Supplementary Information

An inorganic CO_2 diffusion and dissolution process explains negative CO_2 fluxes in saline/alkaline soils

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Supplementary Table S1

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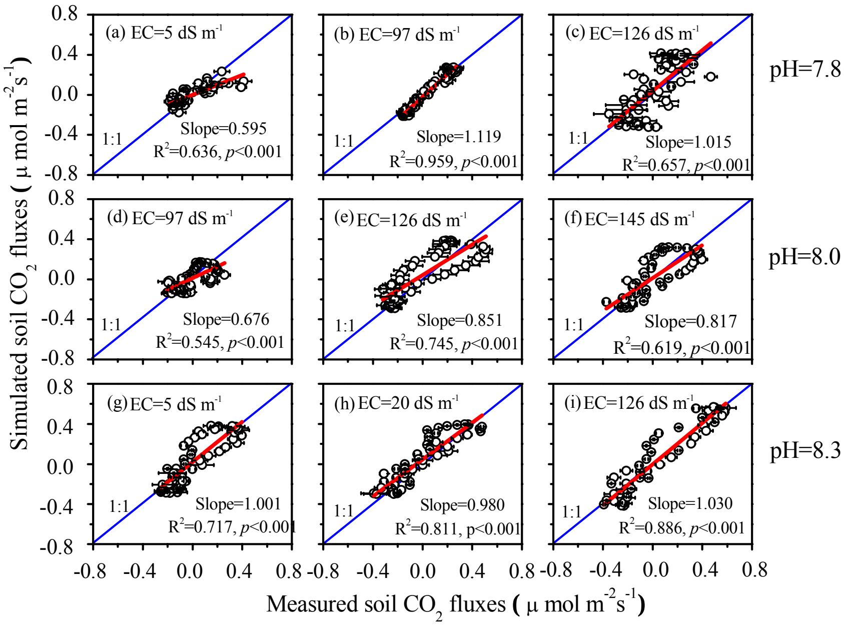
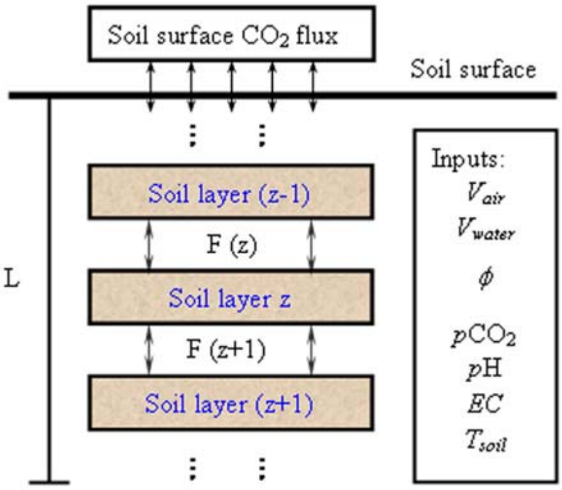
Functions	References
$\log KH = 108.3865 + 0.01985076 \times T - 6919.53/T - 40.45154 \times \log T + 669365/T^2$	ref. 1
$\log K_1 = -356.3094 - 0.06091964 \times T + 21834.37/T + 126.8339 \times \log T - 1684915/T^2$	ref. 1
$\log K_2 = -107.8871 - 0.03252849 \times T + 5151.79/T + 38.92561 \times \log T - 563713.9/T^2$	ref. 1
$K_0 = 1.7 \times 10^{-4}/K_1$	ref. 2

Supplementary Table S1. Temperature dependence of Henry's Law constant and equilibrium constants for saline and alkaline soils



Supplementary Figure S1. Comparison between simulated (ordinates) and directly measured (horizontal axis) inorganic soil CO_2 flux in soils with different pH and EC (a–i). The solid lines represent a line of 1:1. The data is the same as that described in Fig. 6.



Supplementary Figure S2. Conceptual illustration of CO_2 flux model environment. The solid box shows input parameters.

Supplementary Methods

Submodel of heat transport component. The heat transport component of the model approximates the diurnal variation of soil temperature as a sinusoidal curve, and the temperature of each soil layer can be expressed by[3, 4]:

$$T(z,t) = T_0 - \gamma_0 z + \sum_n A_{on} \exp^{\alpha z} \sin(\frac{2n\pi}{\omega} t + \varphi_{0n} - \beta z) \quad (9)$$

where T_0, A_{0n} and φ_{0n} represent the average, amplitude and phase of the soil surface temperature wave, respectively; ω is the period of soil temperature, which equals 86400 in our model; t is the time in units of s; γ_0 is the speed of soil temperature decrease with depth; and α and β are constants for certain soils. However, in actual operation, the soil surface temperature (i.e. at 0 cm) is hard to measure precisely and, along with α and β, may vary with soil type and soil moisture content. So, here we used the difference of soil temperature amplitude for two specific layers, 5 and 20 cm underground, to calculate α and β, and used the temperature at 5 cm underground as the basis. So, each layers' temperature can be expressed as:

$$T(z,t) = T_5 - \gamma_0 (z-5) + \sum_n A_{5n} \exp^{(5-z)\sqrt{\frac{n\pi}{K\omega}}} \sin(\frac{2n\pi}{\omega} t + \varphi_{5n} - (5-z)\sqrt{\frac{n\pi}{KP}}) \quad (10)$$

$$K = \frac{\pi}{\omega} \left(\frac{z_{20} - z_5}{n \frac{A_5}{A_{20}}}\right)^2 \quad (11)$$

where T_5, φ_{5n} and A_{5n} are the initial average, phase and amplitude of the temperature at 5 cm below the soil surface, respectively; z_{20} and z_5 are the depth of these two layers; and A_{20} is the amplitude of soil temperature at a depth of 20 cm.

Supplementary Reference

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2. Wissbrun, K.F., French, D.M. & Patterson, A. The true ionization constant of carbonic acid in aqueous solution from 5 to 45 °C. *J Phys Chem-Us* **58,** 693−695 (1954).
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4. Hillel, D.(eds.). *Environmental soil physics.* (Academic Press, San Diego, CA; 1998).