



*Supplement of*

## **In silico calculation of soil pH by SCEPTER v1.0**

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## S1. Previous example simulations but with cation exchange

As an example simulation, the previous version (v0.9) of SCEPTER has been utilized to reproduce depth profiles of soil organic matter (SOM) and pH at two specific sites (Sites 2 and 3; Fig. 13 of Kanzaki et al., 2022). While the assumption that observed pH represents porewater pH might not necessarily be accurate (see the main text), the tuned models for the two sites are useful for examining the impact of adding cation exchange on model tuning to observations and implications of cation exchange for carbon capture through ERW although not on croplands but natural weathering sites with little human intervention given that the two sites are characterized with cultivated vegetation less than 1% (see Kanzaki et al., 2022, for more details).

Figs. S1a and d compare simulations of porewater pH between v0.9 and v1.0 with/without cation exchange, along with observations. Boundary conditions for simulations with v1.0 are the same as those used for v0.9 (Kanzaki et al., 2022). For v1.0 simulations with cation exchange, we used the default cation exchange capacity and thermodynamics (Tables 1 and 2). Comparison in Figs. S1a and d suggests the following: First, without cation exchange, v0.9 and v1.0 behave essentially the same regardless of the model update that includes modification of aqueous species tracking (Section 2 of the main text); Second, even though we have not performed any additional tuning, simulations with cation exchange are better in reproducing observations at relatively shallow depths.

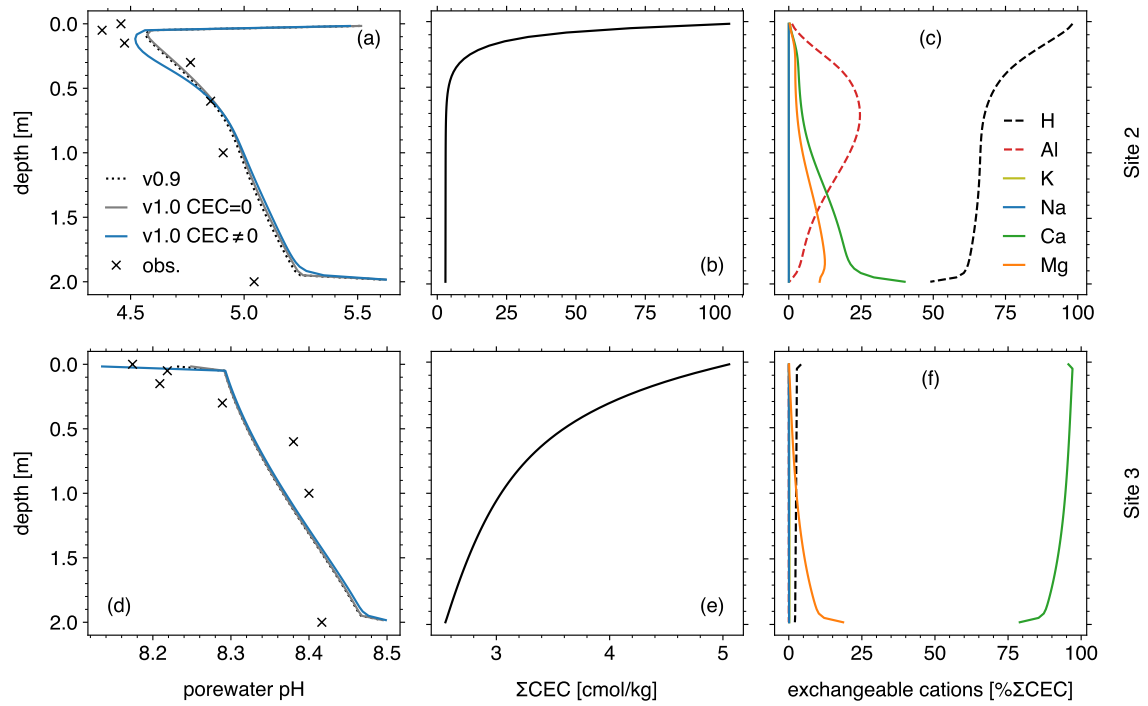
Influences of cation exchange are limited to the top soil because of relatively higher bulk CEC at the surface (Figs. S1b and e), which can be further attributed to the relative abundance of SOM (Figs. 13a and c of Kanzaki et al., 2022) and its dominant CEC contribution to bulk soil in the current default setting (Table 1). Because of the low SOM concentration ( $\leq 0.6$  wt%; Kanzaki et al., 2022), simulated bulk CEC is correspondingly low and the influence of cation exchange is relatively minor at Site 3 (compare Figs. S1b and e). Given the high background pH at this site (Fig. S1d), base saturation is  $\sim 100\%$  (Fig. S1f) and ERW is expected to yield essentially the same carbon capture with and without cation exchange because the expected change in base saturation is limited at this site. In contrast, Site 2 is more acidic containing a larger amount of SOM ( $>20$  wt% at the surface) and the top 50 cm is characterized with  $\sim 0\%$  base saturation (Fig. S1c). Therefore, initial alkalinity addition is expected to be consumed to neutralize the exchangeable acidity and carbon capture is expected to be correspondingly delayed at Site 2.

Expected impacts of cation exchange on carbon capture through ERW described above were confirmed by additional simulations where milled basalt (dominated by 5, 20, 50 and 70  $\mu\text{m}$  particles) is applied to Sites 2 and 3 during initial 0.1 fraction of each year with an annual average rate of  $40 \text{ t ha}^{-1}$  for 100 years (Fig. S2) as in the example experiments shown in Fig. 15 of Kanzaki et al. (2022) but using v1.0 either with or without cation exchange. The same boundary conditions as those for v0.9 (Kanzaki et al., 2022) are applied to v1.0 except that default cation exchange parameters (Tables 1 and 2) are assumed when cation exchange is

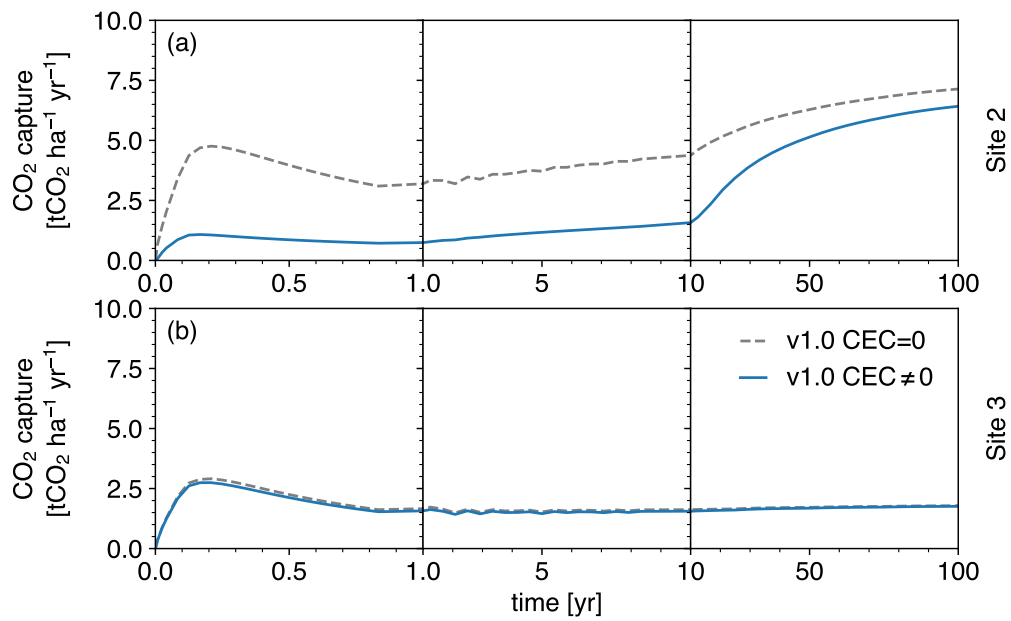
enabled. Among multiple surface area calculation options we consider here only the one with  
40 tracking particle size distributions for individual solid species (see Kanzaki et al., 2022, for more  
details). Fig. S2 clearly shows that including cation exchange can have significant influences on  
carbon capture by ERW. Especially for soils whose initial background states are characterized  
with a large pool of exchangeable acidity as is the case for Site 2, there can be a time lag to  
45 reach a specific carbon capture with cation exchange relative to the case without taking account  
of cation exchange. Delayed carbon capture caused by neutralization of exchangeable acidity  
relative to alkalization in croplands will be studied in more details elsewhere.

## References

Kanzaki, Y., Zhang, S., Planavsky, N. J., and Reinhard, C. T. (2022). Soil Cycles of Ele-  
ments simulator for Predicting TERrestrial regulation of greenhouse gases: SCEPTER v0.9.  
50 *Geoscientific Model Development*, 15(12):4959–4990.



**Figure S1:** Porewater pH (a and d), bulk CEC (b and e) and exchangeable cations (c and f) simulated by SCEPTEr v1.0 at Sites 2 (a–c) and 3 (d–f) of Kanzaki et al. (2022). In (a) and (d), simulations without cation exchange and by v0.9 and observations are also shown for comparison.



**Figure S2:** CO<sub>2</sub> capture simulated by SCEPTEr v1.0 with and without cation exchange for pulsative basalt application experiments at Sites 2 and 3 of Kanzaki et al. (2022).