

Soil aggregates as biogeochemical reactors and implications for soil–atmosphere exchange of greenhouse gases—A concept

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Abstract

Soil–atmosphere exchange significantly influences the global atmospheric abundances of carbon dioxide (CO₂), methane (CH₄), and nitrous oxide (N₂O). These greenhouse gases (GHGs) have been extensively studied at the soil profile level and extrapolated to coarser scales (regional and global). However, finer scale studies of soil aggregation have not received much attention, even though elucidating the GHG activities at the full spectrum of scales rather than just coarse levels is essential for reducing the large uncertainties in the current atmospheric budgets of these gases. Through synthesizing relevant studies, we propose that aggregates, as relatively separate micro-environments embedded in a complex soil matrix, can be viewed as biogeochemical reactors of GHGs. Aggregate reactivity is determined by both aggregate size (which determines the reactor size) and the bulk soil environment including both biotic and abiotic factors (which further influence the reaction conditions). With a systematic, dynamic view of the soil system, implications of aggregate reactors for soil–atmosphere GHG exchange are determined by both an individual reactor's reactivity and dynamics in aggregate size distributions. Emerging evidence supports the contention that aggregate reactors significantly influence soil–atmosphere GHG exchange and may have global implications for carbon and nitrogen cycling. In the context of increasingly frequent and severe disturbances, we advocate more analyses of GHG activities at the aggregate scale. To complement data on aggregate reactors, we suggest developing bottom-up aggregate-based models (ABMs) that apply a trait-based approach and incorporate soil system heterogeneity.

KEYWORDS

aggregate reactor, aggregate-based model, greenhouse gas, individual-based model, microorganism, soil heterogeneity, soil organic matter

1 | INTRODUCTION

Biogeochemical reactions are manifested at spatial scales ranging from molecule to globe (McClain et al., 2003). In the case of the

biogeochemical processes specifically responsible for GHG production/consumption in soils, our understanding, however, is mostly derived from the soil profile level because of methodological constraints (Mosier, Schimel, Valentine, Bronson, & Parton, 1991; Smith

et al., 2003). Larger scale understanding (from landscape through regional to global) is extrapolated from knowledge gained at this scale through scale-up exercises via a combination of land surface modeling and remote sensing of land cover (e.g., McClain et al., 2003). From these scaling efforts, it is clear that soil–atmosphere exchange significantly affects the atmospheric abundances of CO₂, CH₄, and N₂O regionally and globally (Ciais et al., 2013). This conclusion is confirmed by top-down constraints derived from satellite measurements (Ciais et al., 2013). Nevertheless, we still have very poor constraints on the global and regional balances of GHGs (e.g., Ciais et al., 2013; Saunio et al., 2016), though the underlying biogeochemical reactions responsible for the production and/or consumption of these gases in soils are relatively well understood [but see Wang, Lerdau, and He (2017a) for an emerging paradigm of GHG production via nonmicrobial pathways].

These uncertainties necessitate a more complete understanding of GHG activities at the full spectrum of spatial scales, especially the soil aggregate scale which is relatively less understood. Such information is essential for further elucidating complex processes resulting from soil heterogeneity and for guiding bottom-up modeling of soil–atmosphere exchange of GHGs (e.g., Hinckley, Wieder, Fierer, & Paul, 2014; Ebrahimi & Or, 2016). This endeavor will eventually contribute to a better understanding of the mechanisms regulating atmospheric concentrations of GHGs and to improved strategies for mitigating soil GHG emissions in the context of global environmental changes, that is, achieving “climate-smart” soils (Paustian et al., 2016).

The soil system shows extremely high heterogeneity, and microbial activities are not spatially homogeneous in the soil matrix (Young & Crawford, 2004). From the perspective of structure, soil aggregates and pore spaces create fine-scale spatial heterogeneity (e.g., Elliott & Coleman, 1988; Horn, Taubner, Wuttke, & Baumgartl, 1994; Rillig, Muller, & Lehmann, 2017). Primary soil mineral particles (clay, silt, and sand) chemically interact with organic matter (historically classified as “primary organo-mineral complexes”), forming the basic units of soil aggregates. These basic units can accrete into larger aggregates, depending on the availability of a diverse suite of binding agents (e.g., polyvalent cations: Ca²⁺ or Al³⁺) and various forms of organic matter (e.g., polysaccharides, organic acids, plant debris, roots, and hyphae). From these aggregation processes, a hierarchical system of soil aggregates emerges (Lehmann, Kinyangi, & Solomon, 2007; Oades, 1991; Tisdall & Oades, 1982). Such aggregates generate additional soil heterogeneity, along with other “hot-spots” associated with the rhizosphere, detritusphere, and biopores that affect the distribution of substrates and microbial communities (Kuzayakov & Blagodatskaya, 2015).

Since the soil aggregate concept was first proposed about a century ago, extensive studies have been conducted on physiochemical and biological properties at this scale, as well as their responses to disturbances including soil management, land use change, and global change (e.g., Elliott, 1986; Oades, 1991; Jastrow, 1996; Six, Elliott, & Paustian, 2000a; Six, Paustian, Elliott, & Combrink, 2000b; Six, Bossuyt, Degryze, & Denef, 2004; Blanco-Canqui & Lal, 2004; Lehmann,

Zheng, & Rillig, 2017). However, knowledge about aggregate-scale GHG dynamics is still fairly scarce. To address GHG activities at this fine scale and hence their implications for coarse-scale GHG exchange, here we propose that aggregates—as relatively independent micro-habitats in the soil matrix—can be viewed as biogeochemical reactors (hereafter referred to as aggregate reactors) that produce GHGs including CO₂, CH₄, and N₂O. Correspondingly, aggregate reactivity is defined as the potential for GHG production and the rate and duration of these reactions. Because of varying sizes and turnover rates, we further argue that aggregate reactors in a soil system should be viewed in a systematic and dynamic way. By proposing this aggregate reactor concept in a dynamic framework, ecological theory can be applied to studies of GHG exchange by examining both the reactivity of an aggregate reactor (physiology) and the compositional dynamics of differing aggregate reactors (community ecology).

The overarching purpose of this paper is to demonstrate the rationale behind this concept, discuss its implications for soil–atmosphere GHG exchange, and propose ways forward to improve our understanding of aggregate reactors. By synthesizing previous studies, we first examine basic characteristics of aggregate reactors. We then discuss factors influencing aggregate reactivity, such as aggregate size, soil bulk properties, and fractionation methodology. Implications of aggregate reactors for soil–atmosphere GHG exchange are also addressed. In light of increasingly frequent and severe perturbations to soil systems, we emphasize impacts of soil management and global change on aggregate reactors. We conclude by identifying current knowledge gaps and research opportunities, including the potential to develop aggregate-based models (ABMs) that can explicitly incorporate the structural heterogeneity of soil systems. We recommend integration of soil science, ecology, and climate science communities to advance the aggregate reactor concept and to develop a predictive framework based on aggregate reactors in the context of global change. These efforts should eventually help reduce the large uncertainties in GHG exchange associated with soil heterogeneity.

2 | THE AGGREGATE AS A “BIOGEOCHEMICAL REACTOR” OF GHG

Embedded in the soil matrix, soil aggregates exhibit physical, chemical, and biological properties that differ from the bulk soil (Figure 1). Soil aggregates contain a three-dimensional structure with pores of varying sizes (e.g., Ebrahimi & Or, 2016). Organic matter becomes occluded during the aggregation process. Identifiable components of the occluded fraction include small particles of incompletely decomposed organic residues, pollen grains, and particles of plant tissue such as lignin coils and phytoliths. This physically bound organic matter, compared with free organic matter, often has relatively higher carbon and nitrogen concentrations and contains more alkyl carbon that is recalcitrant (Golchin, Oades, Skjemstad, & Clarke, 1994b, 1994a; Six, Guggenberger, et al., 2001b). Further, oxygen (O₂), water, nutrients, and dissolved organic carbon diffuse into the aggregates

from the inter-aggregate voids or macropores of bulk soil (Keiluweit, Nico, Kleber, & Fendorf, 2016). For example, O₂ diffusion from the soil matrix (where the O₂ concentration is further controlled by bulk soil moisture, plant roots, and other factors) is limited by the pore networks of aggregates, whereas O₂ consumption in aggregates is controlled by microbial activities, organic carbon, and nutrient availability. The net result is that aggregates can experience O₂ limitations even within aerobic, well-drained soils, making anoxia the most notable environmental characteristics of aggregates (e.g., Tiedje et al., 1984; Sexstone, Revsbech, Parkin, & Tiedje, 1985; Elliott & Coleman, 1988; Sexstone, Parkin, & Tiedje, 1988; Højberg, Revsbech, & Tiedje, 1994; Diba, Shimizu, & Hatano, 2011; Keiluweit et al., 2016).

A variety of anaerobic metabolic pathways can occur in aggregates (Ebrahimi & Or, 2015; Keiluweit et al., 2016), including processes responsible for CH₄ and N₂O production such as denitrification and methanogenesis (e.g., Sexstone et al., 1988; von Fischer & Hedin, 2007; Keiluweit et al., 2016; summarized in Tables 1–3). Therefore, aggregates can be viewed as segregated biogeochemical reactors of GHG embedded in a complex soil matrix (Figure 1). The connectivity and tortuosity of pores and other bulk soil properties (e.g., soil texture, moisture, and biological activities) determine the micro-environment in aggregates by regulating O₂ diffusion, distribution of water films, and substrate and nutrient accessibility for microbes, as well as the composition and structure of soil microbial community.

Microbial communities inhabit soil aggregates and exhibit dynamics in composition and activity (e.g., Ebrahimi & Or, 2016). Recently, based on aggregates' isolation feature Rillig et al. (2017) proposed that aggregates are "incubators" of microbial evolution that allow processes including genetic drift, natural selection, and mutation to occur and that likely produce an overall effect of an increase in microbial diversity. This microbial evolution dimension further adds complexity to understanding aggregate reactors.

3 | FACTORS REGULATING AGGREGATE REACTIVITY

3.1 | Aggregate reactor size

Aggregate reactor size is typically measured in terms of diameter. Aggregate reactor size is an important factor for GHG reactivity

because of size impacts on other physical, chemical, and biological activities. Just as GHG exchange exhibits substantial variation at coarse spatial scales, aggregate reactivity is also expected to vary across aggregate size classes. Here, we offer a nonexhaustive review of the major differences between macro- (>0.25 mm) and micro-aggregates (<0.25 mm), focusing on the aspects that could potentially result in reactivity differences.

First, aggregates of different sizes have differing geometry. One important aspect of the geometry is mean pore size which is smaller for micro-aggregates than for macro-aggregates (Dexter, 1988). This difference affects diffusion of O₂, nutrients, and dissolved organic carbon (DOC). Compared with macro-aggregates, O₂ diffusion is slower into micro-aggregates (Denef et al., 2001; Diba et al., 2011; Elliott & Coleman, 1988; Højberg et al., 1994; Sexstone et al., 1985).

Second, the chemical composition of substrates for carbon and nitrogen mineralization is different. Macro-aggregates often have higher carbon and nitrogen concentrations (e.g., Elliott, 1986; Gupta & Germida, 1988; Cambardella & Elliott, 1993). Younger and more labile organic matter (with a higher C/N ratio) constitutes more of the organic matter pool in macro-aggregates than in micro-aggregates (Elliott, 1986; Elliott & Coleman, 1988; Six et al., 2004).

Third, microbial community composition and structure are influenced by aggregate size (e.g., Van Gestel, Merckx, & Vlassak, 1996; Mummey, Holben, Six, & Stahl, 2006; Kravchenko et al., 2014; Rabbi et al., 2016; Ebrahimi & Or, 2016). For instance, Mummey et al., 2006 found that micro-aggregates select for specific microbial lineages across disparate soils. Bach, Williams, Hargreaves, Yang, and Hofmockel (2018) reported that micro-aggregates hold more diverse microbial communities than macro-aggregates.

Many studies have found differences in GHG process rates among aggregates of varying sizes, though some studies have found no differences (Tables 1–3). Sexstone et al. (1985) and later studies found that the composition of microbial communities responsible for N₂O production varies with aggregate size. Sey, Manceur, Whalen, Gregorich, and Rochette (2008) suggested that ammonium oxidizers are most abundant in macro-aggregates, while denitrifiers, which preferentially colonize anaerobic environments, are more abundant in micro-aggregates. This study also found that denitrification pathways of N₂O production dominate in smaller aggregates, whereas nitrification dominates N₂O production in larger aggregates. In addition, greater denitrification rates occurred in the smallest aggregate size fractions when acetylene was applied to prevent the complete

FIGURE 1 Schematic of soils as a system of aggregate reactors of different sizes. At the profile level, soils act as a source of CO₂, either a source or a sink of CH₄ (denoted by the upward and downward arrow, respectively), and a source of N₂O. At fine scales, soil consists of aggregate reactors of differing sizes. Each individual aggregate reactor can be described by physical (e.g., pore size, diffusion coefficient, and aggregate size), chemical (e.g., concentration of O₂, H₂O, dissolved organic carbon—DOC, substrates), and biological traits (turnover rate, microbial community composition, and dynamics). Top-down experiment refers to studying these properties by "digging" into soils. Aggregate reactivity depends on aggregate size (denoted by the irregular circles with differing colors) and bulk soil properties including both abiotic and biotic factors, as well as coarser scale anthropogenic disturbances. Different widths of the red arrows denote the reactor size-induced variations in GHGs. Soil systems composed of aggregates of different sizes are dynamically changing because of aggregate turnover (or aggregate stability), which is not illustrated here. Bottom-up modeling refers to building models based on aggregate reactor that can represent soil system composition and dynamics and simulate soil profile GHG exchange as an emergent process

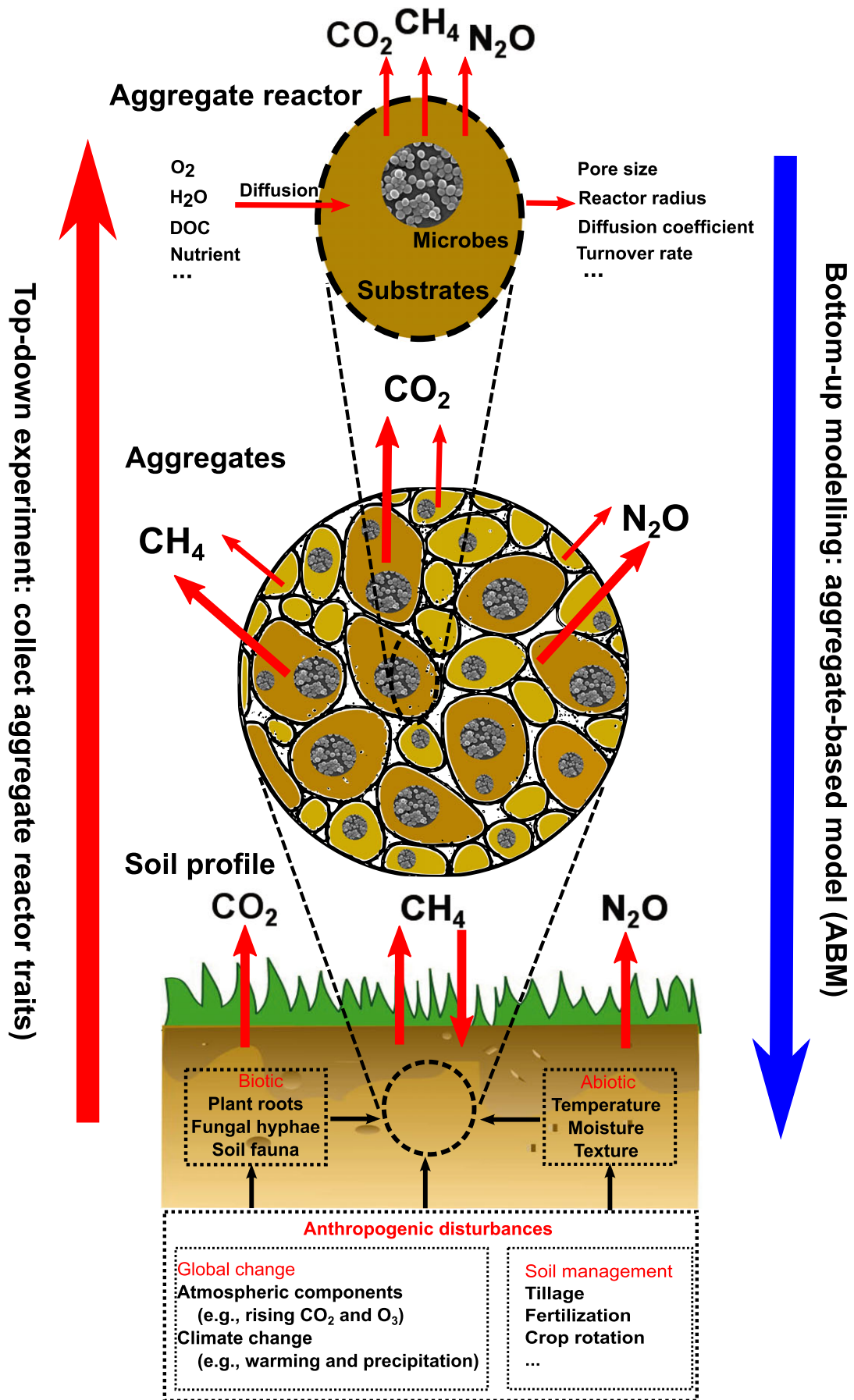


TABLE 1 A compilation of research on aggregate reactors in terms of CO₂

Land use ^a	Soil texture	Method	Size class (mm)	Moisture ^b	Rate versus size ^c	References
Grassland	Silty loam	Dry ^d	6.3–2, <2	FC	+	Bimüller, Kreyling, Kölbl, Lützow, and Kögel-Knabner (2016)
Pasture	Clay	Wet	2–0.25, 0.25–0.053, <0.053	70% FC	=	Rabbi et al. (2015)
Crop	Clay	Wet	2–0.25, 0.25–0.053, <0.053	70% FC	=	Rabbi et al. (2015)
Forest	Clay	Wet	2–0.25, 0.25–0.053, <0.053	70% FC	=	Rabbi et al. (2015)
Crop	Silt loam	Wet	>2, 2–0.25, 0.25–0.053, <0.053	FC	+	Bandyopadhyay and Lal (2014)
Crop (NT)	Silt loam	Wet	>2, 2–0.25, 0.25–0.053, <0.053	FC	+	Bandyopadhyay and Lal (2014)
Forest	Silt loam	Wet	>2, 2–0.25, 0.25–0.053, <0.053	FC	+	Bandyopadhyay and Lal (2014)
NA	Clay loam	Dry	4–2, 2–1, 1–0.5, <0.5	FC	–	Mangalassery et al. (2013)
NA	Sandy loam	Dry	4–2, 2–1, 1–0.5, <0.5	FC	+	Mangalassery et al. (2013)
Crop	Silt loam	Dry	>6, 6–4, 4–2, 2–1, 1–0.5, 0.5–0.25	60% FC	–	Muñoz et al. (2012)
Tropical forest	Peat	Dry	20–8, 8–2, <2	30% & 70% FC	+	Kimura et al. (2012)
Oil palm	Peat	Dry	20–8, 8–2, <2	30% & 70% FC	=	Kimura et al. (2012)
Grassland	NA	Dry	4.5–2, <2	60% & 80% FC	+	Diba et al. (2011)
Crop (NT/CT)	Sandy loam	Dry	>4, 4–1, <1	80% FC	+	Fernández et al. (2010)
Crop	Sandy loam	Dry	6–2, 2–0.25, <0.25	20%–80% WFPS	–	Sey et al. (2008)
Crop	Clay loam	Dry	8–4, 4–2, 2–1, 1–0.5, 0.5–0.25, <0.25	30% GWC	–	Drury et al. (2004)
Crop	Silt loam	Dry	5–2, 2–0.25, <0.25	67% FC	+	Schutter and Dick (2002)
Crop	Loam	Wet	>1, 1–0.5, 0.5–0.25, <0.25	NA	+	Aoyama, Angers, and N'dayegamiye, Bissonnette, (1999)
Crop	Loam	Wet	5.6–1.0, 1.0–0.25, 0.25–0.05, <0.05	FC	+	Franzluebbers and Arshad (1997)
Crop	Silt loam	Wet	5.6–1.0, 1.0–0.25, 0.25–0.05, <0.05	FC	+	Franzluebbers and Arshad (1997)
Crop	Clay loam	Wet	5.6–1.0, 1.0–0.25, 0.25–0.05, <0.05	FC	+	Franzluebbers and Arshad (1997)
Crop	Clay	Wet	5.6–1.0, 1.0–0.25, 0.25–0.05, <0.05	FC	+	Franzluebbers and Arshad (1997)
Crop	Clay loam	Dry	20–10, 10–5, 5–2, 2–1, 1–0.5, 0.5–0.25, <0.25	FC	–	Seech and Beauchamp (1988)
Prairie	Sandy loam	Dry ^d	8–1, 1–0.5, 0.5–0.25, 0.25–0.1, <0.1	Field-moist	+	Gupta and Germida (1988)
Prairie (CT)	Sandy loam	Dry ^d	8–1, 1–0.5, 0.5–0.25, 0.25–0.1, <0.1	Field-moist	+	Gupta and Germida (1988)

Notes. For more detailed information of each study, see Supporting Information Tables S1 and S2.

^aThe blank denotes information not available. NT and CT denote no-tillage and conventional tillage, respectively. ^bIncubation moisture expressed in % field capacity (FC), in water-filled pore space (WFPS), or in gravimetric water content (GWC) based on literature. ^cSign “+” generally denotes a positive relationship of CO₂ production rate with aggregate size, “–” negative, while “=” no significant relationship. ^dThese studies directly used field-moist soils for dry sieving, which remain being labeled as dry sieving.

reduction of N₂O to N₂ during denitrification. Higher denitrification in smaller aggregates was also reported by Seech and Beauchamp (1988) and Uchida, Clough, Kelliher, and Sherlock (2008). Sey et al. (2008) attributed this pattern to a higher proportion of complete denitrification (NO₃[–] → N₂O → N₂) because of very low or effectively absent O₂ in smaller aggregates. An alternative explanation, proposed by Ebrahimi and Or (2016), is that N₂O takes longer to diffuse out of larger aggregates and thus has more time to be completely reduced from N₂O to N₂.

Overall, consistent relationships between aggregate reactor size and reactivity are difficult to establish, even qualitatively (Tables 1–3). Although the majority of studies with different types of soils (>60%) support an overall positive relationship between aggregate size and CO₂ production, some studies observed a negative relationship. For N₂O production, the majority of studies (almost 70%)

support an overall positive relationship with aggregate size, of which more than half found more N₂O production from macro-aggregates than micro-aggregates (Supporting Information Table S3). Regarding CH₄, more studies observe that smaller aggregates act as consumers and larger aggregates as producers, but this is rarely true for the specific comparison of macro- and micro-aggregates (Supporting Information Table S4).

3.2 | Bulk soil properties

Bulk soil properties determine the environment surrounding the aggregate reactors, which largely shapes conditions in the reactors. The observed inconsistent relationships between aggregate reactor size and reactivity across different studies, as discussed above (Tables 1–3), support this postulation; aggregate reactivity is not just

TABLE 2 A compilation of research on aggregate reactors in terms of N₂O

Land use	Soil texture	Method	Size class (mm)	Moisture	Rate versus size	References
Crop	Clay loam	Dry	5.6–4, 4–2, 2–1	Aeration	+	Robinson et al. (2014)
Crop	Silt loam	Wet	>2, 2–0.25, 0.25–0.053, <0.053	FC	+	Bandyopadhyay and Lal (2014)
Crop (NT)	Silt loam	Wet	>2, 2–0.25, 0.25–0.053, <0.053	FC	+	Bandyopadhyay and Lal (2014)
Forest	Silt loam	Wet	>2, 2–0.25, 0.25–0.053, <0.053	FC	+	Bandyopadhyay and Lal (2014)
NA	Sandy loam	Dry	4–2, 2–1, 1–0.5, <0.5	FC	=	Mangalassery et al. (2013)
NA	Clay loam	Dry	4–2, 2–1, 1–0.5, <0.5	FC	=	Mangalassery et al. (2013)
Crop	Silt loam	Dry	>6, 6–4, 4–2, 2–1, 1–0.5, 0.5–0.25	60% FC	–	Muñoz et al. (2012)
Oil palm	Peat	Dry	20–8, 8–2, <2	30% & 70% FC	+	Kimura et al. (2012)
Tropical forest	Peat	Dry	20–8, 8–2, <2	30% & 70% FC	+	Kimura et al. (2012)
Crop	NA	Wet	>2, 2–0.25, 0.25–0.053, <0.053	60% FC	+	Jiang et al. (2011)
Grassland	NA	Dry	4.5–2, <2	60% & 80% FC	+	Diba et al. (2011)
Crop	Sandy loam	Dry	6–2, 2–0.25, <0.25	20%–80% WFPS	+	Sey et al. (2008)
Pasture	Silt loam	Dry	5.6–4, 4–2, 2–1, <1	FC	–	Uchida et al. (2008)
Crop	Clay loam	Dry	8–4, 4–2, 2–1, 1–0.5, 0.5–0.25, <0.25	30% GWC	+	Drury et al. (2004)
NA	Loamy	Wet	5.0–3.0, 3.0–2.0, 2.0–1.0, 1.0–0.5, 0.5–0.25, <0.25	Dry	+	Manucharova et al. (2001)
NA	NA	NA	10–4.0	NA	+	Stepanov, Manucharova, and Polyanskaya (1997)
Crop	Silt loam	Wet	>4.7, 4.7–2, 2–1, 1–0.5, 0.5–0.25, 0.25–0.1, <0.1	FC	+	Beauchamp and Seech (1990)
Crop	Silt loam	Dry	>20, 20–10, 10–5, 5–2, 2–1, 1–0.5, 0.5–0.25, 0.25–0.15, 0.15–0.05, <0.05	FC	–	Beauchamp and Seech (1990)
Crop	Silt loam	Dry	20–10, 10–5, 5–2, 2–1, 1–0.5, 0.5–0.25, <0.25	Saturation	–	Seech and Beauchamp (1988)

Note. See Table 1 notes on information listed. For more detailed information of each study, see Supporting Information Tables S1 and S3.

determined by size but also by the bulk soil properties. These bulk properties can be abiotic or biotic factors that regulate the soil physico-chemical and biological environment.

Although it remains challenging to establish direct causal connections between aggregate reactivity and bulk soil properties, a few studies have addressed these relationships. For instance, soil water content can significantly affect aggregate-level CH₄ activities (Sey et al., 2008). Aggregates with sizes <0.25 mm and 0.25–2 mm consumed CH₄ at low water content but began to produce CH₄ at higher water content (Sey et al., 2008). This same study also observed a maximum CH₄ production rate at 40% water-filled pore space (WFPS) for 2–6 mm aggregates. This pattern can be explained by greater methanogenesis when high water content prevents O₂ diffusion (Yavitt, Downey, Lang, & Sexstone, 1990). Regarding CO₂, studies by Drury, Yang, Reynolds, and Tan (2004) and Mangalassery, Sjögersten, Sparkes, Sturrock, and Mooney (2013) both observed the largest CO₂ effluxes from small-sized aggregates in clay loam soils, in contrast to other studies using different soils (Table 1). This observed difference in CO₂ production may have resulted from texture differences that influence soil porosity and water film distribution.

Many other factors, especially biotic ones, that can also affect aggregate reactor conditions have not been studied at all. For

instance, a soil O₂ concentration decline can be induced directly by root respiration and/or by root exudation that stimulates heterotrophic respiration in the rhizosphere (Keiluweit et al., 2016). Other soil organisms, such as soil fauna and fungal hyphae, can affect soil porosity and change the diffusivity of O₂ into aggregates or significantly affect the formation of soil aggregates and their associated C pools (Lehmann et al., 2017). Based on this reasoning, biological activities should exert a variety of effects on aggregate-level GHG dynamics.

3.3 | Fractionation method

Theoretically, aggregate reactivity should be determined by both soil properties and aggregate reactor size. In practice, however, the observed variability in aggregate reactivity (Tables 1–3) may also reflect differences in fractionation techniques. Separation methods are not uniform across studies; specifically, dry sieving is used more often than wet sieving (Tables 1–3). Separation exerts significant influences on physical, chemical, and biological properties of different sized aggregates (Ashman, Hallett, & Brookes, 2003; Bach & Hofmockel, 2014; Kaiser, Kleber, & Berhe, 2015). For instance, air-drying can increase the mechanical strength of aggregates, and wet sieving can increase potential enzyme activity (Bach & Hofmockel,

TABLE 3 A compilation of research on aggregate reactors in terms of CH₄

Land use	Soil texture	Method	Size class (mm)	Moisture	Rate versus size ^a	References
Crop	Silt loam	Wet	>2, 2–0.25, 0.25–0.053, <0.053	FC	=	Bandyopadhyay and Lal (2014)
Crop (NT)	Silt loam	Wet	>2, 2–0.25, 0.25–0.053, <0.053	FC	=	Bandyopadhyay and Lal (2014)
Forest	Silt loam	Wet	>2, 2–0.25, 0.25–0.053, <0.053	FC	=	Bandyopadhyay and Lal (2014)
NA	Clay loam	Dry	4–2, 2–1, 1–0.5, <0.5	FC	–	Mangalassery et al. (2013)
NA	Sandy loam	Dry	4–2, 2–1, 1–0.5, <0.5	FC	–	Mangalassery et al. (2013)
Tropical forest	Peat	Dry	20–8, 8–2, <2	30% & 70% FC	+	Kimura et al. (2012)
Oil palm	Peat	Dry	20–8, 8–2, <2	30% & 70% FC	+	Kimura et al. (2012)
Crop	Sandy loam	Dry	6–2, 2–0.25, <0.25	20%–80% WFPS	+/=/–	Sey et al. (2008)
Crop	Loam	Dry	<2, 2–4, 4–6, 6–8, 8–10, >10	7%–97% FC	+	Jäckel, Schnell, and Conrad (2001)
Forest	Loam	Wet	>2, 2–0.25, 0.25–0.053, <0.053	Dry	+	Wang, Hou, Liu, and Wang (2013) ^b

Notes. See Table 1 notes on information listed. For more detailed information of each study, see Supporting Information Tables S1 and S4.

^aPattern “+” denotes larger aggregates are CH₄ producers, and smaller aggregates are consumers (or less production than larger aggregates); “–” denotes larger aggregates have less production than smaller aggregates; and “=” denotes no significant pattern is observed. ^bThe only study on aggregate-scale nonmicrobial CH₄.

2014). A recent review by Kaiser et al. (2015) provides further details on air-drying and rewetting effects on soil aggregate stability. Currently, we know of only one study by Beauchamp and Seech (1990) that evaluated impacts of dry and wet sieving methods on aggregate reactivity. They observed decreased denitrification rates as the dry-sieved aggregate size increased, but the opposite relationship for wet-sieved aggregates. More experiments testing the effects of separation techniques on GHG activities across aggregates of different sizes are needed to inform future studies of environmental effects on aggregate reactivity.

4 | AGGREGATE REACTORS AND SOIL–ATMOSPHERE GHG EXCHANGE

To link the fine-scale aggregate reactors and soil profile GHG exchange, here we argue that a systematic, dynamic view of the soil system is required. Specifically, we need to focus on both the reactivity of an individual aggregate and also the composition of aggregate reactors of different sizes in a soil system. This dual focus is necessary because aggregate reactors of different sizes collectively make different contributions to soil profile GHG exchange. For example, Bandyopadhyay and Lal (2014) report a much higher contribution to bulk soil CO₂ emissions from macro-aggregates than micro-aggregates. The relative proportions of different size aggregate reactors in a soil system are dynamically changing, and these changes are determined by the turnover of aggregates (i.e., aggregate stability). Aggregate turnover is strongly influenced by external disturbances to soil systems (Six et al., 2004). This by analogy is similar to the space-lifetime hypothesis for organisms proposed by Ginzburg and Damuth (2008). We should view an aggregate reactor in four dimensions—in addition to its three-dimensional spatial structure, one more temporal dimension, aggregate lifetime, should be included. Therefore, as with ecological systems (e.g., Levin, 1998; Grimm et al., 2005; Wang, Shugart, & Lerdau, 2017b), we need a

dynamic view of aggregate reactors to account for their compositional dynamics (Figure 1).

Current evidence has already unequivocally suggested that aggregate reactors have significant implications for soil–atmosphere exchange of GHG. Formation of these reactors suppresses carbon oxidation and CO₂ release because of oxygen limitation, promoting carbon sequestration (Keiluweit et al., 2016; Keiluweit, Wanzek, Kleber, Nico, & Fendorf, 2017; Six, Conant, Pau, & Paustian, 2002). While revisiting two prior studies (Greenwood Sextstone et al., 1985; Sextstone et al., 1985), Keiluweit et al. (2016) offered an initial estimate of aggregation effects on bulk soil carbon mineralization, showing a striking suppression in the range of 23%–97.5% relative to fully aerobic soils. By contrast, when these reactors are “destroyed” (e.g., by disturbance from tillage), carbon mineralization increases rapidly because of increased O₂ availability (e.g., Elliott, 1986; Beare, Hendrix, Cabrera, & Coleman, 1994, and Drury et al., 2004). In particular, Keiluweit et al. (2017) recently reported that shifting from anaerobic to aerobic conditions leads to a tenfold increase in volume-specific mineralization rate, illustrating the sensitivity of anaerobically protected carbon to disturbance. These results, meanwhile, indirectly substantiate the strong physical protection of organic matter against decomposition offered by the aggregates (Six et al., 2002; Six, Elliott, et al., 2000).

In addition, the aggregate reactor concept illustrates that most field measurements of net soil–atmosphere exchange mask significant gross production and consumption of CH₄ and N₂O. Fine-scale activities are disguised in the traditional metrics of soil–atmosphere exchange of CH₄ at larger scales (von Fischer & Hedin, 2007), where a soil is considered either a sink or a source. Multiple studies have shown that higher in situ gross CH₄ production could stimulate higher gross consumption, resulting in little difference in surface fluxes (Kammann, Hepp, Lenhart, & Müller, 2009; Mangalassery et al., 2013; Yang & Silver, 2016). Similar to CH₄, N₂O could also be both produced and consumed within a soil (Chapuis-Lardy, Wraage,

Metay, Chotte, & Bernoux, 2007), so aggregate-scale production of N_2O may not always increase surface fluxes (Yang & Silver, 2016). In summary, aggregate reactors have significant implications for soil–atmosphere exchange of GHG.

5 | AGGREGATE REACTORS IN THE CONTEXT OF GLOBAL CHANGE

The soils beneath our feet are strongly affected by coarse-scale disturbances including soil management practices (mostly agronomic practices), land use change, and global changes resulting from growing human activities in the Anthropocene Epoch (Bronick & Lal, 2005; Hinckley et al., 2014; Paustian et al., 2016). With the aggregate reactor concept and a systematic view of soil systems as discussed above, coarse-scale perturbations of soil systems are postulated to affect soil–atmosphere GHG exchange both directly by influencing conditions for aggregate reactivity and indirectly by altering the distribution of aggregate reactor sizes (Figure 1). Soil management (e.g., soil cultivation, fertilization, crop rotation, irrigation, biochar addition, and compaction) and land use change can significantly affect the size distribution of aggregates (Six, Elliott, & Paustian, 1999; Six, Paustian, et al., 2000; Wang, Han, et al., 2013; Young & Ritz, 2000). Climate warming increases the soil temperature, while precipitation shifts alter soil moisture content, shaping the environment of aggregate reactors and thus aggregate-level microbial activities (e.g., Fang et al., 2015). Moreover, climate change can also indirectly affect soil aggregate properties by influencing vegetation activity (Torn, Chabbi, & Crill, 2015). Additionally, atmospheric changes can indirectly affect soil structure by influencing above-ground vegetation activities and carbon and nitrogen allocation. Rising CO_2 levels can alter soil structure and increase soil aggregation and carbon sequestration (Cotrufo & Gorissen, 1997; Dorodnikov et al., 2009; Jastrow et al., 2005; Rillig, Wright, Allen, & Field, 1999; Six, Carpentier, et al., 2001). Nitrogen deposition can also shape soil aggregate properties by influencing rhizodeposition, microbial biomass, and microbial activity (Janssens et al., 2010). Increasing abundance of tropospheric ozone (O_3), the most important secondary air pollutant, can modify the soil structure in terms of aggregate properties and distribution and soil–atmosphere GHG exchange (Kou, Wang, Zhu, Xie, & Wang, 2014; Wang, Shugart, & Lerdau, 2017c).

Still, relatively few studies have addressed direct connections between these disturbances and reactions responsible for GHG production from aggregate reactors. The available studies mainly focus on aggregate responses to tillage and fertilization, while the indirect effects mediated by aggregate turnover and size distribution changes are still unknown. In general, macro-aggregates from no-till soils have higher CO_2 production than those from soils under conventional tillage (Fernández, Quiroga, Zorati, & Noellemeier, 2010; Franzluebbers & Arshad, 1997). Moreover, the tillage impact depends upon soil depth. Fernández et al. (2010) demonstrated that differences in CO_2 production between tillage practices disappear for deeper soils. One possible explanation is that no-till soils show a pattern of

decreasing of SOC with depth whereas conventional soils have uniformly distributed SOC (Fernández et al., 2010; Plaza-Bonilla, Cantero-Martínez, & Álvaro-Fuentes, 2014). This pattern might also explain why Plaza-Bonilla et al. (2014) did not observe differences between no-till and conventional tillage.

Similar to CO_2 , CH_4 production and consumption are affected by tillage. A study by Plaza-Bonilla et al. (2014) reported that macro-aggregates act as CH_4 sources under conventional tillage and sinks under no-tillage. This change could be attributed to inhibited methanotrophic activity induced by aggregate destruction under tillage, or alternatively, to a smaller quantity of anoxic microsites within the no-tillage macro-aggregates maintained by intra-aggregate pore architecture and connectivity (e.g., Brewer, Calderón, Vigil, & Fischer, 2018). In contrast, both Jiang, Shi, Liu, and Wright (2011) and Plaza-Bonilla et al. (2014) reported that soil tillage did not affect aggregate N_2O production.

Fertilization has been reported to affect aggregate-level N_2O production with the effects dependent on fertilizer type. For example, Plaza-Bonilla et al. (2014) concluded that mineral and organic nitrogen fertilizers can lead to differences in the relative importance of nitrification versus denitrification in macro-aggregates; nitrification dominates with mineral fertilizer whereas denitrification dominates with organic fertilizer (pig slurry). This difference was attributed to changes in the proportion of C and N substrates and in microbial activities (Plaza-Bonilla et al., 2014).

6 | PROSPECTS AND AGGREGATE-BASED MODELING (ABM)

Generations of research have built a relatively solid knowledge of reactions broadly responsible for GHG production and of aggregates' inherent biophysical and chemical properties. Yet an understanding of the direct relationships between these properties and reactions specifically at the aggregate level remains elusive. Emerging new mechanisms, such as anaerobic oxidation of CH_4 , require additional investigation. Likewise, bulk soil conditions are still not yet fully linked to aggregate reactivity. Aside from the soil hydration- O_2 diffusion relationship (e.g., Ebrahimi & Or, 2018), many abiotic and biotic factors that could regulate aggregate reactivity have not been studied. As pointed out by Torn et al. (2015), two of the most widespread impacts of anthropogenic activities on soils in this century will be warmer temperatures and altered plant allocation belowground because of rising CO_2 and nitrogen deposition. Therefore, more studies are needed to understand how soil temperature and biotic factors (e.g., root activity, plant species, and soil macro-fauna), as well as soil management practices, affect aggregate GHG fluxes. Additionally, how microbial community composition and dynamics control these activities in aggregates is almost unknown (Allison et al., 2013; Buchkowski, Bradford, Grandy, Schmitz, & Wieder, 2017; Ebrahimi & Or, 2016). Finally, future studies should move beyond the reactivity of an individual aggregate. A systematic, dynamic view of these reactors in soil systems is equally important for fully quantifying the implications of aggregate reactors for soil–atmosphere GHG exchange.

Driven by these grand questions, we should simultaneously refine and develop more standardized methodologies for the study of aggregate reactors. Undoubtedly, the ideal route is to conduct in situ measurements, which is a great challenge at the micron scale with current techniques. Therefore, we recommend a combination of the following techniques. First, it is essential to establish a uniform experimental protocol for aggregate fractionation. The approach of optimal moisture fractionation by Bach and Hofmockel (2014) has a high potential to separate aggregates with minimal disturbance to chemical and biological properties and might be ideal for studies of aggregate reactors. As a complement to aggregate fractionation, artificial aggregates are a good means for exploring the relationships between aggregate reactivity and physical structure (e.g., Ebrahimi & Or, 2018; Schlüter et al., 2018). Another area of technique development could exploit isotope pool dilution to measure gross fluxes of GHGs, followed by separation of soil aggregates to determine correlations between aggregate size distributions, physiochemical properties, and the gross gas fluxes [e.g., CH₄ by von Fischer and Hedin (2007) and N₂O by Yang, Teh, and Silver (2011)]. These methods could be combined with technique advancements in computer-aided tomography (CT) and electron microscopy (e.g., SEM and TEM; Williams & Carter, 1996) that provide soil structural information in terms of aggregate reactor size and distribution (e.g., Young & Crawford, 2004; Rabbi et al., 2016).

Finally, a major research need is to develop computational models that can quantify and predict aggregate reactivity. These models could untangle the nonlinearities between aggregate reactors and soil profile GHG exchange. Such research would address the grand challenge of modeling soil biogeochemical processes at larger spatial and temporal scales in the context of global environmental changes. With a systematic, dynamic view of aggregate reactors in soil systems as discussed above, we propose a bottom-up strategy to develop aggregate-based models (ABM) that explicitly represent the “behavior” of aggregate reactors of different sizes (Figure 1). This approach is inspired by the agent-based or individual-based modeling (IBM) strategy that largely originated in ecological systems in the 1960 s (Grimm et al., 2005; Shugart et al., 2018). For a soil system composed of aggregate reactors of different sizes, an ABM framework could be developed to represent these different aggregates. For each aggregate reactor, a single IBM would be developed to explicitly simulate microbial communities and their functions. Therefore, an ABM is expected to be a hierarchy of individual-based models simulating each of an aggregate element and its dynamic properties. Such a hierarchically constructed ABM contrasts with traditional models that represent soils as a set of discrete carbon fractions with an implicit treatment of microbial diversity (e.g., reviewed in Bradford et al., 2016). We also advocate the incorporation of a trait-based approach in the ABM based on trait data from aggregate reactors. These data could include the physical (e.g., aggregate size, pore size, gas diffusion coefficient), chemical (e.g., substrates, enzyme, O₂, and moisture), and biological properties (i.e., turnover rate and microbial diversity) of soil aggregates and could be obtained by the techniques described above (i.e., “top-down experiment”;

Figure 1). We anticipate that a global soil aggregate trait database can be established and that tradeoffs among aggregate traits (e.g., reactor size and O₂ abundance) could be uncovered to facilitate the model construction, similar to previous successful applications with plant traits (e.g., Kattge et al., 2004; Wright et al., 2004) and even litter decomposition (Allison, 2012). Biophysical equations that may be helpful in building such an ABM are listed in the Supporting Information.

Previous workers have built a solid foundation for developing ABMs based on mechanistic modeling of soil processes that occur in aggregate reactors. Smith (1980) developed a model of the variation in the extent of anaerobiosis in aggregated soils by extending previously published models of radial diffusion into individual aggregates (e.g., Currie, 1962). This work assumed a log-normally distributed population of aggregate sizes to calculate denitrification rates. Recently, Ebrahimi and Or (2015) embedded an individual-based microbial model [inherited from Kreft, Booth, and Wimpenny (1998)] into an idealized artificial aggregate and developed an analytical model for biogeochemical processes in aggregates. The model was later expanded to include aggregates of different sizes to simulate CO₂ and N₂O fluxes (Ebrahimi & Or, 2016). Moreover, Ebrahimi and Or (2018) applied their aggregate-based model to scale up microbial processes in aggregates of different sizes. They used spatial data on soil type and land cover to simulate GHG exchange at the landscape scale. Future modeling efforts should dynamically represent aggregate reactivity and distribution and microbial community composition over space. The resulting models should be validated under different soil conditions and management practices across spatial and temporal scales. These efforts will likely require cooperation among modelers, ecologists, microbiologists, and climate scientists to advance a predictive science of land–atmosphere exchange of GHG in the context of global environmental change (BERAC, 2017).

7 | CONCLUSIONS

Soil GHG exchanges are manifested at a wide spectrum of scales from the aggregate through the soil profile to the landscape, region, and globe. Understanding GHG exchange at these different scales is essential for a more accurate quantification of trace gas fluxes and better evaluation of land–atmosphere interactions in the context of accelerating global change. Based on a synthesis of prior studies, we argue that aggregates can be viewed as biogeochemical reactors of GHGs, with reactivities dependent on aggregate size and bulk soil abiotic and biotic factors that shape the reaction environment. We also suggest a systematic, dynamic approach to link the individual aggregate reactor with GHG exchange from the soil profile. Prior work has already revealed implications of aggregate reactors for the soil–atmosphere exchange of GHG—for example, soil carbon oxidation can be suppressed in aggregate reactors to facilitate carbon sequestration. However, our understanding of aggregate reactors is far from complete. We advocate for more research on techniques, environmental drivers, and cross-scale linkages related to the aggregate reactor concept. There is also great potential for developing

mechanistic, aggregate-based models that use a trait-based approach to represent soil systems and reduce uncertainties about soil–atmosphere GHG exchange in the face of human impacts.

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