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Building bottom-up aggregate-based model (ABM) in soil systems with a view of aggregates as biogeochemical reactors

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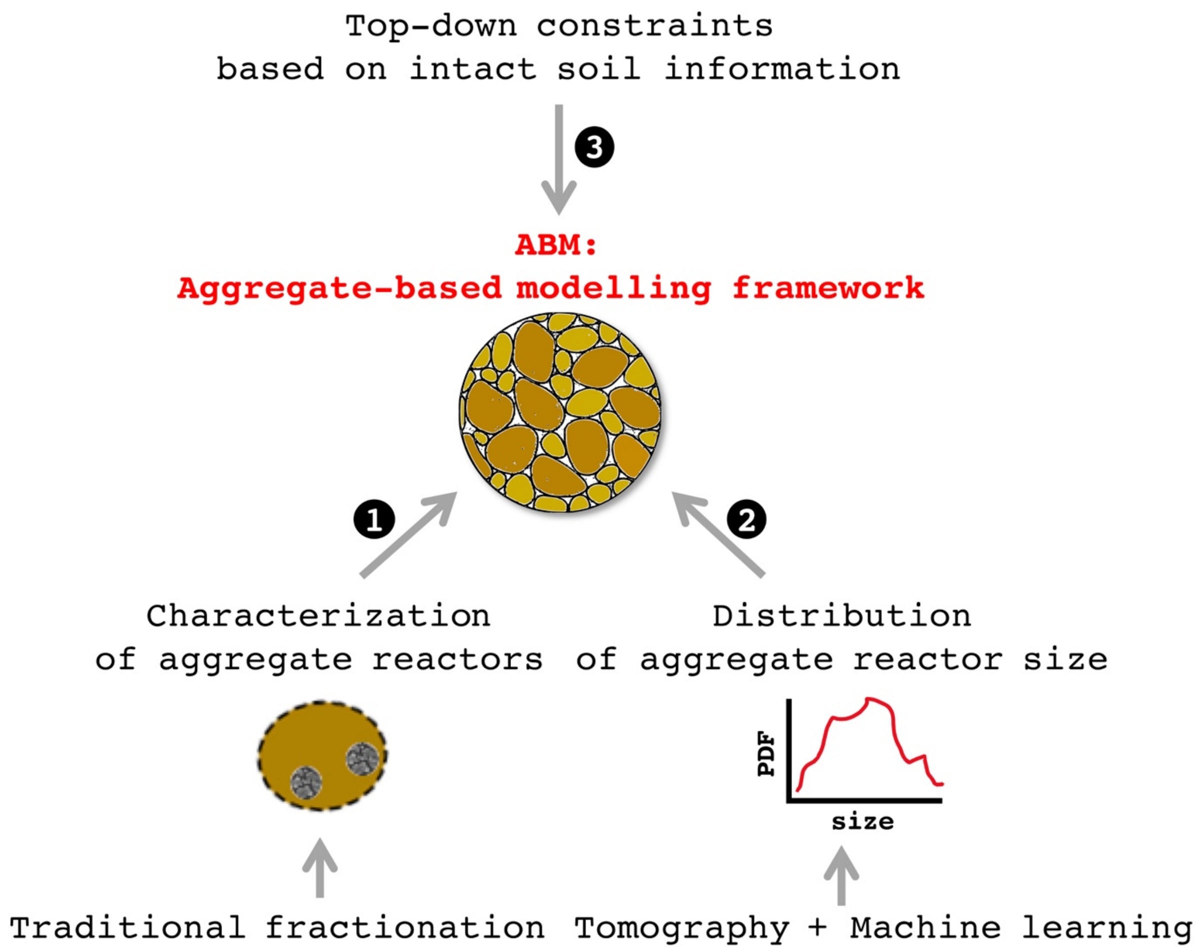

Fig.1 Framework for building aggregate-based models (ABMs) in soil systems. Theories built upon traditional soil fractionation and even artificial aggregates (**Path 1)** and the size distribution of aggregate reactors derived from tomography powered by machine learning (**Path 2**) would inform development of ABMs from the bottom up. This theory can be further constrained by top-down measurements of intact soils through model-data assimilation (**Path 3**).

In our recent article in Global Change Biology (**Wang et al., 2019**), we proposed to develop aggregate-based models (ABMs) based on a view of soil aggregates as biogeochemical reactors in the context of soil heterogeneity. Using a bottom-up philosophy, we argued for developing ABMs based on a systematic and dynamic view of soils as a constellation of aggregate reactors of different sizes. We envision that these ABMs offer the potential to bring new mechanistic perspectives into soil system modelling.

In a letter to the editor by **Kravchenko et al. (2019)** an alternative opinion is articulated, and we appreciate the authors' thoughtful comments. One element of this opinion is that soil system functioning is not a simple sum of soil constituents—we agree with this statement. Another objection from **Kravchenko et al.** is primarily based on indeterminacies of size and boundary conditions of aggregate reactors. We also agree that these limitations are important, and we began to address them in Section 6 of our article (**Wang et al. 2019**). However, we believe that these challenges arising from traditional soil fractionation techniques do not necessarily dilute our confidence in developing ABMs as a prognostic framework that integrates soil processes from the bottom up. We are grateful to have the opportunity here to further clarify our view and share new thoughts on it.

A bottom-up modelling approach is the 'Holy Grail' of soil system modelling that has been difficult to achieve because of soil's opaque and heterogeneous nature. In contrast, there has been a successful infusion of this modelling philosophy into such fields as ecology, sociology, economics, physics, and others (e.g., **Auyang 1998; Shugart et al. 2018**). In soil science, aggregates reflect soil system development ('succession'). Aggregates of different sizes form and collapse constantly during aggregate 'ontogeny', defined by aggregate turnover/stability, while interacting with many endogenous and exogenous factors. In this context we propose that aggregates, as physically distinct units embedded in the complex soil matrix, can be viewed as biogeochemical reactors, in which biogeochemical reactions actively transpire and across which soil macro-pores bridge interactions. By explicitly simulating aggregate reactors of different sizes along with their interactions, soil system functioning can be quantified as an emergent property of finer scale processes. This bottom-up modelling philosophy reflects how we understand soil system composition, structure, function, and dynamics. From this perspective, we firmly believe that viewing soil aggregates as physically independent units is a way forward for understanding soil system functioning.

In building ABMs, aggregate separation techniques and even artificial aggregates have played and will continue to play a pivotal role in gaining theoretical understanding of aggregate reactors and their size-dependent relationships with various factors (**Path 1** in **Fig.1**). Aggregate-based approaches can offer an advantage of measurability relative to current soil carbon models such as CENTURY for which the simulated carbon pools cannot be measured directly (**Parton 1996)**. Although building ABMs based on lab-derived aggregate sizes is a good starting point, **Kravchenko et al.** are legitimately concerned about indeterminacy in real soils. Still, *in-situ* observations of size distributions of aggregate reactors are possible via tomography techniques [e.g., X-Ray CT for bulk soil characterization (**Schlüter et al. 2019**) and SEM for finer structure (**Smith 2008)**] (**Path 2** in **Fig.1**). Even more promising are deep learning techniques for image recognition that can accelerate the retrieval of rich soil structural information from high resolution soil images derived from these tomography techniques (**Reichstein et al. 2019**). Therefore, knowledge from traditional soil fractionations and new data on soil structure powered by machine learning can inform ABM development with aggregate reactors as fundamental units (**Fig.1**).

Moreover, top-down constraints based on data from intact soils can further address shortcomings of the bottom-up approaches (**Path 3** in **Fig.1**). For example, boundary conditions of aggregate reactors (dependent on inter-aggregate spaces or macro-pores) are hard to determine because of methodological challenges in conducting *in situ* measurements. Such a lack of *in situ* information will increase the parameter uncertainty of ABMs. This issue is analogous to the determination of abiotic environment conditions, such as light intensity, surrounding an individual tree crown in a diverse forest system, which, though still hard to measure explicitly, do not hinder explicit model development (e.g., **Wang et al. 2017**). Regarding aggregate reactors, one feasible and efficient approach would be to calibrate ABMs with data derived from intact soils (**Kennedy and O'Hagan 2001**). Our original article therefore emphasized the utility of top-down experiments (**Wang et al. 2019**) as also stressed by **Kravchenko et al. (2019)**.

In summary, because they are mechanistically and structurally explicit, we argue that ABMs are a valuable tool for advancing soil system science [see a recent example by **Ebrahimi and Or (2018)**]. Some of the key challenges facing ABMs can be addressed readily with a combination of theory-driven and data-driven approaches (**Fig.1**). We hope more researchers from soil science, ecology, data science, and beyond will join in this discussion of developing bottom-up ABMs by viewing soil aggregates as relatively distinct units. We maintain that biogeochemical reactors are a useful concept for understanding soil functioning in the context of global environmental changes.

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References

Auyang, S. Y. Foundations of Complex System Theories in Economics, Evolutionary Biology, and Statistical Physics (Cambridge Univ. Press, New York, 1998).

Ebrahimi, A., & Or, D. (2018). On upscaling of soil microbial processes and biogeochemical fluxes from aggregates to landscapes. Journal of Geophysical Research: Biogeosciences, 123(5), 1526-1547.

Kennedy, M. C., & O'Hagan, A. (2001). Bayesian calibration of computer models. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 63, 425-464.

Kravchenko, A., Wilfred Otten, Patricia Garnier, Valérie Pot, Philippe C. Baveye. Soil aggregates as biogeochemical reactors: Not a way forward in the research on soil-atmosphere exchange of greenhouse gases. https://doi.org/10.1111/gcb.14640

Parton W.J. (1996) The CENTURY model. In: Powlson D.S., Smith P., Smith J.U. (eds) Evaluation of Soil Organic Matter Models. NATO ASI Series (Series I: Global Environmental Change), vol 38. Springer, Berlin, Heidelberg

Reichstein, M., Camps-Valls, G., Stevens, B., Jung, M., Denzler, J., & Carvalhais, N. (2019). Deep learning and process understanding for data-driven Earth system science. Nature, 566, 195–204.

Shugart, H. H., Wang, B., Fischer, R., Ma, J., Fang, J., Yan, X., ... & Armstrong, A. H. (2018). Gap models and their individual-based relatives in the assessment of the consequences of global change. Environmental Research Letters, 13, 033001.

Smith, D. J. (2008). Ultimate resolution in the electron microscope?. Materials Today, 11, 30-38.

Steffen Schlüter, Jan Zawallich, Hans-Jörg Vogel, and Peter Dörsch. Physical constraints for respiration in microbial hotspots in soil and their importance for denitrification. https://doi.org/10.5194/bg-2019-2

Wang, B., Brewer, P. E., Shugart, H. H., Lerdau, M. T., & Allison, S. D. (2019). Soil aggregates as biogeochemical reactors and implications for soil–atmosphere exchange of greenhouse gases—A concept. Global Change Biology, 25, 373-385.

Wang, B., Shugart, H. H., & Lerdau, M. T. (2017). An individual-based model of forest volatile organic compound emissions—UVAFME-VOC v1. 0. Ecological modelling, 350, 69-78.