but we also aimed to understand how these predictions come about and which are the dominant drivers. One of the models, Lasso, is a white box model that thus gives insight in the drivers, but the other two applied models, XGB and RF, are not inherently interpretable. We therefore applied explainable artificial intelligence (xAI), more specifically SHAP values, to the best performing model. SHAP values quantify the impact of each feature to the prediction for each datapoint as well as the direction of the impact. SHAP values are determined by assessing the effect of including and excluding each feature on the prediction, while taking all other features into account (Lundberg *et al.*, 2017). The main advantages of this approach are that SHAP values are easy to interpret, account for interactions between features and are model-agnostic (Lundberg *et al.*, 2017). The SHAP values were calculated using Python's SHAP package (Lundberg *et al.*, 2017). This was done for each test set within the outer CV loop, resulting in one set of SHAP values for every datapoint. Adding steel slag seemed to result in very different scales of SIC and DIC. Therefore, SHAP values were also calculated for the subsets with and without steel slag within each test set.

A useful characteristic of SHAP values is that they are additive, meaning that the SHAP values of all features of a certain datapoint sum to the difference between the predicted value of that datapoint and the mean prediction (Lundberg *et al.*, 2017). We used this additivity to explore the general impact of a group of features (e.g., rocks, organic amendments or biota) on the predictions. For each datapoint i, the SHAP value of a group of features G can be calculated using

$$SHAP_G^i = \sum_{feature \in G} SHAP_{feature}^i \quad (2.1)$$

To then determine a general importance of the group of features, we averaged the absolute value of the group's SHAP value over all n datapoints:

$$SHAP_G = \frac{1}{n}\sum_i |SHAP_G^i| \quad (2.2)$$

This group importance does not account for direction of the impact (accelerating or decelerating CDR), but instead represents the general importance of making a good selection of the features within the group on the predictions.

Results and discussion

Data

This study conducted a complex enhanced weathering experiment to reveal the importance of 30 potential drivers in a strongly uneven experimental design with 2000 columns. Initial amounts of DIC, SIC, TIC and TA, added to the system through addition of minerals, biochar, organic amendments and throughput water, could be substantial, especially for SIC (Figure 1b), which mainly originated from the rocks (Table A11 in Extended Data). After taking these initial amounts into account, the calculated targets (ΔSIC, ΔDIC, ΔTIC and ΔTA) only represent the change due to mineral weathering. Negative target values (Figure 1c) indicate that in some batches, carbon was either converted from one form to another (e.g., SIC to DIC), or carbon precipitated or released to the atmosphere as CO_2. ΔTIC predominantly consisted of ΔSIC when steel slag was added, though for the columns without steel slag, ΔDIC became more relevant to ΔTIC.

Model performance

Considering the huge number of possible combinations of column inputs, combinations were generally not repeated to explore the parameter space as much as possible. The resulting uneven experimental design prompted an ML approach to analyse the dataset. To predict the four CDR indicators (ΔDIC, ΔSIC, ΔTIC and ΔTA), we selected one linear model, Lasso, because of its simplicity and inherent explainability, and two ensemble models, RF and XGB, for their proven performance in high dimensional non-linear tabular data and their limited data requirements. Both XGB and RF significantly outperformed the naïve prediction, which is a baseline model that uses the mean target value as its prediction, and in many cases also significantly outperformed the Lasso models (Table 2). For all models, the standard deviations of the performance metrics of the 10 models in the outer CV loop were relatively high (Table 2), which can be attributed to both the relatively small amount of data - compared to the explored input space - and the noise that was present in the measurements (see section B.3 in Extended Data).

Lasso is a white-box model and therefore can be very useful. For the prediction of ΔDIC for instance, Lasso had a performance close to that of the other two models (Table 2). The resulting regression coefficients yield valuable, directly interpretable information. For example, according to the Lasso model, the surface area of added peridotite had the largest effect on ΔDIC, followed by amendment of the alfalfa mixture and straw, and a suite of abiotic and biotic drivers (see Table C2 in Extended Data). However, for the other targets, Lasso exhibited poor performances, with average R^2 values

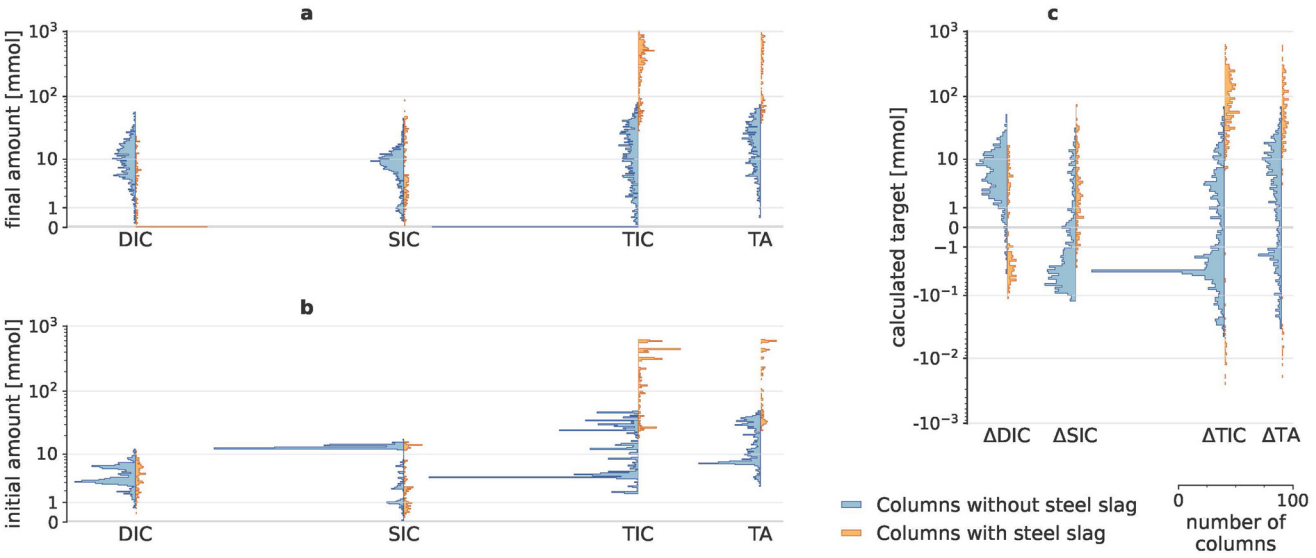

Figure 1. Calculated carbon dioxide removal indicators. Histograms of initial and final dissolved inorganic carbon (DIC), solid inorganic carbon (SIC), total inorganic carbon (TIC) and total alkalinity (TA); with their resulting changes. As adding steel slags resulted in very different scales of SIC, DIC and TA, results for columns with and without steel slags are visualized separately in orange and blue, respectively. (**a**) shows the amounts that were present in the batches at the end of the experiment; (**b**) depicts the initial amounts, i.e., the amounts that were added to the system through addition of rocks, organic amendments and throughput water; (**c**) illustrates the resulting values of the four targets, i.e., the changes in amounts that can be attributed due to mineral weathering.

Table 2. Performance of the predictions of the carbon dioxide removal indicators. Mean absolute error (MAE), mean squared error (MSE), root mean squared error (RMSE), and determination coefficient (R^2) of the prediction of the changes in amount of dissolved inorganic carbon (ΔDIC), solid inorganic carbon (ΔSIC), total inorganic carbon (ΔTIC) and alkalinity (ΔTA), using Least Absolute Shrinkage and Selection Operator (Lasso), Random Forest (RF), and eXtreme Gradient Boosting (XGB) regression. The fourth, naive, regressor, predicts the mean target value for the whole training set and is added as a baseline. Depicted values are the mean and standard deviation of the performance metrics of the 10 models of the outer loop of the nested cross-validation. For each target, the model with best average performances is indicated in blue.

Target	Regressor	MAE	MSE	RMSE	R^2
ΔDIC [mmol]	Lasso	3.0 ± 0.4	20 ± 5	4.4 ± 0.6	0.62 ± 0.09
	RF	2.9 ± 0.5	19 ± 8	4.3 ± 0.9	0.62 ± 0.17
	XGB	2.4 ± 0.4	16 ± 9	3.9 ± 1.0	0.68 ± 0.20
	Naive	5.4 ± 0.6	54 ± 14	7.3 ± 0.9	0.00 ± 0.01
ΔSIC [mmol]	Lasso	25.9 ± 3.3	2776 ± 1136	51.82 ± 10.04	0.42 ± 0.10
	RF	17.9 ± 3.5	1915 ± 988	42.74 ± 9.93	0.61 ± 0.09
	XGB	17.4 ± 2.5	1752 ± 690	41.16 ± 8.02	0.63 ± 0.12
	Naive	39.3 ± 3.9	4864 ± 1939	68.71 ± 12.58	-0.01 ± 0.01
ΔTIC [mmol]	Lasso	24 ± 4.4	2571 ± 1793	48.2 ± 16.6	0.32 ± 0.15
	RF	17.4 ± 5.6	1999 ± 1915	40.9 ± 19.1	0.53 ± 0.21
	XGB	15.6 ± 5.1	1563 ± 1810	35.6 ± 18.2	0.62 ± 0.20
	Naive	29.6 ± 3.9	3690 ± 2323	58.4 ± 17.6	-0.01 ± 0.01
ΔTA [mmol]	Lasso	8.0 ± 1.0	243 ± 100	15.3 ± 3.3	0.41 ± 0.28
	RF	5.7 ± 1.1	125 ± 54	11.0 ± 2.3	0.67 ± 0.23
	XGB	5.3 ± 1.2	119 ± 54	10.7 ± 2.5	0.70 ± 0.17
	Naive	11.5 ± 1.5	471 ± 230	21.1 ± 5.6	-0.01 ± 0.01

below 0.5 (Table 2). Lasso is limited to capturing linear relationships, and while linear regression is a popular tool in ecology, biochemical processes are typically nonlinear (Levin, 1998; Manzoni & Porporato, 2007). RF and XGB allow modeling nonlinear relations and employ ensemble tree learning to improve the prediction accuracy. While RF achieves this through bootstrapping decision trees, XGB iteratively trains new trees to correct the errors of the previous trees, often leading to superior performance. Indeed, although the difference with RF was often small, XGB achieved the best average performance metrics (Table 2). Therefore, the remainder of our analysis is conducted using XGB.

Drivers of enhanced weathering using Shapley Additive exPlanations

As the model with the highest average performance across all targets (Table 2), XGB, is a black box model, we calculated the corresponding SHAP values for the individual features (Figure 2) and for the main groups of features (Figure 3) to understand which of the investigated drivers contributed most to the predictions.

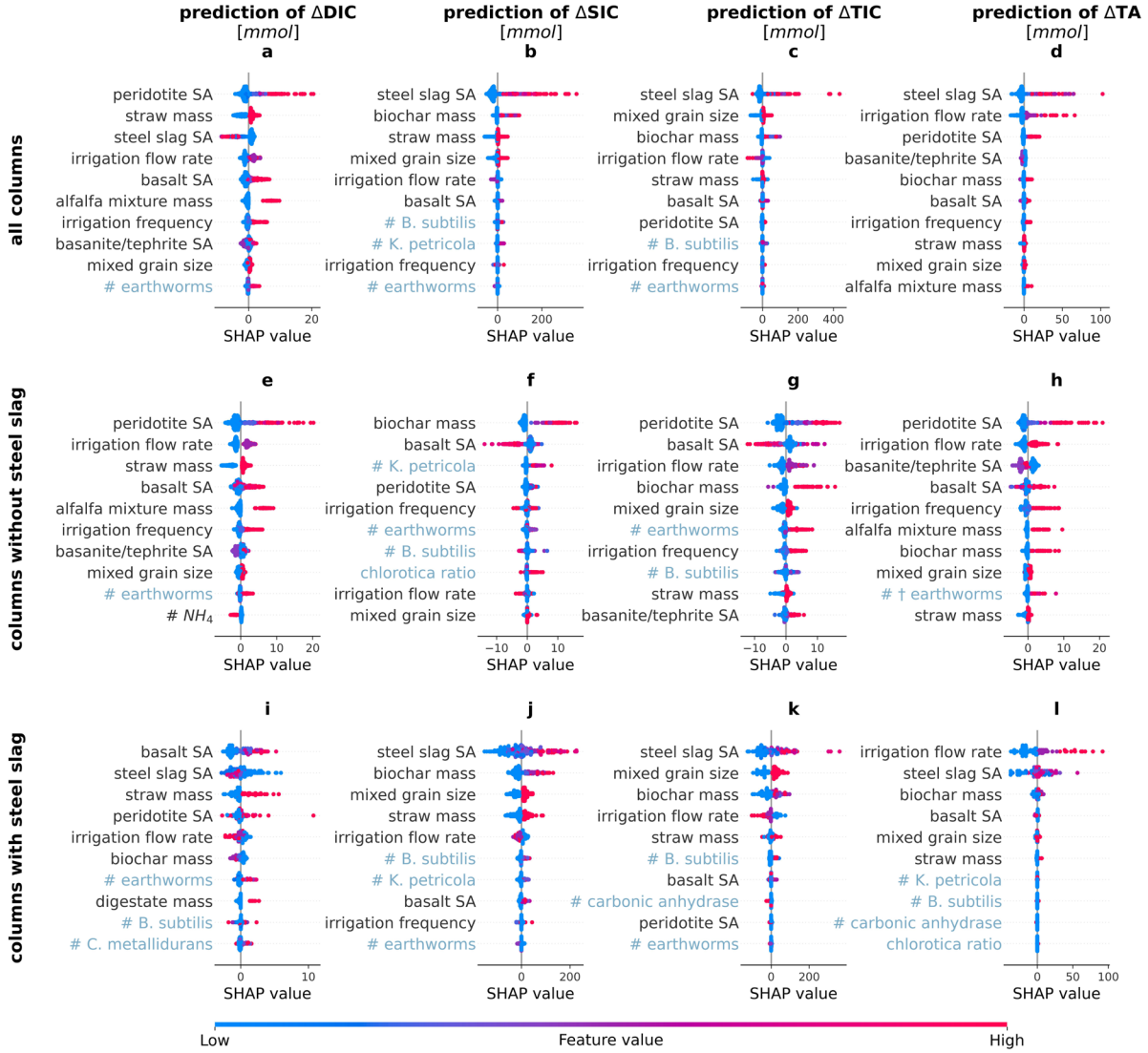

Figure 2. SHapley Additive eXplanation (SHAP) values of the most important drivers of the carbon dioxide removal indicators. SHAP values of the top ten most important features in the eXtreme Gradient Boosting prediction of the changes in amount of dissolved inorganic carbon (ΔDIC), solid inorganic carbon (ΔSIC), total inorganic carbon (ΔTIC) and total alkalinity (ΔTA). The plots depict a SHAP value for each prediction and show the local feature importance and the feature effect. A dot with a high SHAP value for a feature suggests a positive contribution to the prediction, whereas a negative SHAP value leads to a lower prediction. The color of a dot represents the value of the feature in that instance - red indicating relatively high, blue indicating relatively low values (For the binary features, high values = true, low values = false; for chlorotica ratio, red means 100% A. chlorotica earthworms, blue means 100% A. caliginosa earthworms). For example, a red dot with a positive SHAP value implies that a higher value of the feature elicits an increase in the target value. SA stands for surface area, # stands for added amount of biota. The features are ranked in order of descending average importance and biotic features are indicated in light blue for clarity.

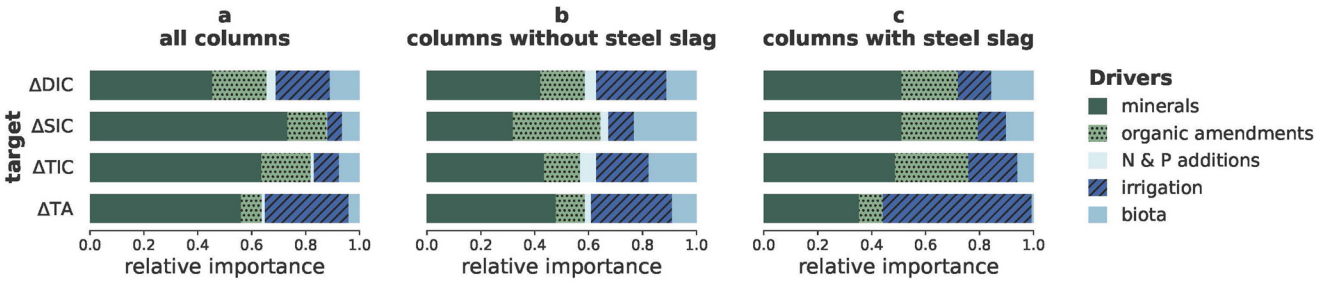

Figure 3. Importance of groups of features to carbon dioxide removal indicators. Relative importance of the main groups of drivers (rocks, organic amendments, irrigation, N and P additions, and biota and biotic products) to the prediction of the changes in amounts of dissolved inorganic carbon (ΔDIC), solid inorganic carbon (ΔSIC), total inorganic carbon (ΔTIC) and total alkalinity (ΔTA); Calculated using Equation 2.2.

In agreement with our hypothesis, the SHAP values revealed that ΔSIC, ΔDIC and ΔTA were indeed driven by different features (Figure 2, Figure 3). Disparities in the drivers of ΔTA and ΔDIC likely indicate a confounding effect of organic alkalinity production or consumption due to the added organics, steel slags or biota. Precipitation of SIC depends on several conditions (saturation, pH, availability of seed crystals (Amann *et al.*, 2022)), and SIC can also be dissolved, leading to ΔSIC being driven by different features than ΔDIC and ΔTA. The target that is most directly related to CDR was ΔTIC, i.e. the sum of ΔDIC and ΔSIC. Its SHAP values are therefore a mix of the SHAP values of ΔDIC and ΔSIC. The next paragraphs discuss in detail the SHAP values of the dominant driver groups of the different targets.

Rocks. Among all potential drivers tested in this experiment, the choice of type of rocks had the biggest impact on the predictions. For ΔDIC, adding peridotite to the rock powder mix had the largest positive effect. This is clearly shown in Figure 2-a, where the columns including peridotite (red dots of peridotite SA) all exhibited higher SHAP values than those without peridotite (blue dots), thus indicating that according to the model, adding peridotite increases ΔDIC the most. In addition to peridotite, also basalt increased ΔDIC predictions (Figure 2-a). As the ultramafic peridotite is known to weather faster than the mafic basalt, these findings are in line with expectations (Hartmann *et al.*, 2013).

In contrast to peridotite and basalt, adding steel slag reduced ΔDIC (Figure 2-a). This is likely because the increased pH shifted the IC equilibrium to carbonate, which precipitated to form SIC (as is indeed seen in Figure 2-b). However, for the other CDR indicators, steel slag was identified as the most important feature, consistently increasing the predicted values (Figure 2-b,c,d). The steel slag used had a high calcium content (Table A6 in Extended Data, XRF), a portion of which was likely present in the form of calcium hydroxide ($Ca(OH)_2$). This phase dissolves quickly in water, increasing solution pH by releasing hydroxide ions. Due to the abundance of cations and the high pH, where CO_3^{2-} is the main species of IC, the solution will be oversaturated with respect to some carbonate minerals. The precipitated $CaCO_3$ can in turn serve as a seed crystal for further $CaCO_3$ precipitation, thereby reducing ΔDIC and increasing ΔSIC and ΔTIC, while the formed hydroxides cause an increase in ΔTA. Interestingly, adding steel slag to the columns led to different SHAP values for some features, such as irrigation flow rate. This is visualized by the blue and red dots (indicating the absence/presence of the feature) switching sign when comparing the SHAP values of some features between the columns with and without steel slag (Figure 2-e,f,g versus Figure 2-i,j,k). Apparently, using steel slag introduced a suite of interactions that altered the impact of these other features, possibly due to the accompanying increase in pH.

In the absence of steel slag, columns that contained more peridotite clearly exhibited faster weathering than average, as indicated by the higher SHAP values for ΔDIC, ΔSIC, ΔTIC as well as ΔTA (Figure 2-e,f,g,h). Columns containing more basalt also exhibited higher SHAP values for ΔDIC and ΔTA, but lower for ΔSIC. For ΔTIC, fine basalt grains (high basalt SA) resulted in lower ΔTIC and coarse grains in higher ΔTIC (medium basalt SA). Adding more basanite/tephrite to the rock mix had no clear effect on ΔSIC and a positive one on ΔTIC (Figures C3–C4 in Extended Data). Coarse grained basanite/tephrite led to a lower ΔDIC and adding basanite/tephrite had a negative effect on ΔTA, especially coarse grains. The negative SHAP values do not necessarily mean that adding the rock decreased CDR, but that it yielded smaller increases in these targets than other rocks, and its addition comes at the expense of a lower content of the other rocks.

Mixing the grain sizes increased the predictions of the CDR indicators (Figure 2). As such, columns with mixed coarse and fine grain sizes may have had similar SA as columns composed of medium-sized grains, yet exhibited higher CDR. While finer grains typically correspond to more nucleation sites for carbonate precipitation, mixing them with coarser grains might have enhanced an efficient water flow (Amann *et al.*, 2022).

Irrigation. The irrigation flow rate and irrigation frequency were also commonly important drivers of weathering rate in the XGB models. The irrigation flow rate had opposing effects on the predicted ΔDIC and ΔTIC for the subsets of columns with and without steel slags. In columns without steel slags, higher irrigation flow rates increased predicted ΔDIC, ΔTIC and ΔTA (Figure 2-e,g,h and Figure C6-a1,i1,m1 in Extended data). This behaviour could be expected, as a higher flow through transports more cations and bicarbonate ions into the leachates, driving the weathering reactions further from equilibrium (Evans & Banwart, 2006; Maher, 2010). However, for ΔDIC and ΔTA, only small differences were detected between the impacts of the medium flow rate and the highest flow rate (100 and 150 ml day^{-1}; equivalent to rainfall fluxes of roughly 10000 and 15000 mm $year^{-1}$). Possibly, 100 ml day^{-1} flushed sufficient dissolved base cations and bicarbonate ions from the column to maintain the solution undersaturated with respect to secondary mineral formation, with stronger dilution only marginally affecting mineral weathering. This suggests that the reactions governing ΔDIC and ΔTA are not transport-limited at flow rates of 0.25 ml $day^{-1}g^{-1}$ rocks (100 ml day^{-1} per 400g rocks) or higher, and that the limit likely lies between 0.125 ml $day^{-1}g^{-1}$ rocks and 0.25 ml $day^{-1}g^{-1}$ rocks.

In the subset including only columns with steel slag, a negative response to irrigation flow rate was observed for ΔDIC, ΔSIC and ΔTIC, whereas for ΔTA, high flow rates exhibited positive SHAP values (Figure 2-i,j,k,l and Figure C6-a2,e2,i2,m2 in Extended data). Possibly, higher flow rates transported more cations to the leachate, increasing ΔTA and lowering ΔSIC and as a result also ΔTIC. The increased pH in the leached solution due to the added steel slags could have brought the system far from equilibrium, leading to continuous precipitation of carbonates in the leachate container (Moras *et al.*, 2022).

In addition to irrigation flow rate, also irrigation frequency was selected as an important driver, exhibiting a positive effect on the predicted ΔDIC, ΔTIC and ΔTA in columns with no steel slag. This was in line with expectations, as a higher irrigation frequency implies more continuous replacement of the saturated pore water. Higher irrigation frequencies may also have accelerated weathering by decreasing average pO_2, possibly retarding formation of oxides that are known to decrease weathering rates by orders of magnitude (Fuhr *et al.*, 2024; Oelkers *et al.*, 2018).

Organic amendments and biochar. The organic amendments (straw, digestate and the alfalfa mixture) were added to create a livable environment for the biota. By providing the substrates used in respiration, they were expected to accelerate CDR. In agreement, adding straw to the columns increased ΔDIC, ΔSIC (when combined with steel slag), ΔTIC, and ΔTA (Figure 2). Digestate had a positive effect on ΔDIC (Figure C2 in Extended Data), and a negative one on ΔTA (Figure C5 in Extended Data), while its other effects were negligible. The alfalfa mixture was only added to batches without steel slag and had a large positive effect on the predicted ΔDIC and ΔTA (Figure 2-e,f,g,h) and a small negative effect on ΔSIC (Figure C3 in Extended Data), resulting in a positive effect on ΔTIC (Figure C4 in Extended Data). Its SHAP values were generally more positive than for straw, possibly because it is a better palatable organic matter source. Organic matter additions, and especially straw and the alfalfa mixture, thus seem to have increased mineral weathering, possibly due to increased CO_2 concentrations following organic matter decomposition and increased porosity and water flow in the column.

Biochar was not added to stimulate microbial activity, but to promote weathering abiotically by adsorbing ions and increasing seed crystals due to its high IC content and pH (Table A8 in Extended Data). It indeed achieved a large positive effect for ΔSIC, ΔTIC and ΔTA (Figure 2), although the increased SIC precipitation logically led to no net increase or even a decrease in ΔDIC (Figure C2 in Extended Data). The absence of a rise in ΔDIC suggests that the increase in ΔTA was of organic origin.

Biota and biotic products. Also certain biota were identified as important drivers of the targets. The number of earthworms, for example, frequently was a positive driver. However, as a substantial part of the added earthworms died during the experiment, their effect on the targets could also be due to decomposing earthworms. To investigate this, also dead earthworms were added to certain columns. The SHAP values revealed that earthworms that were alive at the start of the experiment (# earthworms) positively impacted ΔDIC and, in absence of steel slag, also ΔSIC, ΔTIC and ΔTA, while (initially) dead earthworms (# † earthworms) positively impacted the predicted ΔDIC and ΔTA (Figure 2).

The positive effect of (initially) live earthworms on ΔDIC and ΔTA (Figure 2-a,e,i and Figure C5 in Extended data) agrees with our expectations. Earthworms accelerate organic matter decomposition by fragmenting organic matter, consequently increasing its surface area and inoculating it with microbes in their gut (Edwards & Arancon, 2022). Moreover, earthworms stimulate microbial activity and distribution by producing mucus and concentrating nutrients (Amador & Görres, 2007; Brown, 1995; Frouz *et al.*, 2011; Van Groenigen *et al.*, 2019). This accelerated decomposition of organic matter and higher microbial activity leads to increased release of CO_2 (Ajwa & Tabatabai, 1994; Condron *et al.*, 2010), which could have enhanced mineral weathering (Amann *et al.*, 2022) and led to an increased formation of bicarbonate in solution (Manning *et al.*, 2024). However, as the number of (initially) dead earthworms had similar SHAP values as the number of (initally) live earthworms, the increased ΔDIC and ΔTA could also be a result of decomposing earthworm bodies, e.g., by increasing

the microbial activity due to an immediate pool of available nutrients (Kos *et al.*, 2017; Lin *et al.*, 2022; Sun & Ge, 2021). This higher microbial activity could have further increased decomposition and led to a higher CO_2 release and consequently to ΔDIC formation through weathering (Calogiuri *et al.*, 2025).

The positive effect of (initially) live earthworms on the predicted ΔSIC was only seen for columns in which no steel slag was present (Figure 2-f). In contrast to ΔDIC and ΔTA, the predicted ΔSIC was not substantially impacted by (initially) dead earthworms, indicating that earthworms likely actively increase ΔSIC. This could occur through physical and chemical processes happening within their bodies when earthworms feed on rock particles. First, earthworms possess calciferous glands through which they can produce calcium carbonate minerals and therefore contribute to the formation of SIC (Briones *et al.*, 2008; Versteegh *et al.*, 2014). Second, the rock particles are ground in the earthworms' gizzards, increasing their SA (Suzuki *et al.*, 2003) and removing poorly weathering precipitates by abrasion. These freshly exposed mineral surfaces can then be attacked by microbes living in the earthworms' intestines (Carpenter *et al.*, 2007; Liu *et al.*, 2011; Zhu *et al.*, 2013) and in the surrounding environment once the particles are egested. In the case of Ca-bearing rocks, this results in an increased release of Ca^{2+}, which drives re-precipitation of ΔDIC as carbonate minerals (Manning *et al.*, 2024; Washbourne *et al.*, 2015), thereby increasing ΔSIC. However, when steel slag was present, even in small amounts, the effect of earthworms on the predicted ΔSIC was negative, but negligible with respect to the large importance of the abiotic drivers (Figure 2-j and Figure C6-f2 in Extended data). The positive effect of the earthworms in the absence of steelslags was maximal for ΔDIC for 8 earthworms and for ΔSIC for 4 or 8 earthworms (Figure 2-f and Figure C6-b1,f1 in Extended data). Possibly, a higher earthworm density was detrimental for earthworm well-being and might have created conditions which led to earthworms entering a diapause state instead of feeding on the mineral particles. As ΔTIC is the sum of ΔDIC and ΔSIC, and (initially) live earthworms had a positive effect on both targets for columns with no steel slag, their presence also led to higher ΔTIC (Figure 2-g and Figure C6-j1 in Extended data), especially for 8 earthworms.

Besides earthworms, bacteria and fungi also impacted the CDR indicators, albeit less clearly. For instance, intermediate inoculum densities of *B. subtilis* had a positive effect on ΔSIC and ΔTIC, especially in columns with steel slags (Figure 2 and Figure C6-h,i in Extended data). This is in agreement with previous studies (Ferral-Perez *et al.*, 2020; Keren-Paz *et al.*, 2022; Kim *et al.*, 2005), that showed that *B. subtilis* can promote the formation of solid inorganic carbonates, such as calcium carbonate, through a process called microbially induced calcium carbonate precipitation during the urease-catalyzed urea metabolization. This process may increase the pH and indirectly contribute to the precipitation of $CaCO_3$. (Ferral-Perez *et al.*, 2020; Keren-Paz *et al.*, 2022; Kim *et al.*, 2005).

Other notable effects are the positive impact of *K. petricola* on ΔDIC, ΔSIC and, in absence of steel slag, ΔTIC. *K. petricola* has been demonstrated to increase olivine weathering rates by hindering the formation of iron oxides on the olivine surface (Gerrits *et al.*, 2020). *K. petricola* forms biofilms on rock surfaces, providing a unique micro-environment that could promote the precipitation of carbonate minerals. These biofilms can trap ions and organic material, allowing carbonate nucleation to occur under specific conditions. This process could result in the deposition of carbonate minerals as part of SIC formation on or around the microbial biofilm. *A. pullulans* had a positive effect on ΔDIC and, in columns with steel slag, on ΔSIC, while the effect on ΔSIC was negative in absence of steel slag and no clear net effect was observed on ΔTIC and ΔTA (Figures C2-C5 and C6-c,g,k,o in Extended Data). *A. pullulans* is a versatile fungus that can produce numerous different enzymes and siderophores, which could cause the ΔDIC increase. It has the ability to biomineralize metal nanoparticles, which may be of great importance in an environment rich in metallic ions such as in an ultramafic environment, where toxic metal concentrations may accumulate in a high weathering environment (Gostinčar *et al.*, 2014; He *et al.*, 2021; Nwoko *et al.*, 2021). Since the biomineralized products are oxides rather than carbonates, the negative effect on ΔSIC was expected.

S. variegatus was added to test whether it could enhance weathering by releasing citric acid, which not only helps mobilize nutrients from the mineral but also creates favorable conditions for bacterial growth (Olsson & Wallander, 1998). *C. metallidurans* was tested for its resistance to high metal concentrations and its capacity of using basalt as a source of nutrients (Byloos *et al.*, 2017; Byloos *et al.*, 2018; Olsson-Francis *et al.*, 2010). However, in this study, the effect of *S. variegatus* and *C. metallidurans* on the predicted targets was small (Figures C2–C5 in Extended Data). Therefore, P and N were added to test for microbial nutrient limitation. However, P and urea had no significant effect on the predicted CDR indicators and NH_4Cl even had a large negative effect on ΔDIC, ΔSIC and ΔTIC, which can be attributed to its acidic nature. Consequently, possible P and N deficits were unlikely to have limited microbial activity.

In theory, the added enzymes could play a role in EW; the overexpression of laccase has been reported to enhance quartz weathering (Kirtzel *et al.*, 2020), hydrolysis of urea leads to $CaCO_3$ precipitation (Dilrukshi *et al.*, 2018; Krajewska, 2018), and carbonic anhydrase catalyzes the conversion of CO_2 and H_2O to bicarbonates and protons (or reverse), therefore potentially accelerating the supply of protons to weather the minerals (Peplow, 2024; Watson *et al.*, 2016). In contrast, in this experiment, addition of these three enzymes had negligible, and even negative effects on the predicted CDR indicators.

Limitations

This study also faced limitations, notably the imperfect representations of CDR indicators used, which may have been affected by the open system and unmeasured particulate carbon

accumulation on funnels and tubes. In addition, ΔTA, ΔDIC and ΔTIC were calculated using the irrigated volume and not the volume remaining in the leachate containers, as these volumes did not agree. We assumed all irrigation water passed through the columns and therefore that the volume lost contained the same concentrations. The reader should also bear in mind that the identified drivers that dominate weathering in this experiment may differ from those dominating CDR in the long term. Moreover, this experiment was conducted in the absence of soil to test optimal conditions in reactor settings, which may also have affected the relative importance of the drivers compared to field studies in soils.

Additionally, while the ML and xAI methodology provided valuable insights, they are correlation-based rather than causation-based, which should be considered when interpreting these findings. Last, the nested CV approach provides a robust estimate of model generalization performance and is appropriate for our objective, i.e. uncovering insights from driver importance. However, future applications aimed at model deployment should include evaluation on a separate hold-out test set reserved prior to model development.

Future work should focus on refining these experimental setups and exploring more direct measurements of CDR to quantify the potential of enhanced weathering as a viable CDR technology.

Conclusion

This study presents an extensive enhanced weathering experiment designed to explore how various abiotic and biotic factors influence CDR. ML allowed prediction of key weathering indicators (ΔDIC, ΔSIC, ΔTIC and ΔTA) in a highly uneven dataset. The integration of SHAP value analysis revealed that the four weathering indicators are driven by different features. Nonetheless, the rock-related features consistently dominated all predicted targets. In particular, the addition of steel slags, and to a lesser degree peridotite and basalt, significantly increased weathering rates. Moreover, steel slag introduced complex interactions that led to varying effects on carbon sequestration. This interaction was especially clear in the impact of the irrigation regime. While higher water throughput rates and more frequent irrigation generally increased predicted weathering indicators, higher throughput rates led to lower ΔDIC, ΔSIC, ΔTIC for columns with steel slag. Besides the choice of rocks and irrigation, also biochar and organic amendments, in particular straw and alfalfa-dominated mixtures, positively impacted CDR. Last, earthworms, bacteria and fungi had an impact on the weathering rate, often being one of the top ten drivers of the weathering indicators. However, the effects of the microbes varied depending on the predicted target and on the presence of steel slag. In conclusion, this research underscores the complexity of enhanced weathering processes, offers important insights for future efforts in utilizing enhanced weathering as a carbon removal strategy and demonstrates the potential of ML and xAI in uncovering key drivers of complex biochemical systems.

Ethics and consent

Ethical approval and consent were not required.

Data availability

Underlying data

The column experiment data are produced as part of the Bio-Accelerated Mineral weathering (BAM) project. No data will be released during the project (even upon request) to enable relevant publications or patent filings. In accordance with the BAM project's Data Management Plan, all data will be made openly accessible latest three years after the project's conclusion (2028). At that time, the underlying data repository will be specified on Zenodo: Extended data for 'Machine learning-based identification of key biotic and abiotic drivers of mineral weathering rate in a complex enhanced weathering experiment', https://www.doi.org/10.5281/zenodo.16728794 (Janssens *et al.*, 2025).

Extended data

Zenodo: Extended data for 'Machine learning-based identification of key biotic and abiotic drivers of mineral weathering rate in a complex enhanced weathering experiment', https://doi.org/10.5281/zenodo.16728794 (Janssens *et al.*, 2025).

The project contains the following extended data:

- Extended info.pdf (information about the used materials (A), about the data processing and additional noise analysis (B), and about the machine learning analysis and extended Shapley Additive exPlanation figures (C)).

Data are available under the terms of the Creative Commons Zero "No rights reserved" data waiver (CC0 1.0 Public domain dedication)(http://creativecommons.org/publicdomain/zero/1.0/).

Software availability

Analysis code available from Github: https://www.github.com/STAN-UAntwerp/h2020_bam

Archived software available from: https://doi.org/10.5281/zenodo.14528497 (Janssens *et al.*, 2024)

Software is available under the MIT License

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References

Ajwa HA, Tabatabai MA: **Decomposition of different organic materials in soils.** *Biol Fertil Soils.* 1994; **18**: 175–182.
Publisher Full Text

Amador JA, Görres JH: **Microbiological characterization of the structures built by earthworms and ants in an agricultural field.** *Soil Biol Biochem.* 2007; **39**(8): 2070–2077.
Publisher Full Text

Amann T, Hartmann J: **Ideas and perspectives: synergies from co-deployment of negative emission technologies.** *Biogeosciences.* 2019; **16**(15): 2949–2960.
Publisher Full Text

Amann T, Hartmann J, Hellmann R, *et al.*: **Enhanced Weathering potentials—the role of *in situ* CO_2 and grain size distribution.** *Front Clim.* 2022; **4**: 929268.
Publisher Full Text

Bacanin N, Perisic M, Jovanovic G, *et al.*: **The explainable potential of coupling hybridized metaheuristics, XGBoost, and SHAP in revealing toluene behavior in the atmosphere.** *Sci Total Environ.* 2024; **929**: 172195.
PubMed Abstract | **Publisher Full Text**

Bannigan P, Bao Z, Hickman RJ, *et al.*: **Machine learning models to accelerate the design of polymeric long-acting injectables.** *Nat Commun.* 2023; **14**(1): 35.
PubMed Abstract | **Publisher Full Text** | **Free Full Text**

Basak BB, Sarkar B, Naidu R: **Environmentally safe release of plant available potassium and micronutrients from organically amended rock mineral powder.** *Environ Geochem Health.* 2021; **43**(9): 3273–3286.
PubMed Abstract | **Publisher Full Text** | **Free Full Text**

Beerling DJ, Leake JR, Long SP, *et al.*: **Farming with crops and rocks to address global climate, food and soil security.** *Nat Plants.* 2018; **4**(3): 138–147.
PubMed Abstract | **Publisher Full Text**

Berner RA: **The phanerozoic carbon cycle: CO_2 and O_2.** Oxford University Press, 2004.
Publisher Full Text

Briones MJI, Ostle NJ, Piearce TG: **Stable isotopes reveal that the calciferous gland of earthworms is a CO_2-fixing organ.** *Soil Biol Biochem.* 2008; **40**(2): 554–557.
Publisher Full Text

Brown GG: **How do earthworms affect microfloral and faunal community diversity?** *Plant Soil.* 1995; **170**: 209–231.
Publisher Full Text

Brugere L, Kwon Y, Frazier AE, *et al.*: **Improved prediction of tree species richness and interpretability of environmental drivers using a machine learning approach.** *For Ecol Manag.* 2023; **539**: 120972.
Publisher Full Text

Byloos B, Coninx I, Van Hoey O, *et al.*: **The impact of space flight on survival and interaction of *Cupriavidus metallidurans* CH34 with basalt, a volcanic moon analog rock.** *Front Microbiol.* 2017; **8**: 671.
PubMed Abstract | **Publisher Full Text** | **Free Full Text**

Byloos B, Maan H, Van Houdt R, *et al.*: **The ability of basalt to leach nutrients and support growth of *Cupriavidus metallidurans* CH34 depends on basalt composition and element release.** *Geomicrobiol J.* 2018; **35**(5): 438–446.
Publisher Full Text

Calogiuri T, Hagens M, Van Groenigen JW, *et al.*: **Design and construction of an experimental setup to enhance mineral weathering through the activity of soil organisms.** *J Vis Exp.* 2023; (201).
PubMed Abstract | **Publisher Full Text**

Calogiuri T, Janssens I, Vidal A, *et al.*: **How earthworms thrive and drive silicate rock weathering in an artificial organo-mineral system.** *Appl Geochem.* 2025; **180**: 106271.
Publisher Full Text

Campos MM, Campos CR: **Applications of quartering method in soils and foods.** *Int J Eng Res Appl.* 2017; **7**(1): 35–39.
Publisher Full Text

Carpenter D, Hodson ME, Eggleton P, *et al.*: **Earthworm induced mineral weathering: preliminary results.** *Eur J Soil Biol.* 2007; **43**(Supplement 1): S176–S183.
Publisher Full Text

Chen T, Guestrin C: **XGBoost: a scalable tree boosting system.** In: *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining.* Association for Computing Machinery, New York, NY, USA, 2016; 785–794.
Publisher Full Text

Clarkson M, Larkin C, Swoboda P, *et al.*: **A review of measurement for quantification of Carbon Dioxide Removal by Enhanced Weathering in soil.** *Front Clim.* 2024; **6**.
Publisher Full Text

Condron L, Stark C, O'Callaghan M, *et al.*: **Chapter the role of microbial communities in the formation and decomposition of soil organic matter.** Soil microbiology and sustainable crop production. Springer Netherlands, Dordrecht, 2010; 81–118.
Publisher Full Text

Corbett T, Westholm M, Rosling A, *et al.*: **Organic carbon source controlled microbial olivine dissolution in small-scale flow-through bioreactors, for CO_2 removal.** *Npj Mater Degrad.* 2024; **8**: 34.
Publisher Full Text

Curtis CD: **Stability of minerals in surface weathering reactions: a general thermochemical approach.** *Earth Surf Process.* 1976; **1**(1): 63–70.
Publisher Full Text

Deng H, Sonnenthal E, Arora B, *et al.*: **The environmental controls on efficiency of enhanced rock weathering in soils.** *Sci Rep.* 2023; **13**(1): 9765.
PubMed Abstract | **Publisher Full Text** | **Free Full Text**

Dilrukshi R, Nakashima K, Kawasaki S: **Soil improvement using plant-derived urease-induced calcium carbonate precipitation.** *Soils Found.* 2018; **58**(4): 894–910.
Publisher Full Text

Dontsova K, Balogh-Brunstad Z, Chorover J: **Chapter 2. Plants as drivers of rock weathering.** *American Geophysical Union (AGU).* 2020; 33–58.
Publisher Full Text

Dupla X, Möller B, Baveye PC, *et al.*: **Potential accumulation of toxic trace elements in soils during enhanced rock weathering.** *Eur J Soil Sci.* 2023; **74**(1): e13343.
Publisher Full Text

Edwards CA, Arancon NQ: **Chapter the role of earthworms in organic matter and nutrient cycles**. *Biology and ecology of earthworms*. Springer US, New York, NY, 2022; 233–274.
Publisher Full Text

Evans K, Banwart S: **Rate controls on the chemical weathering of natural polymineralic material. I. Dissolution behaviour of polymineralic assemblages determined using batch and unsaturated column experiments.** *Appl Geochem.* 2006; **21**(2): 352–376.
Publisher Full Text

Ferral-Pérez H, Galicia-García M, Alvarado-Tenorio B, *et al.*: **Novel method to achieve crystallinity of calcite by *Bacillus subtilis* in coupled and noncoupled calcium-carbon sources**. 2020.
Publisher Full Text

Finlay R, Mahmood S, Rosenstock N, *et al.*: **Reviews and syntheses: biological weathering and its consequences at different spatial levels – from nanoscale to global scale.** *Biogeosciences.* 2020; **17**(6): 1507–1533.
Publisher Full Text

Frouz J, Krištůfek V, Livečková M, *et al.*: **Microbial properties of soil aggregates created by earthworms and other factors: spherical and prismatic soil aggregates from unreclaimed post-mining sites.** *Folia Microbiol (Praha).* 2011; **56**(1): 36–43.
PubMed Abstract | **Publisher Full Text**

Fuhr M, Wallmann K, Dale AW, *et al.*: **Alkaline mineral addition to anoxic to hypoxic Baltic Sea sediments as a potentially efficient co_2-removal technique.** *Front Clim.* 2024; **1**: 1338556.
Publisher Full Text

Gastmans D, Hutcheon I, Menegário AA, *et al.*: **Geochemical evolution of groundwater in a basaltic aquifer based on chemical and stable isotopic data: case study from the Northeastern portion of Serra Geral Aquifer, São Paulo state (Brazil).** *J Hydrol.* 2016; **535**: 598–611.
Publisher Full Text

Gerrits R, Pokharel R, Breitenbach R, *et al.*: **How the rock-inhabiting fungus *k. petricola* A95 enhances olivine dissolution through attachment.** *Geochim Cosmochim Acta.* 2020; **282**: 76–97.
Publisher Full Text

Gostinčar C, Ohm RA, Kogej T, *et al.*: **Genome sequencing of four *Aureobasidium pullulans* varieties: biotechnological potential, stress tolerance, and description of new species.** *BMC Genomics.* 2014; **15**: 549.
PubMed Abstract | **Publisher Full Text** | **Free Full Text**

Hartmann J, West AJ, Renforth P, *et al.*: **Enhanced chemical weathering as a geoengineering strategy to reduce atmospheric carbon dioxide, supply nutrients, and mitigate ocean acidification.** *Rev Geophys.* 2013; **51**(2): 113–149.
Publisher Full Text

He C, Zhang Z, Zhang Y, *et al.*: **Efficient pullulan production by *Aureobasidium pullulans* using cost-effective substrates.** *Int J Biol Macromol.* 2021; **186**: 544–553.
PubMed Abstract | **Publisher Full Text**

Heřmanská M, Voigt MJ, Marieni C, *et al.*: **A comprehensive and internally consistent mineral dissolution rate database: part I: primary silicate minerals and glasses.** *Chem Geol.* 2022; **597**: 120807.
Publisher Full Text

Heřmanská M, Voigt MJ, Marieni C, *et al.*: **A comprehensive and consistent mineral dissolution rate database: Part II: secondary silicate minerals.** *Chem Geol.* 2023; **636**: 121632.
Publisher Full Text

Ho TK: **Random decision forests.** In: *Proceedings of 3rd international conference on document analysis and recognition.* IEEE, 1995; 278–282.
Publisher Full Text

Horton P, Long SP, Smith P, *et al.*: **Technologies to deliver food and climate**

security through agriculture. *Nat Plants.* 2021; **7**(3): 250–255.
PubMed Abstract | Publisher Full Text

Huang H, Hong F, Liu J, *et al.*: **FVID: Fishing Vessel type Identification based on VMS trajectories.** *J Ocean Univ China.* 2019; **18**: 403–412.
Publisher Full Text

IPCC: **Global Warming of 1.5°C: an IPCC Special Report on the impacts of global warming of 1.5°C above pre-industrial levels and related global greenhouse gas emission pathways, in the context of strengthening the global response to the threat of climate change, sustainable development, and efforts to eradicate poverty**. Edited by Masson-Delmotte, V., Zhai, P., Pörtner, H.O., Roberts, D., Skea, J., Shukla, P.R., Pirani, A., Moufouma-Okia, W., Péan, C., Pidcock, R., Connors, S., Matthews, J.B.R., Chen, Y., Zhou, X., Gomis, M.I., Lonnoy, E., Maycock, T., Tignor, M. and Waterfield, T, 2018.
Reference Source

Janssens IA, Roobroeck D, Sardans J, *et al.*: **Negative erosion and negative emissions: combining multiple land-based carbon dioxide removal techniques to rebuild fertile topsoils and enhance food production.** *Front Clim.* 2022; **4**: 928403.
Publisher Full Text

Janssens I, Servotte T, Calogiuri T, *et al.*: **Extended data for 'Machine learning-based identification of key biotic and abiotic drivers of mineral weathering rate in a complex enhanced weathering experiment'.** *Zenodo.* 2025.
http://www.doi.org/10.5281/zenodo.16728794

Janssens I, Servotte T, Mortier S: **STAN-UAntwerp.** [Code] h2020_BAM (Version 0.0.1). Github, 2024.
http://www.doi.org/10.5281/zenodo.14528497

Kelland ME, Wade PW, Lewis AL, *et al.*: **Increased yield and CO_2 sequestration potential with the C_4 cereal *Sorghum bicolor* cultivated in basaltic rock dust-amended agricultural soil.** *Glob Chang Biol.* 2020; **26**(6): 3658–3676.
PubMed Abstract | Publisher Full Text

Keren-Paz A, Maan H, Karunker I, *et al.*: **The roles of intracellular and extracellular calcium in *Bacillus subtilis* biofilms.** *iScience.* 2022; **25**(6): 104308.
PubMed Abstract | Publisher Full Text | Free Full Text

Kim J, Mulrooney S, Hausinger R: **Biosynthesis of active *Bacillus subtilis* urease in the absence of known urease accessory proteins.** *J Bacteriol.* 2005; **187**(20): 7150–4.
PubMed Abstract | Publisher Full Text | Free Full Text

Kirschbaum MU: **The temperature dependence of soil organic matter decomposition, and the effect of global warming on soil organic C storage.** *Soil Biol Biochem.* 1995; **27**(6): 753–760.
Publisher Full Text

Kirtzel J, Ueberschaar N, Deckert Gaudig T, *et al.*: **Organic acids, siderophores, enzymes and mechanical pressure for black slate bioweathering with the basidiomycete *Schizophyllum commune*.** *Environ Microbiol.* 2020; **22**(4): 1535–1546.
PubMed Abstract | Publisher Full Text

Koorneef GJ, de Goede RG, Pulleman MM, *et al.*: **Quantifying organic carbon in particulate and mineral-associated fractions of calcareous soils - a method comparison.** *Geoderma.* 2023; **436**: 116558.
Publisher Full Text

Kos M, Jing J, Keesmaat I, *et al.*: **After-life effects: living and dead invertebrates differentially affect plants and their associated above- and belowground multitrophic communities.** *Oikos.* 2017; **126**(6): 888–899.
Publisher Full Text

Krajewska B: **Urease-aided calcium carbonate mineralization for engineering applications: a review.** *J Adv Res.* Biotechnological and medical relevance of ureases, 2018; **13**: 59–67.
PubMed Abstract | Publisher Full Text | Free Full Text

Kruk M, Artiemjew P, Paturej E: **The application of game theory-based machine learning modelling to assess climate variability effects on the sensitivity of lagoon ecosystem parameters.** *Ecol Inform.* 2021; **66**: 101462.
Publisher Full Text

Köhler P, Hartmann J, Wolf-Gladrow D: **Geoengineering potential of artificially enhanced silicate weathering of olivine.** *Proc Natl Acad Sci U S A.* 2010; **107**(47): 20228–33.
PubMed Abstract | Publisher Full Text | Free Full Text

Levin S: **Ecosystems and the biosphere as complex adaptive systems.** *Ecosyst.* 1998; **1**: 431–436.
Publisher Full Text

Lin J, Lin D, Zhu G, *et al.*: **Earthworms exert long lasting afterlife effects on soil microbial communities.** *Geoderma.* 2022; **420**: 115906.
Publisher Full Text

Liu D, Lian B, Wang B, *et al.*: **Degradation of potassium rock by earthworms and responses of bacterial communities in its gut and surrounding substrates after being fed with mineral.** *PLoS One.* 2011; **6**(12): e28803.
PubMed Abstract | Publisher Full Text | Free Full Text

Lucas TCD: **A translucent box: interpretable machine learning in ecology.** *Ecol Monogr.* 2020; **90**(4): e01422.
Publisher Full Text

Lundberg SM, Allen PG, Lee SI: **A unified approach to interpreting model predictions.** *Adv Neural Inf Process Syst.* 2017; **30**.
Publisher Full Text

Luo H, Xiang C, Zeng L, *et al.*: **Shap based predictive modeling for 1 year all-cause readmission risk in elderly heart failure patients: feature selection and model interpretation.** *Sci Rep.* 2024; **14**(1): 17728.
PubMed Abstract | Publisher Full Text | Free Full Text

Maher K: **The dependence of chemical weathering rates on fluid residence time.** *Earth Planet Sci Lett.* 2010; **294**(1–2): 101–110.
Publisher Full Text

Manning DAC, de Azevedo AC, Zani CF, *et al.*: **Soil carbon management and enhanced rock weathering: the separate fates of organic and inorganic carbon.** *Eur J Soil Sci.* 2024; 75(4): e13534.
Publisher Full Text

Manzoni S, Porporato A: **A theoretical analysis of nonlinearities and feedbacks in soil carbon and nitrogen cycles.** *Soil Biol Biochem.* 2007; **39**(7): 1542–1556.
Publisher Full Text

Milici VR, Abiven S, Bauser HH, *et al.*: **The effects of plant–microbe–environment interactions on mineral weathering patterns in a granular basalt.** *Geobiology.* 2024; **22**(6): e70004.
PubMed Abstract | Publisher Full Text

Moras CA, Bach LT, Cyronak T, *et al.*: **Ocean Alkalinity enhancement-avoiding runaway $CaCO_3$ precipitation during quick and hydrated lime dissolution.** *Biogeosci.* 2022; **19**(15): 3537–3557.
Publisher Full Text

Mortier S, Hamedpour A, Bussmann B, *et al.*: **Inferring the relationship between soil temperature and the Normalized Difference Vegetation Index with Machine Learning.** *Ecol Inform.* 2024; **82**: 102730.
Publisher Full Text

Niron H, Vienne A, Frings P, *et al.*: **Exploring the synergy of enhanced weathering and *Bacillus subtilis*: a promising strategy for sustainable agriculture.** *Glob Chang Biol.* 2024; **30**(9): e17511.
PubMed Abstract | Publisher Full Text

Nwoko KC, Liang X, Perez MA, *et al.*: **Characterisation of selenium and tellurium nanoparticles produced by *Aureobasidium pullulans* using a multi-method approach.** *J Chromatogr A.* 2021; **1642**: 462022.
PubMed Abstract | Publisher Full Text

Oelkers EH, Declercq J, Saldi GD, *et al.*: **Olivine dissolution rates: a critical review.** *Chem Geol.* 2018; **500**: 1–19.
Publisher Full Text

Olsson PA, Wallander H: **Interactions between ectomycorrhizal fungi and the bacterial community in soils amended with various primary minerals.** *FEMS Microbiol Ecol.* 1998; **27**(2): 195–205.
Publisher Full Text

Olsson-Francis K, Van Houdt R, Mergeay M, *et al.*: **Microarray analysis of a microbe-mineral interaction.** *Geobiology.* 2010; **8**(5): 446–456.
PubMed Abstract | Publisher Full Text

Park J, Lee WH, Kim KT, *et al.*: **Interpretation of ensemble learning to predict water quality using explainable artificial intelligence.** *Sci Total Environ.* 2022; **832**: 155070.
PubMed Abstract | Publisher Full Text

Pedregosa F, Varoquaux G, Gramfort A, *et al.*: **Scikit-learn: machine learning in Python.** *J Mach Learn Res.* 2011; **12**: 2825–2830.
Reference Source

Peplow M: **Enzymes boost' rock weathering' to trap CO_2 in soil.** *Nat Biotechnol.* 2024; **42**(9): 1326–1328.
PubMed Abstract | Publisher Full Text

Perez-Fodich A, Derry LA: **Organic acids and high soil CO_2 drive intense chemical weathering of hawaiian basalts: insights from reactive transport models.** *Geochim Cosmochim Acta.* 2019; **249**: 173–198.
Publisher Full Text

Raihan J, Khan AM, Kee SH, *et al.*: **Detection of the Chronic Kidney Disease using XGBoost classifier and explaining the influence of the attributes on the model using SHAP.** *Sci Rep.* 2023; **13**(1): 6263.
PubMed Abstract | Publisher Full Text | Free Full Text

Renforth P: **The negative emission potential of alkaline materials.** *Nat Commun.* 2019; **10**(1): 1401.
PubMed Abstract | Publisher Full Text | Free Full Text

Ribeiro MT, Singh S, Guestrin C: **"why should i trust you?": explaining the predictions of any classifier.** In: *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining.* Association for Computing Machinery, New York, NY, USA, 2016; 1135–1144.
Publisher Full Text

Ryo M, Angelov B, Mammola S, *et al.*: **Explainable artificial intelligence enhances the ecological interpretability of black-box species distribution models.** *Ecography.* 2021; **44**(2): 199–205.
Publisher Full Text

Santosa F, Symes WW: **Linear inversion of band-limited reflection seismograms.** *SIAM J Sci Comput.* 1986; **7**(4): 1307–1330.
Publisher Full Text

Shi GY, Zhou Y, Sang YQ, *et al.*: **Modeling the response of negative air ions to environmental factors using multiple linear regression and random forest.** *Ecol Inform.* 2021; **66**: 101464.
Publisher Full Text

Shwartz-Ziv R, Armon A: **Tabular data: deep learning is not all you need.** *Inf*

Fusion. 2022; **81**: 84–90.
Publisher Full Text

Song S, Wang ZA, Gonneea ME, *et al.*: **An important biogeochemical link between organic and inorganic carbon cycling: effects of organic alkalinity on carbonate chemistry in coastal waters influenced by intertidal salt marshes.** *Geochim Cosmochim Acta.* 2020; **275**: 123–139.
Publisher Full Text

Stone M: **Cross-validatory choice and assessment of statistical predictions.** *J R Stat Soc Series B Stat Methodol.* 1974; **36**(2): 111–133.
Publisher Full Text

Sun YQ, Ge Y: **Temporal changes in the function of bacterial assemblages associated with decomposing earthworms.** *Front Microbiol.* 2021; **12**: 682224.
PubMed Abstract | **Publisher Full Text** | **Free Full Text**

Suzuki Y, Matsubara T, Hoshino M: **Breakdown of mineral grains by earthworms and beetle larvae.** *Geoderma.* 2003; **112**(1–2): 131–142.
Publisher Full Text

Tibshirani R: **Regression shrinkage and selection via the Lasso.** *J R Stat Soc Series B Stat Methodol.* 1996; **58**(1): 267–288.
Publisher Full Text

Valavi R, Guillera-Arroita G, Lahoz-Monfort JJ, *et al.*: **Predictive performance of presence-only species distribution models: a benchmark study with reproducible code.** *Ecol Monogr.* 2022; **92**(1): e01486.
Publisher Full Text

Van Groenigen JW, Van Groenigen KJ, Koopmans GF, *et al.*: **How fertile are earthworm casts? A meta-analysis.** *Geoderma.* 2019; **338**: 525–535.
Publisher Full Text

Vanderkloot E, Ryan P: **Quantifying the effect of grain size on weathering of basaltic powders: implications for negative emission technologies via soil carbon sequestration.** *Appl Geochem.* 2023; **155**: 105728.
Publisher Full Text

Versteegh EAA, Black S, Hodson ME: **Environmental controls on the production of calcium carbonate by earthworms.** *Soil Biol Biochem.* 2014; **70**: 159–161.
Publisher Full Text

Vicca S, Goll DS, Hagens M, *et al.*: **Is the climate change mitigation effect of enhanced silicate weathering governed by biological processes?** *Glob Chang Biol.* 2022; **28**(3): 711–726.
PubMed Abstract | **Publisher Full Text**

Vienne A, Poblador S, Portillo-Estrada M, *et al.*: **Enhanced weathering using basalt rock powder: carbon sequestration, co-benefits and risks in a mesocosm study with *Solanum tuberosum*.** *Front clim.* 2022; **4**: 869456.
Publisher Full Text

Wang R, Kim JH, Li MH: **Predicting stream water quality under different urban development pattern scenarios with an interpretable machine learning approach.** *Sci Total Environ.* 2021; **761**: 144057.
PubMed Abstract | **Publisher Full Text**

Washbourne CL, Lopez-Capel E, Renforth P, *et al.*: **Rapid removal of atmospheric CO_2 by Urban soils.** *Environ Sci Technol.* 2015; **49**(9): 5434–40.
PubMed Abstract | **Publisher Full Text**

Watson SK, Han Z, Su WW, *et al.*: **Carbon dioxide capture using *Escherichia coli* expressing carbonic anhydrase in a foam bioreactor.** *Environ Technol.* 2016; **37**(24): 3186–92.
PubMed Abstract | **Publisher Full Text**

White AF, Buss HL: **Natural weathering rates of silicate minerals.** *Treatise on Geochemistry (Second Edition).* Amsterdam: Elsevier, chapter 7.4, 2014; **7**: 115–155.
Publisher Full Text

Wild B, Gerrits R, Bonneville S: **The contribution of living organisms to rock weathering in the critical zone.** *Npj Mater Degrad.* 2022; **6**: 98.
Publisher Full Text

Xie X, Wu T, Zhu M, *et al.*: **Comparison of random forest and multiple linear regression models for estimation of soil extracellular enzyme activities in agricultural reclaimed coastal saline land.** *Ecol Indic.* 2021; **120**: 106925.
Publisher Full Text

Zhu X, Lian B, Yang X, *et al.*: **Biotransformation of earthworm activity on potassium-bearing mineral powder.** *J Earth Sci.* 2013; **24**: 65–74.
Publisher Full Text

Open Peer Review

Current Peer Review Status: ✔ ✔ ?

Version 3

Reviewer Report 23 September 2025

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✔ **Xiying Sun**
Texas A&M University, Texas, USA

I would like to thank the authors for their thorough revisions. They have successfully addressed all of the concerns I raised in my previous review. The manuscript is now a much stronger and more reproducible piece of work. I am pleased to recommend this article for full approval and have no further comments.

Competing Interests: No competing interests were disclosed.

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard.

Version 2

Reviewer Report 26 July 2025

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✔ **David Manning**
Newcastle University, Newcastle upon Tyne, UK

Thank you for addressing my suggested changes so carefully. The Supplementary Information is really informative and would allow other scientists to use this study in a substantial and serious way.

I'd like it if you could rethink some text in the penultimate paragraph of the Introduction: 'implying that the same drivers would induce similar changes in both, albeit with opposite signs.' This is not necessarily so. If calcite (SIC) as the solution are in equilibrium, the concentration of DIC should be constant and will only decrease once calcite has dissolved completely. Precipitation of more calcite will maintain constant [DIC].

Relating to this, in the results section 'Organic Amendments and Biochar', the statement 'The absence of a rise in ΔDIC suggests that the increase in TA was of organic origin' may be wrongly interpreted, as it could instead reflect calcite saturation. Geochemical modelling of the solution composition would tell you this. Can you rule out calcite saturation? If so, please say so.

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: Soil science, mineralogy, petrology, biochar

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard.

Author Response 02 Aug 2025

Iris Janssens

Thank you for your detailed feedback, which has been invaluable in enhancing the quality of our manuscript.

- We agree with the referee: if a solution is at equilibrium, adding IC to it would increase SIC with constant DIC. However, we had in mind driver-induced changes relative to the controls. Take the example of using steel slag as mineral substrate instead of basalt. Its weathering increases pH so strongly that all formed IC (released from added substrates or by heterotrophic respiration in the columns) is immediately precipitated as calcite. In this case, as the referee suggests, inside the pot DIC remains constant (in fact zero), while SIC increases strongly. However, compared to the starting concentrations and to the pots with basalt, DIC declines and SIC increases. Another example: adding a chelate would mask part of the DIC, effectively increasing the equilibrium constant at which calcite precipitates, and thereby increasing DIC and decreasing SIC precipitation. To avoid similar criticisms by the readers, we rephrased the sentence as: "*Moreover, in a purely abiotic system, DIC and SIC are in equilibrium (yet controlled by kinetic rate constants of carbonate precipitation and dissolution), implying that a driver that accelerates or decelerates SIC formation would induce opposite changes in DIC and SIC, relative to comparable columns without the driver.*"

- Indeed, the absence of a rise in ΔDIC may come from calcite precipitation, but this could not explain why ΔTA increased simultaneously, because calcite precipitation is an alkalinity sink. So if calcite saturation were at play, both ΔTA and ΔDIC should decline with increasing ΔSIC, which we did not observe. The three figures below show for three different ΔDIC ranges the corresponding ΔSIC and ΔTA values, revealing no correlations and suggesting that TA can change substantially also in absence of large

values of ΔSIC or ΔDIC. A manuscript dedicated to the importance of the organic fraction of TA using a subset of this dataset and showing clear evidence for a major contribution of organic alkalinity has been submitted for publication elsewhere. Unfortunately, that manuscript is still under review so we cannot give a definite citation for it, but together with the absence of correlation with ΔSIC, it does rule out that carbonate saturation is causing these observations.

Fig-https://openreseurope-files.f1000.com/linked/258401.Fig_2_19252.png

Competing Interests: No competing interests were disclosed.

Reviewer Report 15 July 2025

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Xiying Sun
Texas A&M University, Texas, USA

The authors have done an excellent job addressing most of my previous concerns. The added details on the input materials and the new machine learning results in the Extended Data have substantially strengthened the manuscript.

The paper is very close to being ready for full approval. However, I recommend a few final revisions to ensure the analysis is fully transparent and reproducible.

1. SHAP interaction plots: To directly visualize the conditional effects that are central to the paper's conclusions, I still strongly recommend including SHAP interaction plots. As the authors are already using the shap library in Python, this can be implemented with the standard shap.dependence_plot() function and should not require significant additional work.

2. Justification for data omission: My previous review raised a major point about the potential bias from omitting data from rounds 1-3 for some targets. This remains unaddressed. A brief discussion of this choice and its potential limitations should be added to ensure the methodology is fully transparent.

3. Correction of potential error in Extended Data: The newly added "Extended Data" file is very helpful. However, potential error is in Table A6, where the error reported for SO3 in basalt is ±1.00% on a value of 0.01%, which is scientifically implausible.

For these reasons, I recommend maintaining the status of Approved with reservations. I am confident that if the authors address these points, I will be able to recommend the article for full approval.

Competing Interests: No competing interests were disclosed.

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.

Author Response 02 Aug 2025

Iris Janssens

We sincerely thank you for the in depth review that helped us strengthen our manuscript.

1. We have now added several SHAP interaction plots to the Extended data (figure C6) and added references to these plots to the discussion. This indeed added clarity to some of the discussion points.

2. Sorry for this, we misunderstood your previous question and provided a response explaining why it was OK to omit them instead. The justification for omitting these three rounds was given in the second paragraph of the section on data pre-processing: “In rounds 1 to 3, additional samples were taken from the leachate after three weeks, which affected the measurements after eight weeks. Therefore, data of rounds 1 to 3 were omitted for the prediction of ΔTA, ΔDIC and ΔTIC.” However, we now see that the justification for the omission and its potential introduction of bias in the dataset indeed needed strengthening. We therefore elaborated the sentence as follows: "In rounds 1 to 3, additional samples for chemical analyses were taken from the leachate after three weeks, which affected the measurements after eight weeks. Therefore, data of rounds 1 to 3 were omitted for the prediction of ΔTA, ΔDIC and Δ TIC. Because the leachate sampling happened in the leachate container, it did not impact the column with solid matter above, whose data were still used. As we realized early in the project that the leachate data from the first three rounds could not be used in this analysis, many input combinations covered in these first three rounds were repeated in later rounds. As a result, this information was not lost for the ΔDIC, ΔTA and ΔTIC models. While the ΔSIC data contained more replicates, these were properly dealt with in the cross validation (CV) approach (see next section, 'Predictive models') to avoid bias in our analyses. Therefore, we believe that excluding the first three rounds did not introduce biases in this study. "

3. Thank you for spotting this. This was indeed wrong, and should be 0.01%. We have changed this in the Extended Data.

Competing Interests: No competing interests were disclosed.

Version 1

Reviewer Report 14 June 2025

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Nate Looker
Stanford University, Stanford, USA

This manuscript presents new analyses of a high-dimensional enhanced mineral weathering experiment, a portion of which was previously analyzed in Calogiuri et al. (2025). The complex study design allows exploration of the response of weathering rates (inferred using DIC, SIC, and TA) to 29 independent variables. The inclusion of several biological variables is an important distinction from previous lab-based enhanced weathering studies, as soil-dwelling organisms and biologically derived compounds (e.g., enzymes and organic acids) may play underappreciated roles in determining in-field weathering rates.

Overall, the study is well designed and executed. My primary recommendation is that the authors further leverage the design and statistical analyses to deliver more interpretable insights. For example, what design-based comparisons can be made, if any? I understand that the design was not full-factorial (i.e., treatments represent a subset of all possible combinations of factor levels), but of the treatments that were explored, are there subsets that can be analyzed as varying in only one variable (e.g., mineral grain size, presence/absence of a particular additive)? Additionally, I was left wondering what the three sets of models can tell us about interactions (e.g., effect of earthworm biomass as mediated by mineral feedstock type) and the functional form (or at least direction) of effects. The Lasso regression models did not perform as well as the more sophisticated ML models, but did Lasso-estimated coefficients agree with the direction of effects inferred with ML? Partial dependence plots (as the authors previously presented in Calogiuri et al. 2025) or bivariate SHAP plots could be effective ways to explore these questions. I also encourage the authors to consider including a conceptual model to synthesize their hypotheses and/or results (e.g., expanding the earthworm-specific model in Calogiuri et al. 2025 to include the other variables analyzed here).

Specific comments:

Portions of the introduction (starting with the fifth paragraph on page 5) present study-specific details that would fit better in the methods section. Consider instead using the introduction to review the state of the science of interactive/nonlinear controls on enhanced weathering (i.e., the motivation for a complex study like this).

Hypotheses (page 6): different features were hypothesized to drive change in each of the weathering indicators—can you get more specific about which features you expected to drive each indicator?

How were treatments allocated temporally (across rounds)?

Was autoclaving one of the 29 treatments (page 7)?

How long and at what temperature were samples combusted for LOI? How was removal of organic C verified?

The text states that leachate concentrations were calculated using irrigated volume (which to me means the volume of water applied), rather than the leachate volume: is this correct? Does this differ from the approach the authors used previously (Calogiuri et al. 2025)?

What processes gave rise to missing data? If some analytes were “missing-not-at-random” (e.g., related to treatment outcomes), omitting columns with missing data could introduce bias.

How sensitive are the effects of the enzymes studied here to pH?

Is the work clearly and accurately presented and does it cite the current literature?
Yes

Is the study design appropriate and does the work have academic merit?
Yes

Are sufficient details of methods and analysis provided to allow replication by others?
Yes

If applicable, is the statistical analysis and its interpretation appropriate?
Partly

Are all the source data underlying the results available to ensure full reproducibility?
No

Are the conclusions drawn adequately supported by the results?
Yes

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: Soil carbon cycling, pedology, forest soils, biogeochemistry

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.

Author Response 23 Jun 2025

Iris Janssens

We thank the referee for the insightful suggestions, which helped to improve the quality of the manuscript.

- As the number of possible combinations of treatments was extremely large (see all features and used amounts in Table 1), it was impossible to test them all in a full factorial design. The experimental design was therefore set up with the machine learning approach in mind. As a result, for many combinations the number of similar combinations with only one different variable is limited. For simple combinations (for example, containing no biotic inputs, but instead only one type of mineral (with one grain size), organic matter and biochar), such subsets can be extracted. Other studies have been -or are being- conducted using subsets of the data, for example Calogiuri et al. (2025), which indeed provide more specific results. However, the objective of this study is to test whether machine learning can be leveraged to maximally extract information from the entire dataset. This way, potential interactions between treatments are not excluded.
- We agree that more results on the interaction effects and functional forms would be interesting.
    - The direction and size of the effects is given by the SHAP plots (Figure 3). If a red dot (= adding (more of) the input) has a positive SHAP value, it means that the target is positively impacted by adding the input; if it has a negative SHAP value, adding the input decreases the impact.
    - The models don't give functional forms, except from Lasso, which only performed reasonably well for ΔDIC. Its coefficients are given in the Extended data (section C2). Comparing these coefficients with the SHAP plots of the XGB model (Figures 2, C2 in Extended data), we see that the most important features generally agree (e.g. dunite has the largest positive effect in both models), with slight deviations in the rankings (e.g. alfalfa mixture mass has a large positive effect in both models, but is ranked second by Lasso and sixth by SHAP). The latter can be explained by a difference in the meaning of the rankings: the rankings in the SHAP plots do not only include the size of the importance, but also the abundance of this value in the data set. However, there also are some differences. For example, urea is the sixth most important feature in the lasso model, while it has no impact in the XGB model.
    - Other kinds of plots, such as partial dependence plots and SHAP dependence plots, can indeed indicate interactions between two features. We have studied these SHAP dependence plots but only found clear interactions with steel slag surface area. However, as we had already calculated and plotted the SHAP values separately for the subsets with and without steel slag, these dependence plots did not give additional information. Other interactions, though possibly present, were unclear in the dependence plots.
- We do agree with the referee that a conceptual model would be beneficial. However, due to the absence of direct CDR data, which is now circumvented by looking at four CDR indicators, and the fact that the importances of the 30 investigated drivers differ across targets and in some cases depend on interactions with other drivers, it is at this point extremely difficult to extract a full conceptual model that describes the whole system. However, other studies focus on subsets of the data to develop conceptual models about specific aspects. One of this studie is Calogiuri et al., 2025, but more studies are still in progress.

Specific comments:

- Thank you for suggesting this. We revised the first sentences of the fifth paragraph to make it better suited for an Introduction section, but did not move the paragraph because it introduces the rationale for selecting the chosen variables. Moreover, we did elaborate the third and seventh paragraphs, citing new papers on the interactions between minerals and biota that introduce non-linearities in the weathering rates.
- This is an interesting suggestion, but after internal discussion we opted not to adopt it. Our main reasons are: 1. The requested indicator-specific hypotheses are the subject of targeted studies in preparation and 2. This manuscript focuses on the leverage potential of machine learning to identify key drivers in the presence of a multitude of possibly interacting features. By shifting towards indicator-specific mechanisms, we fear that the focus on machine learning leverage would be lost. We hope the referee will understand.
- Treatments were predominantly chosen by the researchers in the project, either randomly or based on hypotheses and interests which changed through time based on intermediate results. Some subsets were also computationally determined, amongst others randomly through Latin hypercube sampling, to fill the input space as much as possible, or through optimal experimental design. This was used in later rounds and is the subject of a separate manuscript in preparation. Last, previously failed experiments were often repeated in a later round. Thus, determining the treatments was done through a mix of different methods, which could change over time. However, as the possible 'ingredients' were determined at the start of the project (with the exception of initially dead earthworms), all rounds had comparable input combinations.
- Yes, the number of treatments was determined as the number of features in the models, and whether autoclaving was done or not was given by the feature 'sterilized' (see Tab. 1). However, your question made us realize that the number of treatments mentioned (29) did not agree with the number of features (30; Tab. 1), so we changed this to 30 in the text.
- Samples were combusted for three hours at 550°C. This protocol is standard and was therefore not verified by alternative methods. We added this information to the Methods section.
- Indeed, your interpretation is correct. We observed that the leachate volume did not consistently agree with the irrigated volume, which could have been due to different evaporation from containers across placements in the climate chamber, leakage after passing through the column, and small deviations of the irrigation system. However, most likely, most of these discrepancies originated after passing through the column, which would indicate that the irrigation volume is a more accurate quantity of the volume that passed through the system. Moreover, this also meant that using the irrigated volume to calculate the amounts of DIC [mmol] and TA [mmol] from their measured concentrations would give a more accurate estimation than using the leachate volume. This was added to the Limitations subsection of the manuscript.
- Missing data could have different reasons. Sometimes errors in measurements of SIC, DIC and TA lead to the experiments being discarded for the corresponding target. Sometimes the experiment failed for some columns due to the irrigation system malfunctioning, a leak in the system, flooding of columns and human errors in the set up and during the experiment. The flooding of columns was investigated,

as it could be related to the inputs, but no pattern was found. Moreover, as the experiment was conducted in different rounds, many of the failed experiments were successfully repeated in a later round. We are therefore confident that our dataset did not show a bias due to 'not random missing data'. We have now clarified in the manuscript that the missing target data was due to measurement errors.
- The following figure plots the SHAP values of the concentrations of the three enzymes as a function of the pH of the leachate. Generally, the SHAP values are or are close to zero, and no pH effect is observed.

Figures- https://openreseurope-files.f1000.com/linked/258400.Fig_19252.png

Competing Interests: No competing interests were disclosed.

Reviewer Report 27 May 2025

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Xiying Sun
Texas A&M University, Texas, USA

This study represents an ambitious and carefully designed contribution to understanding the complex drivers of enhanced weathering. The combination of a multifactorial experimental setup with machine learning provides a promising approach to disentangle the roles of biotic and abiotic variables in carbon transformation processes. The methodology is well-matched to the complexity of the system, and the findings are likely to be of broad interest within the fields of biogeochemistry and carbon dioxide removal. However, there are some important areas where clarification and additional detail would strengthen the manuscript.

Major points requiring attention include:

1. The term "basalt (basanite), lava (basanite)" is unclear since basalt is a type of lava (solidified), are they from different sources? Do they have different textural properties despite both being basanite (e.g., one is more vesicular, hence broadly termed "lava", while the other is a more standard "basalt")? I recommend the authors improve the clarification and provide detailed chemical characterization.
2. The feature "# earthworms" reflects the number of initially live earthworms (Table 1). However, the manuscript acknowledges that "a substantial part of the added earthworms died during the experiment". As a result, the SHAP importance for this feature in Figure 2 and discussed in the "Biota and biotic products" subsection likely captures both the effects of live worm activity (e.g., mineral grinding, $CaCO_3$ production) and post-mortem decomposition (e.g., CO_2 and nutrient release). Attributing the entire SHAP signal to active biological processes may therefore be misleading. I recommend clarifying this point and reconsidering the interpretation of this feature's contribution to carbon cycling outcomes.

3. The manuscript explains the reason for omitting rounds 1-3 from the ΔTA, ΔDIC, and ΔTIC targets due to intermediate sampling affecting 8-week measurements. However, it does not explicitly address the potential biases this exclusion may introduce. Since rounds 1-3 account for a substantial portion of the experimental timeline and may contain distinct early-phase weathering dynamics or unique input combinations, their omission could limit the model's ability to capture the full variability of system behavior. This could affect both model generalizability and the interpretation of driver importance for key CDR indicators. I recommend the authors explicitly discuss these possible limitations and qualify any conclusions drawn for these targets accordingly. Also, why were these rounds not omitted for ΔSIC? If leachate sampling affected the system, it could potentially influence SIC precipitation/dissolution as well by altering solution chemistry.
4. While Extended Info B (Table B1) helpfully lists the names of tuned hyperparameters for RF and XGBoost, the manuscript would benefit from including the full value grids used during tuning and a summary of the selected optimal values for each outer fold. Additionally, adding predicted versus actual scatter plots for the best-performing models, particularly XGBoost, would provide valuable visual insight into model fit and error structure. Including these elements, even in the supplementary materials, would enhance reproducibility of the machine learning workflow.

Some minor points for consideration:

1. The manuscript's current use of SHAP value comparisons across subsets (e.g., with vs. without steel slag) offers useful insights into potential feature interactions. The paper would benefit further from incorporating SHAP interaction plots (plotting a feature's SHAP value against its value, colored by an interacting feature), which directly visualize how the effect of one feature on model predictions varies depending on the value of another. This would strengthen the interpretation of conditional effects already discussed in the text, such as the differing impacts of irrigation flow rate or biotic inputs depending on the presence of steel slag or organic amendments. Including a few targeted SHAP interaction plots in the supplementary materials could enhance the clarity and depth of the paper's explainable AI analysis.
2. The "mixed grain size" feature is marked as important, but its definition and distinction from the detailed surface area (SA) features are unclear. Since SA already reflects grain size composition, it is not evident what unique information this feature adds. To clarify its role, the manuscript would benefit from addressing: (1) Does "mixed grain size" refer to mixing within a single mineral or across different minerals? (2) What does it capture that SA features do not-such as effects on column packing or flow? Clarifying these points would help ensure the SHAP importance of this feature is not misinterpreted or confounded with other inputs.
3. Extended Info B includes SHAP plots for XGBoost across most targets and for RF only in the case of ΔTA. Since RF performed comparably to XGBoost for several outcomes, the manuscript would benefit from a brief comparison of SHAP feature importance rankings between the two models for another key target such as ΔTIC. Including this in the supplementary material could strengthen confidence in the robustness of the identified drivers.
4. A small typo in "the concentrations of and TA" in the Method section.
5. The caption for Figure 1 explicitly states it includes histograms for "dissolved organic carbon (DOC)". However, DOC is not displayed in any of the Figure 1 panels. Also, the "five targets" should be four accordingly.

6. While the study offers a valuable snapshot of early-stage mineral weathering dynamics, the temporal scope constrains conclusions about the durability of carbon sequestration and the evolving role of key drivers over time. A discussion of these limitations, particularly regarding the permanence of ΔTIC and the potential shifts in driver importance beyond the experimental window, would help appropriately qualify the interpretation of "CDR potential" and provide clearer context for future studies aiming to translate lab-scale findings to field-scale applications. For discussion on the long-term sequestration potential of DIC and its fate in natural systems, please refer to Beerling et al. (2020)
7. The use of nested cross-validation in this study is appropriate and provides a robust estimate of model generalization performance. However, if the authors intend to deploy or highlight a final, single predictive model beyond the evaluation framework, it would be ideal to validate that model on a separate hold-out test set that was set aside prior to any model tuning or training. While not essential for the study's current focus on driver importance and methodological insights, clarifying this point or outlining such a step for future applications would strengthen the reproducibility and potential downstream utility of the modeling approach.
8. "Biochar was not amended to stimulate microbial activity, but to promote weathering abiotically by adsorbing ions and increasing seed crystals due to its high IC content and acidification of the system." Biochar is generally alkaline and tends to increase soil pH (Rashid et al., 2020), so the observed acidification in the presence of biochar should be explicitly explained.

References

Beerling, D. J., Kantzas, E. P., Lomas, M. R., Wade, P., Eufrasio, R. M., Renforth, P., et al. (2020). Potential for large-scale CO2 removal via enhanced rock weathering with croplands. *Nature*, *583* (7815), 242–248. https://doi.org/10.1038/s41586-020-2448-9

Rashid, M., Hussain, Q., Khan, K. S., Al-Wabel, M. I., Afeng, Z., Akmal, M., et al. (2020). Prospects of Biochar in Alkaline Soils to Mitigate Climate Change. In S. Fahad, M. Hasanuzzaman, M. Alam, H. Ullah, M. Saeed, I. Ali Khan, & M. Adnan (Eds.), *Environment, Climate, Plant and Vegetation Growth* (pp. 133–149). Cham: Springer International Publishing. https://doi.org/10.1007/978-3-030-49732-3_7

References

1. Beerling DJ, Kantzas EP, Lomas MR, Wade P, et al.: Potential for large-scale CO2 removal via enhanced rock weathering with croplands.*Nature*. 2020; **583** (7815): 242-248 PubMed Abstract | Publisher Full Text
2. Rashid M, Hussain Q, Khan K, Al-Wabel M, et al.: Prospects of Biochar in Alkaline Soils to Mitigate Climate Change. 2020. 133-149 Publisher Full Text

Is the work clearly and accurately presented and does it cite the current literature?

Yes

Is the study design appropriate and does the work have academic merit?

Yes

Are sufficient details of methods and analysis provided to allow replication by others?

No

If applicable, is the statistical analysis and its interpretation appropriate?
Yes

Are all the source data underlying the results available to ensure full reproducibility?
No

Are the conclusions drawn adequately supported by the results?
Partly

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: Oceanography, Machine Learning, Carbon Cycle, Silicate Weathering

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.

Author Response 23 Jun 2025

Iris Janssens

Thank you for the thorough evaluation and the constructive suggestions that helped us improve the manuscript. Major points:

1. The rocks were indeed not properly described. We have renamed lava to basanite/tephrite (and dunite to peridotite) and added a clearer explanation to the methods. Moreover, we added a new section (A) to the Extended Data, containing amongst others a TAS diagram and XRF and XRD results for the rocks (section A.2).
2. We indeed realized that earthworms died during the experiment. To distinguish the impacts of living versus decaying earthworms, we also conducted experiments where only dead earthworms were added. Then, we always compared the SHAP values of the initially live earthworms with the initially dead earthworms and interpreted the results accordingly. This is discussed in the 'Biota and biotic products' subsection.
3. To answer you last question; the data of the first three rounds could be used for the ΔSIC models, because the leachate sampling happened in the leachate container, which did not impact the column with solid matter above. To adress your first point; as we realized early in the project that the first three rounds would not be used in this analysis, many of the input combinations covered in these three rounds were repeated in later rounds. As a result, this information was not lost for the ΔDIC, ΔTA and ΔTIC models, while the ΔSIC data contained more replicates, which were properly dealt with in the train test splits. Based on this, and the fact that the amount of data after omitting the first three rounds remains large, we believe that this exclusion did not introduce biases in the data sets.
4. We agree that this enhances the reproducibility. I have expanded the hyperparameter table to include the selected values in each fold of each of the models (Table C1); and added the scatter plots to the Extended data (Fig C1).

Minor points:

1. We agree that in many cases such interaction plots are very informative. However, we

looked at these plots, and besides the interaction with steel slag, no clear interactions were found. Since these interactions with steel slag were already clear in the summary plots, we opted not to provide redundant display items.

2. (1) The mixed grain size refers to both. Whether a coarse mineral A was mixed with a fine mineral B, or a fine mineral A with a coarse mineral B, is reflected in the respective total SA of minerals A and B; therefore this information was captured by the SA. However, information on mixing or no mixing needed to be provided because: (2) Whether the grain sizes were mixed or not provides additional information to the SA, both within the same rock type and across mixed rock types. For example, mixing minerals with a high and a low SA can yield a similar SA as minerals with a medium SA, but combining large and small grains can have a big impact on the water flow (Amann et al., 2022).
   We have clarified this in the revised manuscript in the 'Rocks' subsection of the 'Results and discussion' section.
3. We agree that comparing the SHAP values of RF with those of XGB strengthens the robustness and have added these plots for all targets to the Extended Data (Figs. C6-C9). The SHAP values of both models generally agree: the direction of the effects consistently agree, though there are small changes in sizes of impacts and as a result in the rankings.
4. Thank you for spotting this. This is now corrected.
5. This was indeed a wrong version of the caption and is corrected now.
6. We agree with the referee that our results are only valid for the first 8 weeks of weathering and should not be extrapolated in time nor to field applications. We added the following text to the Limitations subsection: “The reader should also bear in mind that the identified drivers that dominate weathering in this experiment may differ from those dominating CDR in the long term. Moreover, this experiment was conducted in the absence of soil to test optimal conditions in reactor settings, which may also have affected the relative importance of the drivers compared to field studies in soils.
7. Thank you for this suggestion. We agree that clarifying this can be useful and we have added the following sentences to the Limitations subsection: “The nested CV approach provides a robust estimate of model generalization performance and is appropriate for our objective, i.e. uncovering insights from driver importance. However, future applications aimed at model deployment should include evaluation on a separate hold-out test set reserved prior to model development.”
8. Thank you for spotting this. This was indeed a mistake in the text. The pH, measured in $CaCl_2$ was 8.6 (this was added in a new table A8 in the extended data). The text is now corrected to: “Biochar was not added to stimulate microbial activity, but to promote weathering abiotically by adsorbing ions and increasing seed crystals, due to its high IC content and pH (see Table A8 in Extended data).”

Competing Interests: No competing interests were disclosed.

Reviewer Report 09 May 2025

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David Manning
Newcastle University, Newcastle upon Tyne, UK

This manuscript reports a really nice piece of work that addresses a fundamental problem associated with experiments that investigate enhanced rock weathering – how do you work with so many variables. I am not an expert in AI, but I can see the value of the approach taken here, and I find it exciting. I am confident that once the work is indexed, it will be widely regarded as a pioneering paper that will be widely cited, the approach being emulated and developed by many other researchers.
I always look at the supplementary material, Extended Data in this case, to see if there is enough information to allow others to repeat the experiments. In this case insufficient information is made available either in the Extended Data or in the paper that describes the experimental work, Calogiuri et al 2023. The following information must be provided, and its disclosure will have no effect on the project's protection of intellectual property:

1. The rocks used MUST be properly described in the Methods section. A basanite is as different from a basalt as a lion is from a tiger. You must use the International Union of Geological Sciences' classification of volcanic rocks, published by Le Bas et al many years ago: Refer:1. Here you will see that a basanite has a different chemical composition to a basalt. At the very least, the chemical analysis of the rocks and slag used should be provided in the Extended Data in the conventional way (as oxides with the Loss on Ignition and the Sum), together with the location that these materials came from (or the name of the company that supplied the slag). In each case, a reference should be cited to geological literature that describes the rocks in more detail – there will be plenty to choose from. Similarly, 'dunite' has a precise definition (>90% olivine), and the source should be stated again with a reference to its description. You need to take similar care to that taken when describing the earthworms or the microbes.
2. Clearly explain what is the difference between the basanite that is a 'basalt' and the basanite that is a 'lava'. What is written in the Methods section (page 7, top left) is meaningless as it stands, and will only confuse a reader who only knows a little petrology.
3. Similarly, the biochar needs to be described in more detail, as different biochar feedstocks (e.g. wheat straw, softwood etc) lead to very different properties. Please state what the feedstock is, and provide a reference that gives the basic properties of biochar prepared from that feedstock.
4. And in Table 1, the type of straw needs to be stated.
5. The sand: again, give a full description of the sand, in terms of its chemical and mineralogical composition and its source. Sand is a really variable material. It often contains calcite and aragonite as shells, and it often contains feldspars, rock fragments and other confounding components.
6. The water used needs to be clearly described. I don't think its description is stated anywhere. I assume it was deionised water – but say so. If tap water was used, give its chemical analysis as a lot of Belgian tap water is close to calcite saturation, which would perturb the interpretation enormously.

In terms of the processes that take place in weathering experiments of this type, a clear description of some of these is given in the paragraph beginning 'Lasso…'. Here the ability of Lasso to address linear relationships is described in the context of ecological processes, stating that biogeochemical processes are non-linear. It is a point of discussion that should be developed. In the absence of biological factors, weathering reactions are driven by thermodynamics, with a reduction in the Gibbs free energy of the system. These reactions are highly linear, with appropriate transformation of the data. Curtis (1976) provides an elegant approach to this: Refer 2. The kinetics of the reactions then is well developed by Oelkers and coauthors, exemplified by recent publications in Heřmanská et al (2022, Refer 3; 2023, Refer 4). The bottom line is that abiological weathering reactions are not random. They are controlled by thermodynamic and kinetic processes that can be described precisely using an algebraic approach. It would be fantastic if AI could extract evidence for this from experiments of the type reported here – you are probably the best placed research team to be able to do this.

Other points include:

1. 'However, care must always be taken to ensure that the minerals used do not pollute the soil with heavy metals (Dupla et al., 2023; Vienne et al., 2022).' I agree with this sentence, but great care needs to be taken when talking about possible contamination. First, very large areas of agricultural land have basaltic rocks as the soil parent material, providing populations of millions with crops grown on effectively 100% basalt (from the inorganic point of view). Secondly, soils naturally contain 'pollutants' so any risk assessment must include determination of the natural background levels of these elements. You could also cite Gastmans et al's elegant description refer 5) of the geochemistry of basalt aquifers that supply millions of people in São Paulo state with clean safe drinking water. Please consider revising the text at this point, bearing in mind the reaction you want from the reader – which should be that 'I don't really need to worry about this for these rocks'.
2. 'Notwithstanding that DIC resembles TA in most organic-poor systems, in organic-rich systems, TA has an inorganic and organic component (Song et al., 2020).' I think this could be developed, and that you should provide evidence of the amounts of DOC in your water samples. Was this information available from the FormacsHT TOC analyser?
3. Data Preprocessing section: Table A2 does not describe minerals, as implied by the text, but the rocks. Make sure you acknowledge that the individual particles of both rock and slag whose characteristics are given in Table A2 are each a composite mixture of different mineral grains. This comes through in Table 1, where the term 'mineral' should be replaced by 'rock' or 'material'.
4. 'In contrast to dunite and basalt, adding steel slag reduced ΔDIC (Figure 2a).' Did you check for the presence of carbonate? It is easy to do, using thermal analysis, which is very sensitive (much more so than XRD).
5. 'Steel slag typically contains free CaO and MgO (Wang et al., 2024)'. Please check that this is not a misunderstanding of the conventional way in which chemical compositions of slags are reported – as % oxides. It is extremely unlikely that the slag used in these experiments contained free CaO and MgO, as these oxides will hydrate or carbonate very rapidly during preparation of the material prior to use in the experiments.
6. 'Adding more lava to the mineral mix had no clear effect..' I don't know what you are referring to here – please be more precise.
7. 'Biochar was not amended' – replace 'amended' with 'added'. 'Amended' suggests that you amended the biochar before use.
8. 'Biota and biotic products.' How dd you stop the earthworms from migrating from one pot to another or escaping altogether? I have experience of them behaving in this way, a real

nuisance.

9. ‘Second, the rock particles are grinded in the earthworms’ gizzards,’ Use ‘ground’, not ‘grinded’.

References

1. BAS M, MAITRE R, STRECKEISEN A, ZANETTIN B, et al.: A Chemical Classification of Volcanic Rocks Based on the Total Alkali-Silica Diagram. *Journal of Petrology*. 1986; **27** (3): 745-750 Publisher Full Text
2. Curtis C: Stability of minerals in surface weathering reactions: A general thermochemical approach. *Earth Surface Processes*. 1976; **1** (1): 63-70 Publisher Full Text
3. Heřmanská M, Voigt M, Marieni C, Declercq J, et al.: A comprehensive and internally consistent mineral dissolution rate database: Part I: Primary silicate minerals and glasses. *Chemical Geology*. 2022; **597**. Publisher Full Text
4. Heřmanská M, Voigt M, Marieni C, Declercq J, et al.: A comprehensive and consistent mineral dissolution rate database: Part II: Secondary silicate minerals. *Chemical Geology*. 2023; **636**. Publisher Full Text
5. Gastmans D, Hutcheon I, Menegário A, Chang H: Geochemical evolution of groundwater in a basaltic aquifer based on chemical and stable isotopic data: Case study from the Northeastern portion of Serra Geral Aquifer, São Paulo state (Brazil). *Journal of Hydrology*. 2016; **535**: 598-611 Publisher Full Text

Is the work clearly and accurately presented and does it cite the current literature?
Yes

Is the study design appropriate and does the work have academic merit?
Yes

Are sufficient details of methods and analysis provided to allow replication by others?
No

If applicable, is the statistical analysis and its interpretation appropriate?
Partly

Are all the source data underlying the results available to ensure full reproducibility?
No

Are the conclusions drawn adequately supported by the results?
Partly

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: Soil science, mineralogy, petrology, biochar

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.

Author Response 23 Jun 2025

Iris Janssens

We appreciate the referee's support for our innovative approach and the good suggestions. We have assessed the constructive remarks as follows: 1-2. We agree that some information was missing here. We have added more information to the Methods section and added a new section to the Extended data (section A). Specifically,

- We have renamed lava into basanite/tephrite and dunite into peridotite; and have added a clearer description of the rocks to the methods section.
- The Extended data (section A2) now contains the TAS diagram of the basalt and basanite/tephrite rocks is added to the Extended data (Fig. A1), references and sources of the rocks and slags (Tab. A3), the qualitative and normative compositions (XRD) (Tab. A4-5), the XRF composition (Tab. A6-7). Additional samples are now being analyzed by XRD for modal mineral results.
- We have added the sources of the earthworms and microbes to the methods section.

3. The biochar source (Verora, Germany) and feedstock (natural wood) are now added to the methods, and tables with its basic properties and elemental composition are added to the Extended data (Tab. A8, A9). Its IC content is given in Tab. A11 and the DIC, DOC and TA that result from columns with sand and biochar are given in Tab. A10. 4. The type of straw (wheat straw) is now added to the table, and its elemental composition is added to the Extended Data, Tab. A9. 5. We agree that knowing the full mineralogical characterization of the sand would be interesting; however, comparing TA and DIC of the input ground water (Tab. A2 in Extended Data), and the measurements after leaching through the sand bed (Tab. A10 in Extended Data), does not show an increase in TA and DIC. Hence, if calcite and aragonite or other confounding components were present in the sand, they did not leach TA and DIC. This is also expected as the mean pH of the ground water was 7.85 (Tab. A2). 6. In the revised manuscript, we have specified that the used water was natural ground water and have added tables with its properties (Tab. A1-A2 in Extended data). (7.) We thank the reviewer for this insightful remark. We have now included this in the introduction: “Weathering reactions, such as those promoted in enhanced weathering experiments, are driven by thermodynamics and are, in absence of biotic interactions, highly linear such that their kinetics can be modelled well (Curtis et al., 1976; Heřmanská et al., 2022; Heřmanská et al., 2023). Model outputs may be transformed to yield linear relationships or normal distributions, enabling parametric statistical approaches to elucidate results from experiments or variability in time series. However, in situ, microbes will respond to the altered environmental conditions and availability of elements in soils, among others by altering their respiration, exudation of organic acids, or taking up reaction products. These microbial responses thus elicit a suite of feedbacks that the current generation of geochemical models cannot reproduce, rendering some geochemical reactions unpredictable and highly non-linear. Under these real-world conditions where reaction kinetics cannot be reproduced by existing models, machine learning that can cope with non-linear relationships may enable the attribution of observed changes in weathering reactions to potential drivers.” Other points: 1. We thank the reviewer for these insights and have changed the sentence to: “care must always be taken to ensure that the added minerals will not increase heavy metal availabilities beyond risk-bearing thresholds (Gastmans et al; Dupla et al., 2023; Vienne et al., 2022).” 2. DOC was indeed measured. We

have added the DOC measurements of the blank columns (Table A9 in Extended data). Moreover, we have added a new section to the Extended data (C.5), with a plot of the relation of ΔDIC and ΔDOC with ΔTA (Fig. C10) and used linear regression to predict ΔTA from ΔDIC and ΔDOC (Fig. C11). Results for data with steel slag have a low accuracy (either due to the limited data size, noise, or absence of a linear relation due to rapid precipitation), while a clear linear relation is found for columns without steel slag. Here, ΔDIC dominates the prediction, but ΔDOC also contributes. Given that DOC is outside the scope of our study, we did not further elaborate on this in the manuscript. 3. We indeed wrongly used minerals and rocks interchangeably. We have now corrected this issue throughout the text and in the tables. 4. Indeed, ΔDIC is low due to rapid precipitation of carbonates, which is indicated by the high ΔSIC (indicating an increase in SIC). This is shown by the high SHAP values of steel slag in the prediction of ΔSIC (Figure 3b). This is discussed in the Rocks subsection in the Results and discussion section. 5. Thank you for this suggestion, which was correct. We reformulated the text as follows: “The steel slag used had a high calcium content (Table A6 in Extended Data (Janssens et al., 2025), XRF), a portion of which was likely present in the form of calcium hydroxide ($Ca(OH)_2$). This phase dissolves quickly in water, increasing solution pH by releasing hydroxide ions.”
6. We have added a reference to Figs. C3, C4 in Extended Data. 7,9. We have corrected the words. 8. A mesh was placed on top of the columns, which is now added to the methods.

Competing Interests: No competing interests were disclosed.