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An overlooked mechanism underlying the attenuation of temperature response of heterotrophic soil respiration

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S1. Soil structure parametrization

Soil water content appears in the model is a result of volumetric average of the microscopic processes throughout the hydrated soil pore space. Soil structure is parameterized via its impact on wetted pore wall for providing microbial habitat, water-air interfacial area for dissolving O_2, and hydraulic distance separating the two surficial areas. Increasing soil water content increases both substrates and the numbers of microsites monotonically. In contrast, water-air interfacial area increases with soil water content initially; when soil water content reaches a threshold, a further increase reduces the air-water interface for O_2 to dissolve while increasing the distance for dissolved O_2 to reach microsites. As an illustrative example, Figures S1(C-E) shows how these three parameters change with soil saturation for two soils acquired using X-ray CT imagery shown in Figures S1A, B. Pore geometries of the two soils differ, but the above three parameters vary with soil saturation in similar trends: as soil saturation increases, the hydraulic distance between the water-air interfacial area and the wetted walls increases gradually followed by a rapid increase once the saturation exceeds a threshold, approximately 55% - a saturation deemed optimal for aerobic microbes.

S2. The feedback factor

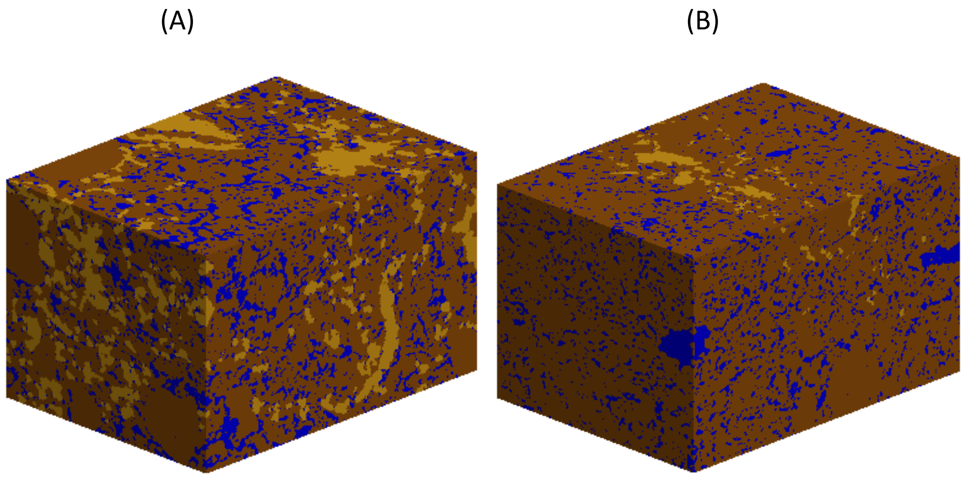
Kinetic reactions at microsites are independent of each other but the volumetric average couples them nonlinearly. For example, the potential demand of respiring microbes associated with a unit area of wetted pore wall for O_2 is k, but summing k over all microsites in a soil sample is not equivalent to the total respiration; it needs to be scaled back by the feedback factor E_r. To elucidate how E_r varies with soil water content and k, we take the soil sample in Figure S1A as an example, calculating their impact on E_r. For ease of analysis, k was normalized by molecular diffusion coefficient of O_2 in water and the hydraulic distance λ, i.e., $k' = 2\lambda k / D$, which represents the ratio of potential demand for O_2 and to the O_2 supply. Figure S2A shows the change in E_r with soil saturation under different k'. As envisaged, E_r decreases asymptotically as the saturation increases regardless of k'. When the demand at individual microsites for O_2 is low with respect to O_2 diffusion, i.e., when k' is small, E_r is close to 1.0 except when soil is nearly saturated where E_r drops sharply due to rapid reduction in water-air interfacial area for O_2 to dissolve. Figure S2B compares the changes in E_r with k' under different soil saturations, where the feedback factor decreases exponentially as the potential demand of the individual microsites for O_2 increases.

S3. Comparison with experimental data

The mechanistic model was derived by volumetrically averaging the microscopic processes occurring in pore space. It differs from previous models which use independent moisture and temperature functions to describe the respective influence of soil water and temperature on soil respiration. Since soil respiration is the consequence of microscopic processes occurring in the pore space, congruence between measurements and model results can be used as a criterion to assess if the model correctly captures the microscopic processes underpinning the response of respiration to soil water, temperature and other factors measured at macroscopic scale.

The model incorporates soil structure and microbial activity at the pore scale, with the former parameterized by water-air interfacial area, wetted pore-wall area, and the hydraulic distance between them; the latter is described collectively by the potential demand of microsites for O_2, which depends on temperature and SOC quality/quantity, as described by the Arrhenius kinetic equation and the Michaelis-Menten formula [1]. These factors are independent of each other at microsites in soil pores, but the volumetric average nonlinearly integrates them. Mathematically, each soil structure parameter can take an arbitrary value, but we treated them as a set, calculating their values by mining soil image database for a sample that best matches the experimental data.

The potential demand at each microsite for O_2 depends on many factors including microbial abundance and substrate quality and quantity, but these factors are difficult to separate experimentally. Thus, for incubation experiments where the temperature was kept constant, or field experiments where the temperature was not controlled, we used a single parameter to collectively describe their combined effects. Substrates and microbial distributions in the pore space are heterogeneous, and we represent such heterogeneities by allowing the potential demand for O_2 at microsites to vary with pore size. Quantitative data regarding how microbes and substrates vary with pore size are sparse, and we adopted a simple, yet rational approach, that for incubation experiments with repacked soil samples, the potential demand of microsites for O_2 was assumed to be independent of pore size. For field experiments or incubation experiments using field-structured soil samples, the potential demand for O_2 microsites increased with pore size to produce the “Birch phenomenon” where the respiration surges after rewetting dry soils [2].



Soil 1 **Soil 2**

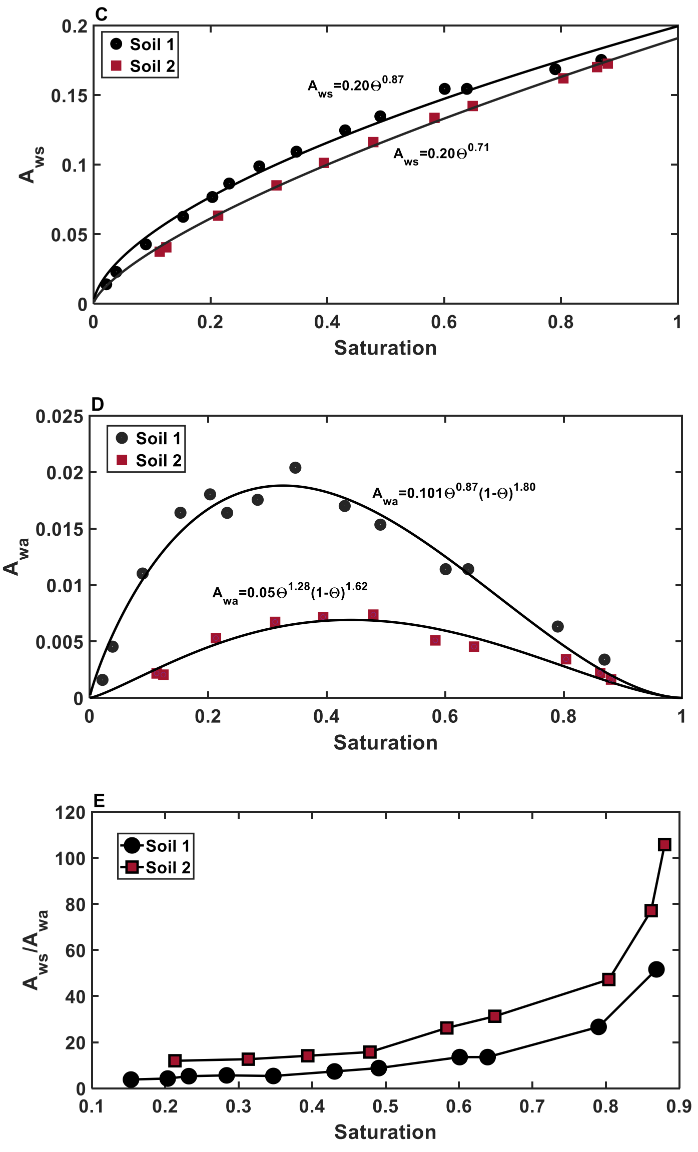


Figure S1. Water distribution in soils of different structures (A, B). Variation in specific wetted pore wall areas - A_{ws} (C), water-air interfacial area - A_{wa} (D), and hydraulic distance (E), as saturation increases in the two soils.

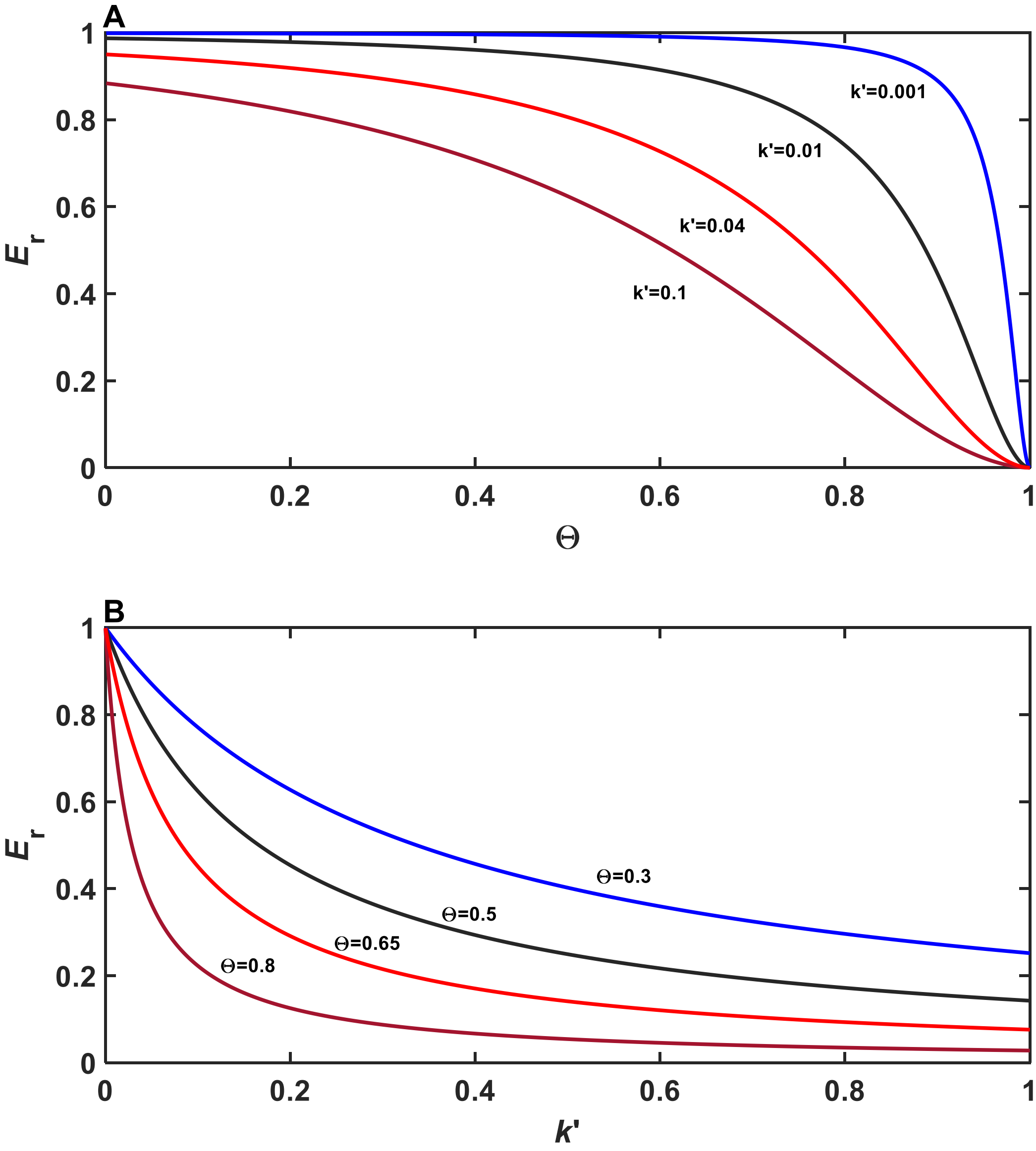


Figure S2. (A) Change in the feedback factor (E_r) with soil saturation (Θ) at different normalized potential demand of microbe for oxygen (k') at the microsites. (B) Decrease in E_r with the normalized potential demand of the microbes at reactive microsites for oxygen (k') under different soil saturations (Θ).

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