

Chapter 6

Advances in Biogeochemical Modeling for Intensively Managed Landscapes



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6.1 Introduction

The study of biogeochemistry in intensively managed landscapes (IMLs)—those landscapes which are dramatically altered and managed through human effort to provide economic benefit—is a study of transitions. Large-scale industrialized agricultural practices have induced significant shifts in the transport and transformation of water, carbon, and nutrients across landscapes in order to maximize our ability to extract from the land the richest, most fruitful agricultural and bioenergy products to address the food and energy needs of an ever-growing global population. Since the Industrial Revolution, the Earth has seen a five-fold surge in land cover dedicated for agricultural use, and recent estimates of crop- and pastureland area range between 500 million and 2.7 billion hectares (5 and 27 million km²) globally (Ramankutty et al. 2018) [However, it should be noted that conversion of natural landscapes to IMLs has slowed in recent decades, due most likely to technological and engineering advances that increase yield and production efficiency (Ramankutty et al. 2018)].

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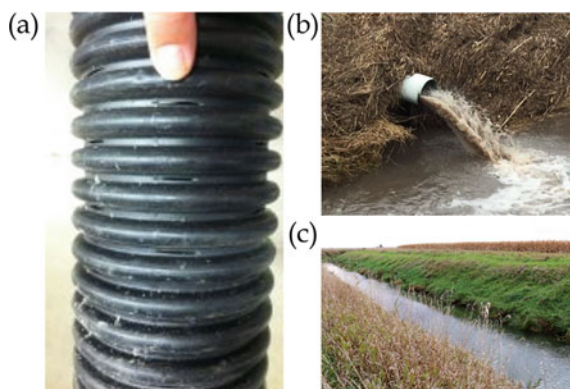
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In IMLs, the Critical Zone (CZ), the bedrock-to-canopy top living layer of Earth's crust, encompasses not only the landscape's natural underlying lithology, evolving land surface, and energy, nutrient, and hydrologic flows and fluxes, but also incorporates human amendments to the natural system. These include seasonal changes in land cover and vegetation type associated with, for example, row crop agriculture and chemical treatments like soil liming or fertilization, which can have an overwhelming effect on natural biogeochemical processes. Understanding CZs experiencing intensive management and characterizing them through modeling can lead to improved management techniques and improved insights into their long-term sustainability. In the Chapter, we discuss the unique challenges to studying the biogeochemistry of CZs in IMLs and summarize several recent modeling efforts made by researchers in the Intensively Managed Landscape Critical Zone Observatory (IMLCZO) <http://criticalzone.org/iml/>.

The degree and manner by which a natural ecosystem is modified to become an IML depends on both the pre-existing topographic and climatological characteristics inherent to the landscape as well as the ultimate purpose for which it is modified. Two contrasting IMLs located in the American Midwest and in China's Loess Plateau illustrate this accelerated give-and-take relationship between humans and their environments. IMLs typical of the Midwestern United States, which are host to billion dollar annual food, feed, and biofuel crop production, are generally topographically planar with rich, deep soil horizons (Wilson et al. 2018). They are subject to precipitation and temperature fluctuations characteristic of humid-continental climates. Poorly drained soils means that intensive management practices in this region are generally aimed at artificially promoting drainage and reduction of long residence times of water, carbon, and nutrients. Farmers and landowners in the Midwestern US began in the 1820s the practice of removing excess moisture from the soil via tile drains (Fig. 6.1), comprised of perforated tubes installed over a meter beneath the ground surface (Woo et al. 2019; Kratt et al. 2020). Twelve American Midwestern states are presently implemented with tile drainage systems to the extent that more than half of the total 170 million *ha* of cropland shared between them is artificially drained (Nakagaki and Wiczorek 2016). The presence of tile drains enables improved crop productivity and nitrogen use efficiency through increased rooting depth. However, extensive tile drainage results in unintended consequences. Tile drains increase nutrient losses through channelized subsurface water fluxes (Castellano et al. 2019) and disrupt the landscape's moisture and transport dynamics by dramatically increasing drainage rates and overall moisture efflux (Davis et al. 2014). They flush fields of carbon, nutrients, and excess fertilizer, which are then swiftly deposited into receiving waterways adjacent to fields. Topographic dips associated with constructed roadside and agricultural ditches support rapid surface water removal and nutrient movement, as well (Rhoads et al. 2016).

In addition to tile drains, other surficial anthropogenic inputs such as fertilizer application and mechanical tillage accelerate nutrient and sediment flux. The landscape's naturally-occurring nutrient cycling is often overhauled by widespread fertilizer application. However, only about 40% of nitrogen fertilizer applied to grain crops is ultimately used by the grain crops (Gardner and Drinkwater 2009). The

Fig. 6.1 **a** Perforated tile drain tube [Picture credit: What is a tile drain? 2021]; **b** video still of tile drain outflow immediately following a rain event (Courtesy: Bruce Rhoads 2016); **c** edge-of-field drainage ditch (Courtesy: Praveen Kumar 2016)



ensuing large scale excessive losses of chemicals from fields have resulted in well-documented water quality issues, such as blue baby syndrome (Mahvi et al. 2005) and ongoing challenges such as the Gulf of Mexico Dead Zone (Fausey et al. 1995; Woo and Kumar 2019; Li et al. 2008; Radcliffe et al. 2015).

The above-mentioned human inputs are in no way an exhaustive list of anthropogenic amendments to the landscape. It has been estimated that in American Mid-western IMLs, humans directly input and expend nearly 2 MJ per m² of cropland in order to overcome rate-limiting processes associated with water, nutrients, and biogeochemical cycling (Richardson and Kumar 2017). This massive energetic influx converts the planar landscape into one that is more productive than the Amazon (Guanter et al. 2014), and importantly, it catalyzes a “critical transition” in the overall function of the landscape, converting it from one which had longer residence times to one that swiftly moves water, nutrients, and carbon through it. This transition is referred to as the *transformer-to-transporter* hypothesis (Kumar et al. 2018).

In contrast, IMLs such as those found in the arid Loess Plateau of China aim to achieve a *transporter-to-transformer* transition in order to overcome high erosion rates and limitations in arable space that accompany the region’s hilly topography (Kumar et al. 2018). The Loess Plateau, which has been referred to as “the most erodible area on earth” (Tian and Huang 2000), is located in the highly tectonically active North Central China. It is characterized by steep hills and valleys and an abundance of highly erodible, largely degraded loess deposits (Li and Shao 2006). Intense rainfall in summer months accounts for 60–70% of annual precipitation, which contributes to soil erosion problems (Shi and Shao 2000). The average annual rate of soil loss from the region has been estimated to be between 2000 and 2500 tons per km² (Shi and Shao 2000), which inhibits much-needed agricultural and industrial activity in the region. The most widely used management practice to combat such high erosion has been the implementation of check-dams (Chen et al. 2007), dams constructed across drainage structures to trap sediment and mitigate losses (Wang et al. 2014a). Although check-dam construction began over 400 years ago, its implementation has dramatically increased in recent decades: over 110,000 check-dams were constructed

between 1962 and 2012 alone (Jin et al. 2012). Check-dams, which can essentially act as depositional centers, alter the landscape's soil organic carbon stocks, nitrogen stocks, and pH (Liu et al. 2017). Additional measures to combat erosion, including vegetation rehabilitation, strategic artificial irrigation, limited ploughing, and terracing impact the region's biogeochemical profile, as well (Qiang-guo 2001; Zhao et al. 2017).

Regardless of overall land-use aims, massive efforts across IMLs in more recent times have led to the widespread adoption of an additional goal: to protect and maintain the long-term resilience of ecosystems under intensive management. Comprehensively addressing this goal requires an understanding of the interplay between underlying natural processes, which have occurred over geologic time scales, relative to the overprinting of intensive agricultural practices that have dominated the landscape in recent centuries. This interplay has a unique and fascinating effect on the biogeochemistry of IMLs, particularly in the notoriously complex and poorly constrained section of the near surface CZ. The shallow CZ is an interface across which mass and energy are transferred and transformed from surface to subsurface through both biotic and abiotic pathways according to natural forcings, such as hydroclimatological variability, and anthropogenic forcings, such as tile drainage or check-dam usage. A suite of top-down impetus associated with surface transformations propagate the reactive signal from nutrient and solute responses to surface inputs through the dynamic shallow subsurface CZ. These top-down impetus can take the form of seemingly innocuous, centuries-long spatiotemporal patterns of deposition or erosion of sediment, or the swift, violent passage of a mechanical plough. Water also routinely infiltrates this zone and promotes biological activity and chemical transformations, only to be redistributed or transpired back out of the soil surface. Carbon enters the shallow subsurface CZ daily or seasonally in the form of litter, roots, and associated exudates only to be re-emitted as a terrestrial CO₂ flux or stored in the shallow subsurface over a wide range of timescales. The solid phase soil itself is the product of a series of water-rock-life hydrobiogeochemical interactions emanating from an unweathered supply of fresh reactive material at the base of the weathering zone. The modern-day biogeochemistry of IMLs is, therefore, the result of the convolution of long-term dynamics, such as soil formation, long-term carbon stock replenishment or depletion, and landscape evolution, with short-term dynamics, such as seasonal or intra-annual land management practices, natural and human inputs at the soil surface, and vegetation dynamics such as root exudation.

Long-term biogeochemical dynamics are imbued with the geologic legacy of the landscape's development. In IMLs in the Midwestern United States, the natural progression and evolution of CZs in prairie and mesic hardwood forests has shaped the development of floodplains and gradual establishment of native grasses and vegetation since the last glacial retreat (Pielou 2008; Kumar et al. 2018). After European settlement began in the mid to late 1800s, the landscape experienced rapid erosion and deposition of sediment commonly referred to as Post Settlement Alluvium (PSA) (Hansel and McKay III 2010). The massive shift from natural riparian wetland to agricultural land resulted in PSA effectively burying pre-existing soils (Yan et al. 2019). In some areas, PSA deposits reach up to 4 m of thickness (Knox 1989). PSA essen-

tially constitutes modern-day initial soil conditions, and we can expect that it reflects dramatically shifted rates and magnitudes of hydrologic, geomorphologic, and ecobiologic cycles affecting soil organic carbon transport and transformation compared to pre-existing soils. In addition to direct alterations of hydrologic and sediment fluxes, human replacement of natural vegetation by annual crops with vastly different nutritional needs and rooting depths contributes to dramatic subsurface biochemical changes, as well. Higher biodiversity associated with natural vegetation supports a more diverse soil microbiome (Dornbush and Wilsey 2010). Therefore, conversion from natural prairie grasses, whose rooting depths often extend well past two meters below the surface (Nippert et al. 2012), much deeper than the roots of annual crops like maize and soybean, can change biogeochemical processes deep into the CZ. Indirect effects associated with the reduction of subsurface biodiversity can induce significant changes in above- and below-ground productivity, carbon sequestration rates, and other ecosystem services (Allan et al. 2015).

Short-term dynamics encompass the immediate response of biotic and abiotic features in the shallow CZ to both natural and anthropogenic inputs. Microbially-mediated processes are strongly influenced by temperature and moisture fluctuations in the soil, as well as changes in land cover (Herzberger et al. 2014), vegetation type (Kim et al. 2020), and management practices (Kraut-Cohen et al. 2020). In the presence of tile drains, moisture removal rates can exceed the rates of assimilatory processes. The structure and function of the soil microbiome is also heavily influenced by root exudation, the highly variable process by which roots deposit organic C into the soil (Sasse et al. 2018; Vives-Peris et al. 2020). Root exudates can also affect soil pH and drive the weathering of solid phase soil (Hinsinger et al. 2003; Haque et al. 2019).

Despite the advances that new technologies afford [e.g. extensive data collection via sensor networks and flux towers (Wilson et al. 2018; Math and Dharwadkar 2017; Vuran et al. 2018), utilization of autonomous vehicles and drones (Candigo et al. 2015; Bacco et al. 2018), GIS-based services (Sharma et al. 2018), and even smartphone-based tools (Mendes et al. 2020)], a knowledge gap remains in our ability to determine the long-term impacts of overprinted anthropogenic activity on the natural CZ architecture and function (Anders et al. 2018; Kumar et al. 2018). We identify several key areas that have emerged from research at the IMLCZO that have challenged our ability to interpret biogeochemical transformations: (1) The co-evolution of surface transport of soil and soil organic carbon and its influence on the dynamics of soil carbon profiles; (2) The ability of (a) microtopographic surface features and (b) natural and artificial subsurface drainage pathways to reroute subsurface hydrology and drive below-ground geochemical gradients and reactivity; and (3) Vegetation dynamics—particularly root exudation—and their role in shaping the soil microbiome and subsurface biogeochemical environment subject to the unique seasonal cycles of growing and harvesting crops. While not necessarily a comprehensive list for IMLs with fundamentally different features than the IMLCZO (e.g. a forested IML), these areas, which encapsulate both surface and subsurface features and inputs, are important segments of a vast, interconnected landscape in transition.

Disentangling the signals from natural biogeochemical cycling and human-imposed alterations to the rates of mass transport and transformation through management practices, phreatic tile drain surface depth, fertilizer nutrient loading, and seasonal disturbances from cropping systems (from planting through harvest) requires the use of novel, comprehensive tools. Models can synthesize and help us visualize simultaneous signals recorded through extensive data collection to improve our interpretations of those measurements and inform subsequent experimental design. In this chapter, we highlight modeling efforts from the IMLCZO which have made advancements in the study of biogeochemistry in intensively managed landscapes.

6.2 Long-Term Carbon Dynamics

Piecing together the backstory of the legacy of a modern landscape's C content holds an important key to understanding its present-day biogeochemical properties. To this end, C stocks and vertical C profiles across a landscape can serve as historical landmarks built into the landscape that can potentially anchor back-calculations of a landscape's evolution over long periods of time. While researchers are in general agreement that the dynamics of soil organic carbon (SOC) stocks and vertical profiles are determined by their physical transport and biogeochemical transformation (Stallard 1998; Van Oost et al. 2007; Doetterl et al. 2016; Quinton et al. 2010), exactly how the interplay of the lateral, vertical, and biogeochemical processes affects landscape evolution has long remained unclear.

We may expect in an undisturbed natural system that this interplay would exist in a dynamic equilibrium (Amundson et al. 2015). Surface roughness characteristics determine overland flow pathways and dictate where and how soil and SOC are redistributed through lateral fluxes. These lateral fluxes break aggregates apart, mobilize SOC through erosion, redistribute SOC, and bury already existing layers of SOC in depositional areas. Erosional sites formed up-slope by soil transport generate concentrated locales of newly exposed subsoil across a landscape, which could favor C sequestration and even provide local net sinks of atmospheric C given a slower rate of decomposition than accumulation (Van Oost et al. 2007; Doetterl et al. 2016; Quinton et al. 2010). At depositional sites down-slope, topsoil layers with relatively high SOC content are gradually buried, increasing the total amount of SOC while suppressing SOC turnover rates. This imbalance can either reduce or enhance SOC decomposition rate, meaning that depositional sites could either serve as local net sinks or sources of atmospheric CO₂ (Van Oost et al. 2007; Berhe et al. 2008; Berhe and Torn 2017; Wiaux et al. 2014; Wang et al. 2014b; Zieger et al. 2017; David et al. 2009). Acting simultaneously with physical transport processes, the biogeochemical transformation of SOC can be described as a bi-directional vertical flux of C at the soil-atmosphere exchange: carbon is either inserted into the soil system via plant litter or rhizodeposition and allowed to accumulate, or it is decomposed by the soil microbiome and released into the atmosphere as CO₂. The rate of accumulation or decomposition of C in the soil is regulated by soil physical properties, such as aggre-

gate size (Wilson et al. 2009), soil moisture content and fluxes, and overall land use and land cover changes. It is also indirectly controlled by lateral soil transport, which alters the turnover rate of SOC.

This give-and-take becomes more convoluted in intensively managed systems where agricultural practices accelerate soil erosion rates by up four orders of magnitude compared to rates in relatively undisturbed landscapes (Amundson et al. 2015; Papanicolaou et al. 2015). In particular, mechanical tillage, the process by which land managers agitate the top layers of soil in order to improve certain physical characteristics for the benefit of planting, modifies surface roughness and accelerates soil and associated organic carbon redistribution in the vertical profile, which also indirectly influences the organic matter transformation rate. Tillage is not the only culprit, however; the formation and maintenance of grassed waterways significantly modifies overland flow pathways and material transport rates, altering where on the landscape material is delivered and the rate at which it is delivered (Papanicolaou et al. 2018). These surface disruptions happen in tandem with natural disturbances to surface roughness, including raindrop splashes and overland flow, which redistribute SOC by controlling lateral fluxes across interconnected soil-scapes (i.e., vertical soil columns).

Yan et al. (2019) developed the first process-based model of its kind to describe the interplay of lateral and vertical transport with biogeochemical processes (Fig. 6.2). The SCALE (Soil Carbon and Landscape co-Evolution) model (Yan et al. 2019) couples hydrologic, biogeochemical, and geomorphologic processes to characterize how soil transport, biogeochemical transformation, and the emergent landscape evolution born of the interplay of these processes affect the lateral and vertical SOC dynamics under both natural and human influences. SCALE's quasi 3-D framework couples five major components (Fig. 6.2): 2-D overland flow, 2-D SOC lateral transport, 1-D soil moisture dynamics, 1-D soil organic matter (SOM) transformation, and 2-D soil transport and resultant landscape evolution. SCALE additionally considers spatial and temporal variability in the water cycle, C cycle, and topographic evolution on temporal scales varying from days to centuries. While previous models have quantitatively assessed SOC budgets based on erosion, respiration, mineralization, and litter incorporation (Van Oost et al. 2007; Doetterl et al. 2016), SCALE additionally incorporates the enrichment ratio (ER) concept, which considers preferential carbon mobilization and deposition based on an empirically-determined ratio of the concentration of SOC in the eroded material to the concentration of SOC of the in-situ soil (Papanicolaou et al. 2018). SCALE uniquely quantifies the carbon exchange fluxes between the soil and atmosphere, and provides insights into the locations of hotspots of sinks and sources of atmospheric CO₂. Most importantly, SCALE can target broader questions regarding landscape evolution, the impact of mechanical mixing, and their resultant implications to SOC heterogeneity in IMLs.

Many previous conceptual models of SOC dynamics have been built on the concepts of 'humification', disregarding the idea that SOC is a continuum of progressively decomposing organic components ranging from labile compounds that rapidly decompose to recalcitrant compounds which, in turn, decompose extremely slowly (Lehmann and Kleber 2015). SCALE addresses SOC characterization by categoriz-

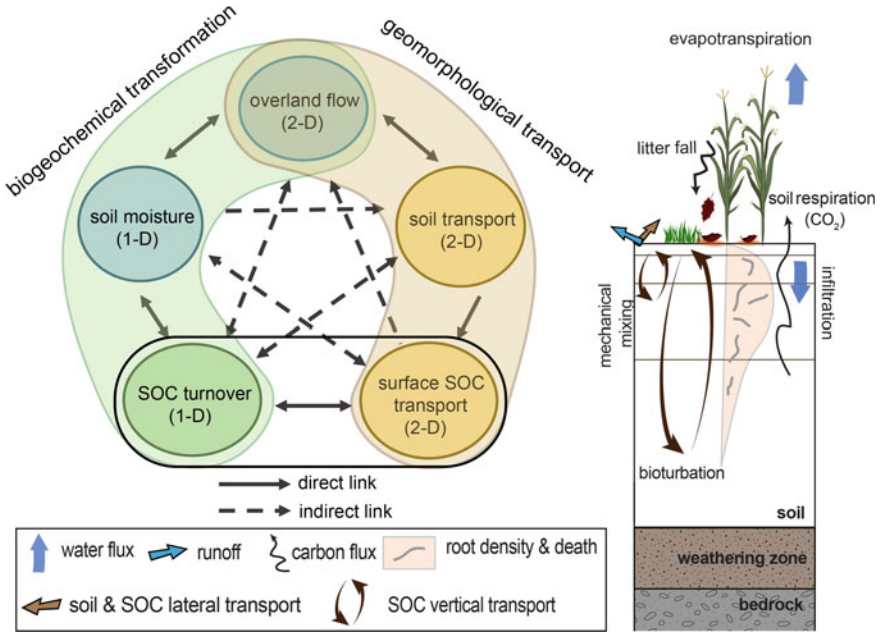


Fig. 6.2 Illustration of the modeling framework that couples biogeochemical transformation related processes of SOC throughout the soil columns with geomorphological transport at the surface. The computational approach discretizes the surface processes as 2-D matrix and below-ground processes using a 1-D array, where the surface processes include overland flow, soil transport and surface SOC transport, and below-ground processes include soil moisture and SOC transformation. SOC turnover is controlled by plant residue input (e.g. leaf litter-fall, dead root, and stover), soil water content, bioturbation via soil fauna, mechanical tillage, and SOC surface erosion/deposition. Overland flow depth and soil water content are co-dependent through precipitation, infiltration and evaporation. Soil transport and resultant landscape evolution are directly controlled by overland flow, wind, and rain splash. The associated SOC transport provides an upper boundary condition for the below-ground biogeochemical transformation [Figure is modified from (Yan et al., 2019)]

ing SOC into three pools—fast (C_l), slow (C_h), and microbial biomass (C_b) (Porporato and Odorico 2003)—and their feedbacks between each other. Combining the biogeochemical transformation, soil erosion/deposition (and resultant landscape evolution), and bioturbation by soil fauna, the SOC mass conservation in a soil column is summarized as (Yan et al. 2018):

$$\frac{\partial}{\partial t} \int_0^z \mathbf{C} dz = \int_0^z \mathbf{g} dz - \nabla \cdot \mathbf{q}_C + \int_0^z \nabla \cdot [D(z) \nabla \mathbf{C}] dz \quad (6.1)$$

where $\mathbf{C} = [C_l, C_h, C_b]^T$ is the SOC concentration, C_l , C_h , C_b represents the fast (or litter), slow (or humus), and microbial biomass pool, respectively [ML^{-3}]; $\nabla \cdot \mathbf{q}_C$ is the sum of surface SOC flux by overland flow erosion and diffusive-like erosion (e.g.

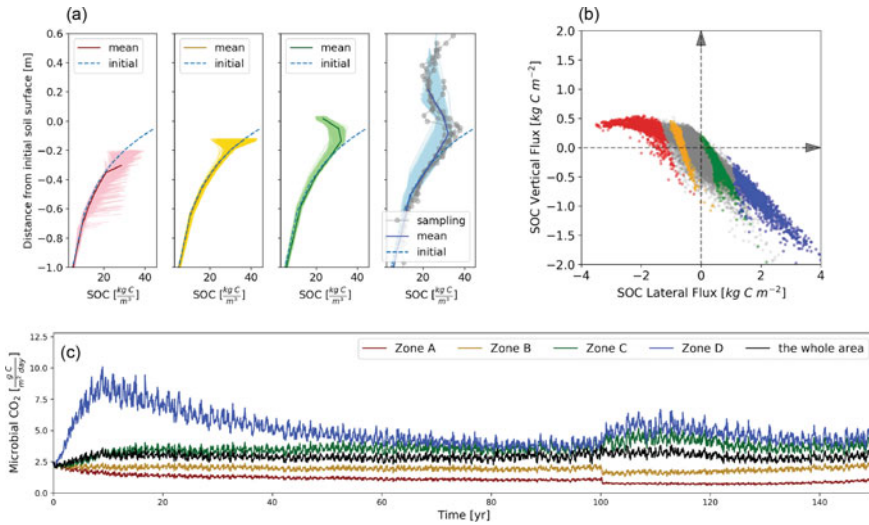


Fig. 6.3 Simulation results from the SCALE model in a sub-catchment in the Clear Creek Watershed (CCW), Iowa. **a** and **b** are from (Yan et al., 2019), and **c** is under preparation (Yan and Kumar, 2020)). Subfigure **a** shows four ensemble simulations of SOC profiles in areas in CCW that are highly eroded (red), moderately eroded (yellow), moderately depositional (green), and highly depositional (blue). Simulations for the area with highest levels of deposition (blue) are validated by the field sampling data collected in CCW. **b** Comparison of the SOC fluxes between the lateral redistribution (driven by soil transport) and the vertical carbon exchange (the net carbon change rate between litter input and decomposition rate). Colors indicate erosional/depositional areas as indicated in **(a)**, and grey dots encompass all possible points in the study area. This shows that erosional areas tend to accompany positive SOC vertical flux, meaning that those areas can be sources of atmospheric C. Depositional areas generally indicate negative SOC vertical flux, meaning that they can be atmospheric C sinks. **c** The SOC decomposition rate (i.e., the CO_2 production from soils) changes at a mean monthly rate. At year-100, a mechanical mixing experiment (which uniformly mixes 20 cm of near-surface soil) is conducted to the subcatchment at DOY 104

raindrop splash and wind) (Yan et al. 2018); $\nabla \cdot [D(z)\nabla \mathbf{C}]$ is the vertical diffusion process resulting from bioturbation by soil fauna, where $D(z)$ is the bioturbation diffusivity, parameterized as $D(z) = D_{top}e^{-0.1Z}$ (Quijano et al. 2013a), where D_{top} is the bioturbation diffusivity at the surface [$\text{m}^2 \text{T}^{-1}$]; and $\mathbf{g}$ is the net carbon flux of the biogeochemical transformation process.

More recently, numerical modeling of SOC dynamics have moved away from characterizing fast and slow C pools in favor of active or passive pools or more measurable pools (Abramoff et al., 2018). Future funding permitting, the SCALE model will be updated to incorporate more accurate approaches. Nevertheless, the novel simulation capabilities of SCALE help elucidate differences in spatio-temporal patterns of SOC content in erosional and depositional sites and how those patterns are affected by mechanical tillage. It also provides researchers a tool to help determine C hotspots across a landscape which could potentially lead to better land management practices. A 100-year SCALE model simulation based on an IMLCZO hillslope

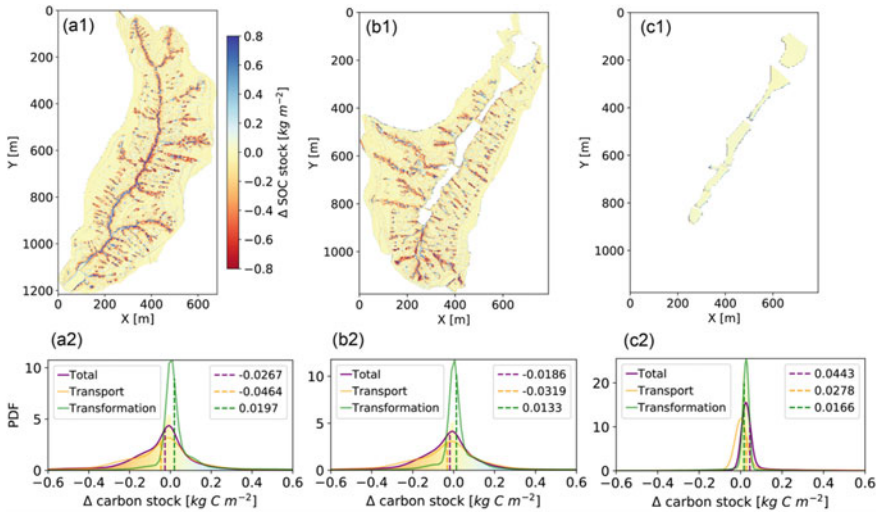


Fig. 6.4 The total SOC stock change after a 50-years evolution in the Reference Watershed (a), GLC Watershed excluding the consolidated gully (b), and the consolidated gully only (c). (a1–c1) Spatial map of total SOC stock change. (a2–c2) Probability distribution functions (PDFs). The dashed lines represent spatial mean values. The purple line corresponds to the PDF of total SOC stock change, the orange line corresponds to lateral transport, and the green line corresponds to biogeochemical transformation. Shared with permission from (Yan et al., 2020)

demonstrated the give-and-take between transport and transformation of SOC stocks in intensively managed Midwestern soils (Fig. 6.3). Figure 6.3a reveals lower SOC content in depositional centers relative to their initial SOC profile and higher SOC content associated with eroded soils. Figure 6.3b echoes this spatiotemporal result, indicating that erosional sites correspond to a positive SOC vertical flux (meaning SOC accumulation is higher than decomposition), while depositional sites tend to lose SOC through decomposition (Yan et al. 2019). Further, SCALE results suggest that this spatiotemporal difference in the rates of accumulation/decomposition vs lateral transport is exacerbated by the practice of mechanical tillage (Fig. 6.3c) (Yan and Kumar 2020). When applied to a natural watershed and consolidated gully in China's Loess Plateau, the SCALE model was able to highlight mechanistic differences between SOC stock changes in natural watersheds and consolidated gully areas. A 50-year simulation indicates that although the consolidated gully experiences higher rates of SOC transport than in the natural watershed, it had a relatively lower effect on SOC transformation rates (Fig. 6.4). This implies that the consolidated gully behaves as a sink for atmospheric carbon in addition to serving as a depositional area (Yan et al. 2020).

6.3 Event-Scale Biogeochemical Dynamics: The Impact of Microtopography and Artificial Drainage

Ultimately, linking the lateral and vertical flux of C with its turnover is an important step towards merging long timescale processes and landscape evolution with short time scale transformations. The landscape resulting from the above co-evolutionary processes directly influences the biogeochemical dynamics occurring at shorter time scales. These can be seasonal or intra-annual in scale, such as seasonal climate fluctuations whose signals propagate into the soil, or daily or subdaily processes, such as rates of infiltration, biotic transformations, and vegetation dynamics. One prime example of this link between landscape evolution and resulting biogeochemical traits can be found in Midwestern IMLs, which are typically situated on converted prairie land and floodplains and are characterized by flat to mild topographic inclines capping deep layers of post-settlement alluvium and glacial till. The generally flat topography typical of the region presents a uniquely challenging geospatial system: micro-topographic features, such as topographic depressions and drainage structures, govern the landscape's ecohydrologic and biogeochemical dynamics through their influence over the water balance and associated response of inorganic nitrogen dynamics. Surface heterogeneity associated with these areas contributes to unique biogeochemical traits, such as localized nutrient hot-spots and dramatic gradients in nutrient and moisture availability. Surface ponding, a keystone feature of micro-topographic depressions, creates pockets of prolonged anoxic conditions which result in reduced aerobic microbially-facilitated processes, such as nitrification and mineralization (Li et al. 1992; Grant 2004; Grant et al. 2010). The reduction of microbial activities, in turn, results in a decrease in the concentration of inorganic soil nitrogen (Woo and Kumar 2017).

These modest topographic features are often ignored in models that utilize lower resolution or coarse computational grids, which limits our understanding of biogeochemical dynamics in the root zone. However, the advent of high-resolution measurements of topographic features enables us to resolve micro-scale structural characteristics over large areas, providing an opportunity to capture the hydrologic and biogeochemical responses to micro-topographic variability. These high resolution measurements are incorporated into the *Dhara* model (Le and Kumar 2017) (Fig. 6.5), which links the vertically-resolved canopy-root-soil biophysical vegetation model MLCan (Drewry et al. 2010a) with a 3-D coupled surface and subsurface transport model (Le et al. 2015). MLCan resolves the vertical radiation, thermal, and environmental regimes of the canopy and soil-root system of both C3 and C4 photosynthetic pathways (Drewry et al. 2010a), and can be parameterized for a variety of row crops, including soybean and corn (Drewry et al. 2010a,b) and bioenergy crops, such as switchgrass and miscanthus (Le et al. 2011; Woo et al. 2014), and forest (Quijano et al. 2012, 2013a). In addition to plant water uptake, hydraulic redistribution (Quijano et al. 2012) is included to simulate the passive transport of moisture throughout the root and soil column according to water potential gradients. The model also incorporates carbon and nitrogen dynamics for multi-species

Table 6.1 List of key governing equations in *Dhara*

Hydrology	Biogeochemistry
Overland flow $\frac{\partial H}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial H}{\partial x} \right) + \left(D \frac{\partial H}{\partial y} \right) - q_e - q_r$	Age model of reactive transport dynamics $\frac{\partial c_i}{\partial t} + \frac{\partial c_i}{\partial \tau} + \nabla \cdot (D_i \nabla c_i + u c_i) = g - l$
Variably-saturated flow $S_s \frac{\partial \psi}{\partial \phi} \frac{\partial \psi}{\partial t} + \frac{\partial \theta}{\partial t} = \nabla \cdot K(\theta) [\nabla \psi + \hat{k}] + q_s + q_e$	$\frac{\partial C_i}{\partial t} + \nabla \cdot (D_i \nabla C_i + u C_i) = \int_0^\infty g d\tau - \int_0^\infty l d\tau$
Soil heat $C_s \frac{\partial T_s}{\partial t} = \nabla \cdot \lambda (\nabla T_s)$	$\frac{\partial E_i}{\partial t} + C_i \nabla \cdot (D_i \nabla E_i + u E_i) = \int_0^\infty \tau g d\tau - \int_0^\infty \tau l d\tau$
Canopy processes	Root exudate processes $\frac{\partial C_{gl}}{\partial t} = \underbrace{-\nabla \cdot \vec{u} C_{gl}}_{\text{Advection}} + \underbrace{\nabla \cdot (D_{gl} \nabla C_{gl})}_{\text{Diffusion}} + \underbrace{S_{gl}}_{\text{Source}} - \underbrace{L_{gl}}_{\text{Loss}}$ $\frac{\partial C_{flav}}{\partial t} = \underbrace{-\nabla \cdot \vec{u} C_{flav}}_{\text{Advection}} + \underbrace{\nabla \cdot (D_{flav} \nabla C_{flav})}_{\text{Diffusion}} + \underbrace{S_{flav}}_{\text{Source}} - \underbrace{L_{flav}}_{\text{Loss}}$
• Radiation regime • Leaf level biophysics • Micro-Environment • Soil surface fluxes	

Here, t represents time and τ represents age. (Left column) H : water elevation above the datum; D : diffusion coefficient; q_e : exchange fluxes between surface and sub-surface domains; q_r : general source/sink term; ψ : sub-surface pressure head; θ : is the soil moisture; ϕ : porosity; $\hat{k}$: unit-upward vector, S_s : the specific storage coefficient, K : unsaturated hydraulic conductivity, q_s : general source/sink term for subsurface, T_s : soil temperature., C_s : soil volumetric heat capacity. (Right column) c_i represents a concentration density of a $c_i(t, z, \tau)$ of a reactive constituent that depends on time t , depth z , and age τ ; C_i represents concentration; E_i : age concentration. Constituents modeled include: nitrate (n^-), immobile ammonium (n_{im}^+), and mobile ammonium (n_{mo}); D_i represents diffusion coefficient for a particular constituent i ; u : velocity; g : gain rate; l : loss rate, $\vec{u}$: water flux, C_{gl} : concentration of glucose, D_{gl} : diffusivity coefficient of glucose, C_{flav} : the concentration of flavonoids, D_{flav} : the diffusivity coefficient of flavonoids. See references (Le and Kumar 2017; Woo and Kumar 2017, 2019; Roque-Malo et al. 2020) for more details about the governing equations

vegetation compositions that share common resources, such as below-ground soil moisture and nutrient pools (Quijano et al. 2013a; Woo et al. 2014). It includes a coupled surface-subsurface model that simulates hydrologic and thermal processes below the vegetation canopy. *Dhara* utilizes a Compute Unified Device Architecture (CUDA) interface on Graphics Processing Units (GPUs) to exploit high resolution lidar topographic data to simulate integrated surface and subsurface transport of soil moisture and heat.

The governing equations for overland flow on the land surface and mixed form, variably saturated subsurface flow in the soil domain is shown in Table 6.1 (left column). Soil temperature regimes, primarily driven by downward ground heat fluxes, are modeled by solving the three-dimensional diffusive heat equation (Table 6.1). The biogeochemical module in *Dhara* captures the coupled dynamics of nitrogen (nitrate, mobile and immobile ammonium, and ammonia) and carbon mediated by microbial action in the soil. These processes are coupled to below-ground moisture transport to understand the distribution of concentration (hot spots) and timing (hot moments) across landscapes (Woo and Kumar 2017).

To go beyond the spatial characterization of microtopographic features themselves and examine their role in observed nutrient dynamics, researchers at the IMLCZO

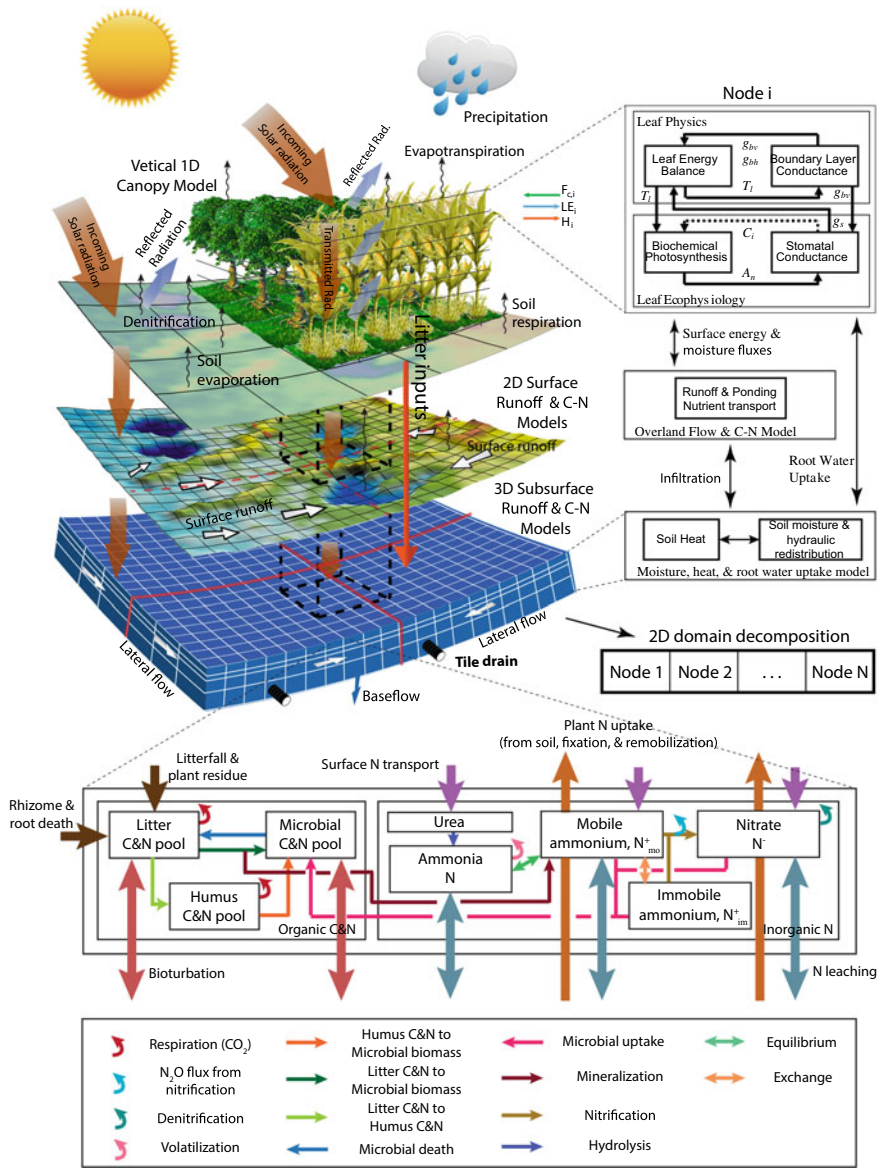


Fig. 6.5 Illustration of *Dhara* model which presently includes energy, moisture, and C-N dynamics supported through CPU-GPU hybrid computing to resolve impacts of micro-topographic variability. This figure is modified from previous studies (Le and Kumar 2017; Woo and Kumar 2017, 2019)

incorporated another variable into the equation: age (Table 6.1 right column). Woo and Kumar (2016) connect the prevalence of microtopographic features in Midwestern agricultural areas to the spatial distribution of nitrogen age in the soil, positing that age of inorganic nitrogen, the time elapsed since its introduction into a control volume, is a uniquely useful tool for the characterization of soil nitrogen dynamics. For a transient system driven by storm events and periodic application of fertilizers, the spatial distribution of age provides a dynamic attribute not captured by estimates of residence times, which are better suited for systems in equilibrium. Examination of subsurface nutrient concentration-age dynamics allows for (i) analysis of the historical footprint of nitrogen dynamics (Woo and Kumar 2016), and (ii) for exploration of the spatial and temporal distributions of nutrient stagnation and expulsion (Woo and Kumar 2017). Taken together, knowledge of both age and concentration of inorganic nitrogen can serve as an indicator for spatially-variable efficiency of nitrogen use and mobility through the soil matrix. Analysis of age along with its concentration is particularly important for any reactive constituents where different chemical species (i.e. nitrate, ammonia, and ammonium) can have widely varying age dynamics due to their varying solubility, mobility, and reactivity through the soil matrix, thereby introducing significant lateral and vertical heterogeneity. Higher concentration and age would reflect low mobility and low utilization by vegetation and, therefore, greater availability. Lower concentration and age would correspond to high mobility and/or high utilization. Age studies using reactive constituents are distinctive from age analysis using nonreactive tracers, such as chloride and bromide (Delhez et al. 1999; Duffy 2010), which flow through the system as dissolved constituents and are an indicator of the travel time of the solvent (water).

Both lower nitrate concentration and age were modeled in areas that are classified as topographic depressions due to surface flow convergence (Fig. 6.6). That is, nitrate leaching from these areas is higher than elsewhere, reducing the amount of old nitrate from the soil. This consequence, combined with increased soil moisture and lower soil temperature in the low-lying areas of flow convergence catalyze denitrification. However, for the case of mobile ammonium, lower concentration and higher age are observed in depression areas relative to other locations. Cation exchange partitions ammonium between mobile and immobile pools, leading to an increased mobile ammonium age in topographic depression areas. The estimation of nitrogen age along with its concentration can thus serve as a tool to further disentangle complex nitrogen dynamics by providing the time-scales of nitrogen transformation and transport processes. However, the data necessary to validate nitrogen age simulations is not yet available.

While the spatial distribution of surface topographic depressions determine the overall dynamics of soil inorganic nitrogen across the landscape, the short-term hydrologic and nutrient fluxes of Midwestern IMLs are governed by the overwhelming effect of another anthropogenic structure: subsurface tile drainage systems. The *Dhara* framework allows researchers to show that the presence of subsurface tile drainage systems reduces the age of nitrate in the soil. Results indicate that at the rising limb of tile drainage, relatively young nitrate, such as that derived from fertilizer application and mineralization, is associated with drainage flux (Fig. 6.7). After

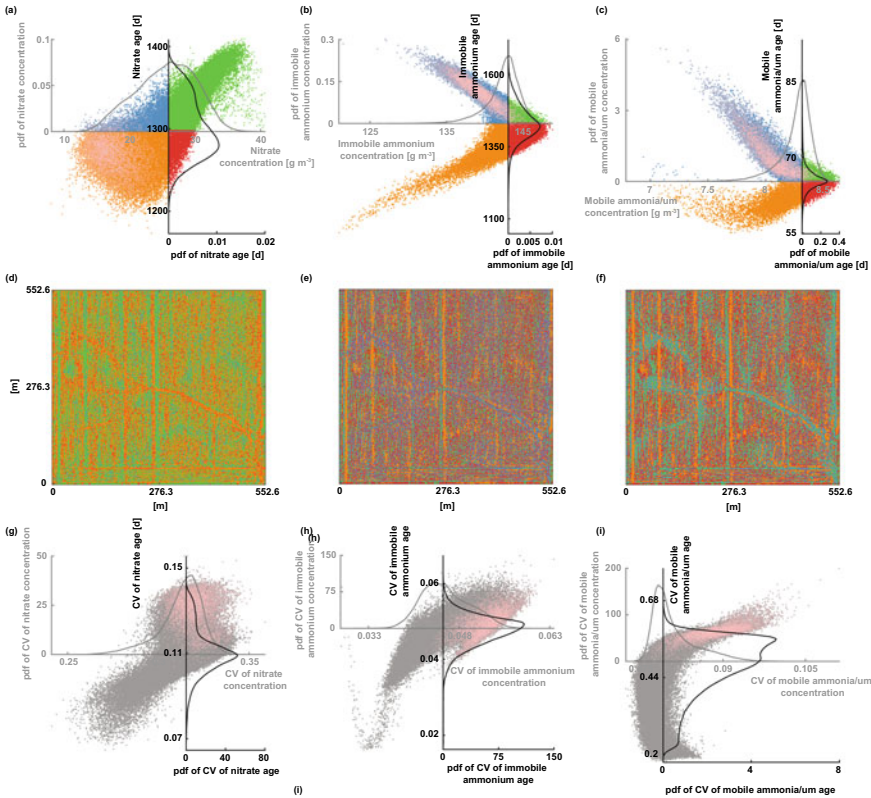


Fig. 6.6 Illustration of the variability of the age of nitrate (left column), immobile ammonium (middle column) and mobile ammonium (right column). Each plot in the top row shows the marginal distribution (solid curve) of concentration and age along two orthogonal axes that intersect at their respective median. The four quadrants in each plot, therefore, capture the combinations of high and low concentrations and ages for **a** nitrate, **b** immobile ammonium, and **c** mobile ammonium. Each individual point in a plot corresponds to a specific spatial grid, and together they illustrate the joint distribution of concentration and age in the study domain. Points in each quadrant are plotted in a different color to identify the four different combinations of concentrations and age. These points are mapped to the spatial domain (middle row) to capture the corresponding spatial patterns for **d** nitrate, **e** immobile ammonium, and **f** mobile ammonium, respectively. To assess the temporal variability, a joint distribution of coefficient of variance (CV) of the column averaged concentration (x-axis) and column and mass-weighted average of the age (y-axis) for **g** nitrate, **h** immobile ammonium, and **i** mobile ammonium, is also shown. The pink dots overlaid in **a**, **b**, **c**, **g**, **h**, and **i** indicate areas that are classified as topographic depressions (these are not marked in **d**, **e**, and **f**). Shared with permission from (Woo and Kumar, 2017)

the peak of tile drainage, however, the drainage flux carries relatively old soil nitrate to receiving surface water. In the case of ammonium, results showed an unexpected trend: tile drains increase the age of soil mobile ammonium. This surprising result is rooted in the cation exchange of ammonium: an increase in the loss of mobile ammo-

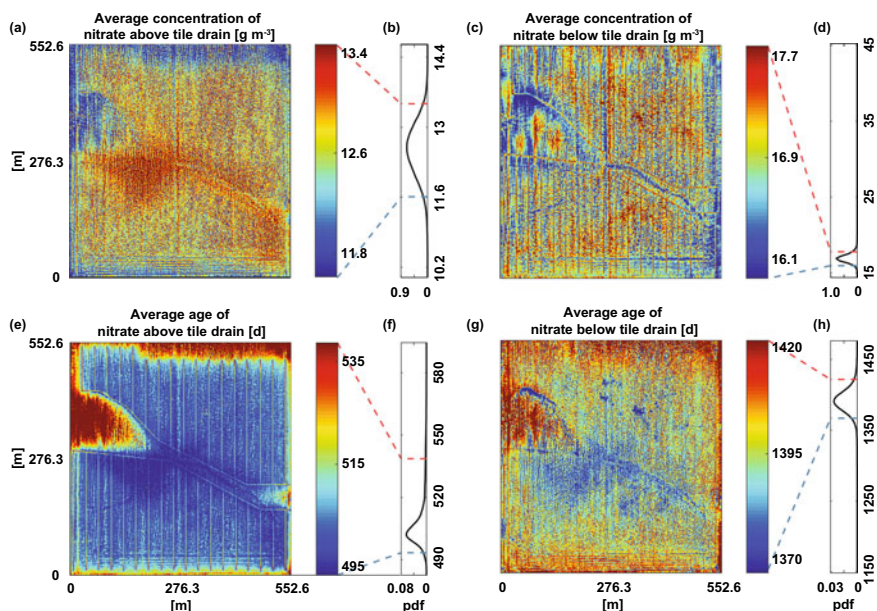


Fig. 6.7 Illustration of the spatial distribution of nitrate concentration (top row) and age (bottom row) above (left column) and below (right column) the tile system. Column averaged (**a** and **c**) nitrate concentrations and (**b** and **d**) their probability distribution functions (pdf) above and below the tile drains over the study period, respectively. (**e** and **g**) Mass-weighted averages of the ages of nitrate and (**f** and **h**) their pdfs above and below the tile drains, respectively. The blue and red dashed lines represent the corresponding 5th and 95th percentiles of the given pdfs, respectively. Shared with permission from (Woo and Kumar, 2019)

nium leads to increased ammonium flux from immobile ammonium to mobile. Since the age of immobile ammonium is approximately 10 times older than that of mobile ammonium, this flux increases mobile ammonium age in the soil. *Dhara* simulations also show that the age of nitrate in tile drain flow ranges from 1 to 3 years while that of mobile ammonium is less than a year (Woo and Kumar 2019). One of the nitrate sources is nitrification, a nitrogen transformation from mobile and immobile ammonium to nitrate. The age of immobile ammonium in the soil is the oldest among nitrogen species because its positive charge causes it to adhere to clay in the soil. Therefore, the age of nitrate in tile drainage is older than that of mobile ammonium. The rapid transport of mobile ammonium through tile drainage leads to a decrease in immobile ammonium and thus an increase in the age of mobile ammonium. These results indicate that practices and policies for reducing nitrogen loading have time lags between the implementation of mitigation plans and their responses, thus requiring mid- and long-term strategic plans. The research found in this study can be used as a guide for iterative and interactive learning processes to refine recommendations for adaptive management.

6.4 Root Zone Biogeochemistry

Another actor in biogeochemical processes in the short term is vegetation. Vegetation and their roots serve as dynamic bi-directional conduits linking above- and below-ground processes. Roots and rhizosphere processes, such as root exudation, are fundamental regulators of microbial activity and the movement and transformation of moisture and nutrients (Li et al. 2017; Lynch 2007; Manzoni and Porporato 2009; Philippot et al. 2009; Wieder et al. 2013; Vereecken et al. 2016). Root exudation, the process by which plant roots secrete an array of organic chemical compounds into the soil to influence and optimize their immediate environment, is a particularly important component of biogeochemical cycling. Nutrient gradients and fluxes across the vertical structure of the CZ are heavily influenced by root exudation, also called rhizodeposition. Root exudation is a highly variable but ubiquitous process which serves as an active driver for soil C and nutrient cycling (el Zahar Haichar et al. 2014) and of the structure of the rhizome, influencing the appearance and sustenance of the soil microbiome and the rate and magnitude of their functions (Sasse et al. 2018). It has been recognized as one of the central factors in maintaining healthy ecosystem functioning under future climate, particularly in terms of sustaining healthy microbial biomass populations under extreme conditions (Preece and Peñuelas 2016). Rumpel and Kögel-Knabner (2011) identify root exudates as one of the four main sources of organic matter in soil, along with plant roots, dissolved organic matter, and mixing of surface C through bioturbation. Root exudates commonly include sugars, amino acids, vitamins, and other organic compounds (Shukla et al. 2011). The concentration, type, and purpose of these exudates can vary as a function of plant phenology and species (Baetz and Martinoia 2014). Additional factors such as age of the root, vegetation type, bacterial growth, soil/regolith type and structure, and water availability (Toal et al. 2000; Jones et al. 2004) all contribute to make rhizodeposition a highly variable process that is not easily generalized between different study sites.

Vegetation in agricultural landscapes is no different. Crops like soybean and maize are known to secrete compounds that assist in nutrient acquisition (Cesco et al. 2010; Wen et al. 2019; Li et al. 2016), plant defense (Kidd et al. 2001), and induction of soil microbial community behaviors and structure (Guo et al. 2011; Wang et al. 2012; Sugiyama 2019; Zhalnina et al. 2018). Switchgrass, a bioenergy crop, promotes soil carbon sequestration and significantly alters soil carbon and nutrient cycling below-ground (Garten and Wulfschleger 2000; Ma et al. 2000). Perennial crops, too, can increase labile carbon in soil and strongly influence the soil microbiome, possibly to a greater degree than annuals (Sprunger et al. 2019; Szymanski et al. 2019). A growing body of literature recognizes these features as a potential avenue to exploit with respect to agricultural crop improvement and protection (Rasmann and Turlings 2016; Lanfranco et al. 2018; Zhalnina et al. 2018). This is especially true for agricultural plant species for which it has been suggested that a better understanding of root exudation and its effects on soil nutrient cycling can lead to reduced N runoff via better-informed plant breeding and land management practices (Lynch and Whipps 1990; Sugiyama et al. 2014; Bodner et al. 2015). However, in addition to the

above-mentioned subsurface dynamics, the below-ground biogeochemical systems of IMLs are subjected to drastic episodic overhauls characterized by bursts of carbon and nutrient inputs from post-harvest litterfall or root death, soil priming practices and fertilization, and supplantation of plant species.

Despite the recognition of the role of root exudation as a driver of critical biogeochemical processes, it is not entirely well modeled (Bardgett et al. 2014). The computational characterization of rhizosphere processes generally falls into two broad categories: either high-resolution models describe root behavior in detail or roots are crudely represented or are fixed as non-dynamic factors in global-scale models (Finzi et al. 2015). In a recent review of nine different agroecosystem biogeochemical models frequently implemented by the European Union's Joint Programming Initiative on Agriculture, Food Security and Climate Change (FACCE-JPI), researchers found that root distributions (but not their chemical contributions to the soil microbiome) were included in seven of nine models and that all of the models were found to over- or underestimate total nitrate leaching (Brilli et al. 2017). The absence of roots and root exudation in ecosystem- and larger-scale models is thought to be one of many factors contributing to shortcomings in predictions regarding biogeochemical cycling and transformations (Finzi et al. 2015).

The biogeochemical models described in previous sections of this chapter similarly represent vegetation as passive features in subsurface nutrient cycling. To address this, the model REWT (Root Exudation in Watershed-scale Transport) developed by Roque-Malo et al. (2020) builds upon the ecohydrologic framework developed by Drewry et al. (2010a); Le et al. (2015); Quijano et al. (2013b); Woo and Kumar (2017), and others and incorporates the active role of vegetation in driving biogeochemical and nutrient dynamics through root exudation. REWT characterizes the bidirectional feedbacks between microbial biomass dynamics, organic C turnover, root exudation, and subsurface water and nutrient transport. It is presently coupled to the 1-D MLCan model with plans to couple to the 3-D *Dhara* model (Le et al. 2015). REWT's forward predictive framework makes it the first of its kind to offer prognostic capabilities regarding vegetation-driven hydrobiogeochemical dynamics. However, as is the issue with many root exudation models, the data necessary to validate such a model is not readily available. The model is expected to contribute to experimental design.

REWt models the transport dynamics of root exudates, such as glucose (a polysaccharide that directly fuels microbial biomass growth) and flavonoids (a type of biological nitrification inhibitor). The basic form of these exudates' transport equation is provided in Table 6.1. A thorough description of REWT's governing equations are presented in Roque-Malo et al. (2020). Descriptions of rhizodeposit transport fit into a suite of equations describing the transport and transformation of carbon and other nutrients in a spatially heterogeneous framework. REWT simulations indicate that the explicit consideration of root exudation in shallow subsurface biogeochemistry can result in dramatic differences in the estimation of microbial biomass or solute export (Fig. 6.8(a, c) and (b, d), respectively). By mapping the effect of root exudates on biogeochemical transformations, REWT's simulations can inform the design of experiments related to notoriously difficult in-situ root exudation sampling. They can

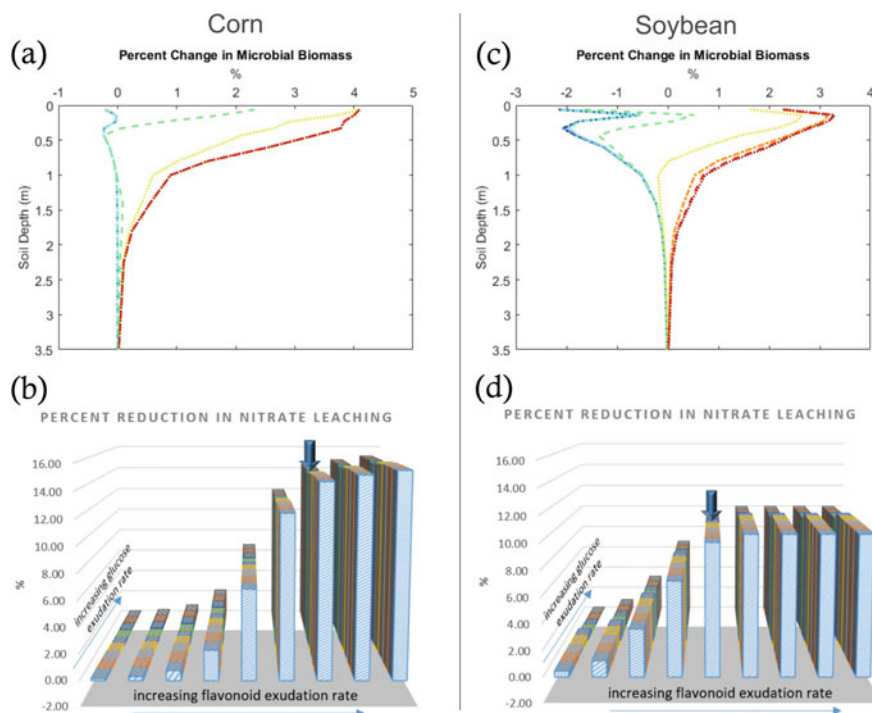


Fig. 6.8 Sensitivity analyses for change in microbial biomass and leached nitrate for corn (**a, b**) and soybean (**a, c**) based on varying rates of exudation of glucose and flavonoids. Percent changes in microbial biomass and percent reduction in nitrate leaching are calculated with respect to model results in which root exudation was not considered. Red, orange, and yellow lines in **a** and **c** indicate rates of exudation of glucose that are larger than the one found in literature. Blue, cyan, and green lines indicate rates of glucose smaller than those found in literature. The blue arrow in **b** and **d** indicates the exudation rate found in literature. Shared with permission from (Roque-Malo et al., 2020)

also assist researchers in determining the role of vegetation on solute fluxes, which ultimately informs the interpretation of concentration-discharge relationships.

Future work

The grand challenges faced by IMLs, including long term soil health, agroecosystem resilience, and perturbation responses in row crop agriculture, can be studied more effectively with improved simulations of evolving land surface topography and disturbance, subsurface hydrologic fluxes and flow pathways, and plants' active role in shaping the biogeochemical landscape. In particular, the theoretical constructs presented in the above modeling frameworks offer an advantage to understanding the region at the core of these challenges: while empirical, point-scale measurements may capture signals from many different physical and biogeochemical drivers, the above models can synthesize and help us visualize simultaneous signals in the shal-

low subsurface to improve our interpretations of those measurements. Additionally, we need a new type of model that can embrace a new era of data growth since models evolve as the quantity, quality, resolution, and density of data increases. To expand and explore opportunities across a vast variety of data sources, models like MLCan, *Dhara*, SCALE, and REWT have potential to inform laboratory and field-scale experimental design necessary for more sophisticated characterization of biogeochemical dynamics.

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