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Research papers

Integrating field observations and process-based modeling to predict watershed water quality under environmental perturbations

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ABSTRACT

Watersheds play a critical role in supplying water resources needed for human use and ecosystem health. Understanding and predicting how, when, and where changes in the quantity and quality of water resources occur under different environmental stresses including extreme events is crucial for sustainable management of water resources under a changing environment. However, few studies have attempted to quantify or identify the factors and process interactions controlling the impact of extreme events across watershed systems. Only few large-scale studies include coordinated monitoring and modeling efforts, which limits our ability to assess the large-scale impact of extreme events on water supply and quality. Methods are lacking to propagate uncertainty in process understanding through an integrated hydro-biogeochemical model framework and evaluate its importance, thus failing to take full advantage of the information potentially available through transformative advances in characterization technologies from high-resolution mass spectrometry to airborne and satellite-based remote sensing. There are consequent risks to our nation's water security and to human and ecosystem health that may become exacerbated with the increasing frequency of extreme events that is projected for the coming decades. This paper reviews the current status of watershed science for both water quantity and quality and identifies critical gaps in our current knowledge and modeling capability in addressing the emergent needs in predicting watershed hydrologic and biogeochemical responses (i.e., water quantity and quality) under natural and anthropogenic perturbations. We highlight the need to (1) understand how environmental perturbations including extreme events like floods and droughts and anthropogenic changes such as deforestation and urbanization propagate through watershed systems and assess their short- and long-term impacts on watershed biogeochemistry, water quality and their recovery pathways; (2) develop and improve a watershed water quality model that reflects the state of scientific understanding gained from observations; and (3) construct a data-model fusion system for watershed characterization, process identification, and mechanistic model parameterization. A large base of modeling, monitoring and data capabilities have been built by various federal government agencies given the relevance of water to their critical missions. An emerging need is to build an integrated national capability for watershed water availability and quality that can address water-related missions across multiple federal agencies.

1. Introduction

Watersheds are the key functional units for water resources management. Hydrological processes in watersheds mediate biogeochemical cycling of carbon, nutrients, and metals; vegetation growth; and fate and transport of contaminants, all of which can affect water quality. A schematic in Fig. 1 illustrates some key components to conceptualize the hydrologic and biogeochemical processes within a complex watershed.

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We define watershed function as the response of a watershed to the water entering its control volume (Wagener et al., 2007). Typically, watershed functions involve (a) partitioning of accumulated water into separate flowpaths such as infiltration, percolation, runoff, and interception; (b) storing water in different sub-compartments such as snow, soil moisture; (c) releasing water through evapotranspiration and surface water-groundwater interactions (Sivapalan, 2005; Wagener et al., 2007). Apart from these, watersheds also perform an essential function of retaining and releasing nutrients, metals, and contaminants, which determines river water quality downstream (Hubbard et al., 2018). In general, coupled transport of water and dissolved substances (e.g., nutrients, organic matter, and contaminants) from different locations in the watershed controls hydro-biogeochemical reaction rates and consequently impacts downstream water quantity and quality (Kirchner, 2006). Understanding and predicting how, when, and where changes in the quantity and quality of water resources occur requires deep insight into the physical and biological mechanisms that govern the cycling and transport of water and elements across watersheds under a wide spectrum of environmental stresses (Laudon and Sponseller, 2018). Gaining such insight requires field-based information that resolves how water moves across landscapes, its residence time, and what the biogeochemical properties are along various flow paths. Long-term monitoring efforts should be tightly coupled with process-based models that span the disciplinary boundaries of hydrology, geochemistry, microbiology, ecology, and atmospheric sciences (Bao et al., 2017; Seibert and McDonnell, 2002), to pursue causation, identify when and where the hydrological and biogeochemical processes are most sensitive to environmental changes at various severities (Laudon and Sponseller, 2018; Murdoch et al., 2014), account for uncertainty ranges (Fatichi et al., 2016), and get "the right answers for the right reasons" (Kirchner, 2006).

Watershed science has advanced significantly over the last 50 years, leveraging both high-resolution spatial and temporal data obtained using surface and subsurface sensors and remote sensing, availability of high performance computing resources including simulation codes, and the emerging statistical methods for integrating modeling and observations to extract knowledge in advancing predictive understanding (Kirchner, 2006; Wagener et al., 2007; Kirchner et al., 2004; Hubbard et al., 2018; Gooseff et al., 2007; Beven, 2006; Bear, 2013). Such efforts have furthered our understanding of watershed function by linking climate, hydrology, ecology, biogeochemistry, and biodiversity (Graham et al., 2019).

Despite these advances, climate change, extreme weather, anthropogenic activities (e.g., agriculture, energy production, land-use change, and contaminant exposure), and other perturbations lead to huge uncertainties regarding how watersheds respond to such perturbations (Page et al., 2012). For instance, climate change has not only shifted average meteorological conditions but also led to an increased number of extreme events, illustrated by the recent examples of Hurricane Katrina, Hurricane Irene, Tropical Storm Lee, and Hurricane Harvey, all of which resulted in record-breaking rainfall totals and billions of dollars in loss and damages (Vidon et al., 2018; Paerl et al., 2018). Watershed responses to environmental changes may vary depending on the intensity, duration, and magnitude of an event (Kaushal et al., 2018b). High-intensity events, such as tropical cyclones, usually lead to pulse responses in water quality, with large changes in chemical concentrations and fluxes occurring over relatively large areas and over short time periods. For example, Hurricane Irene and Tropical Storm Lee led to unprecedented increases in the concentrations and loads of total suspended solids (TSS), particulate organic carbon (POC), and dissolved organic carbon (DOC) as they moved through Maryland and Pennsylvania (Vidon et al., 2018). Ten-fold increases in DOC and hundred-fold increases in POC were observed in Maryland; hundred-fold increases in TSS concentrations occurred in Pennsylvania. High runoff induced by tropical cyclones had large impacts on annual N and phosphorus (P) fluxes and mobilized and transported terrestrial-derived C to estuaries.

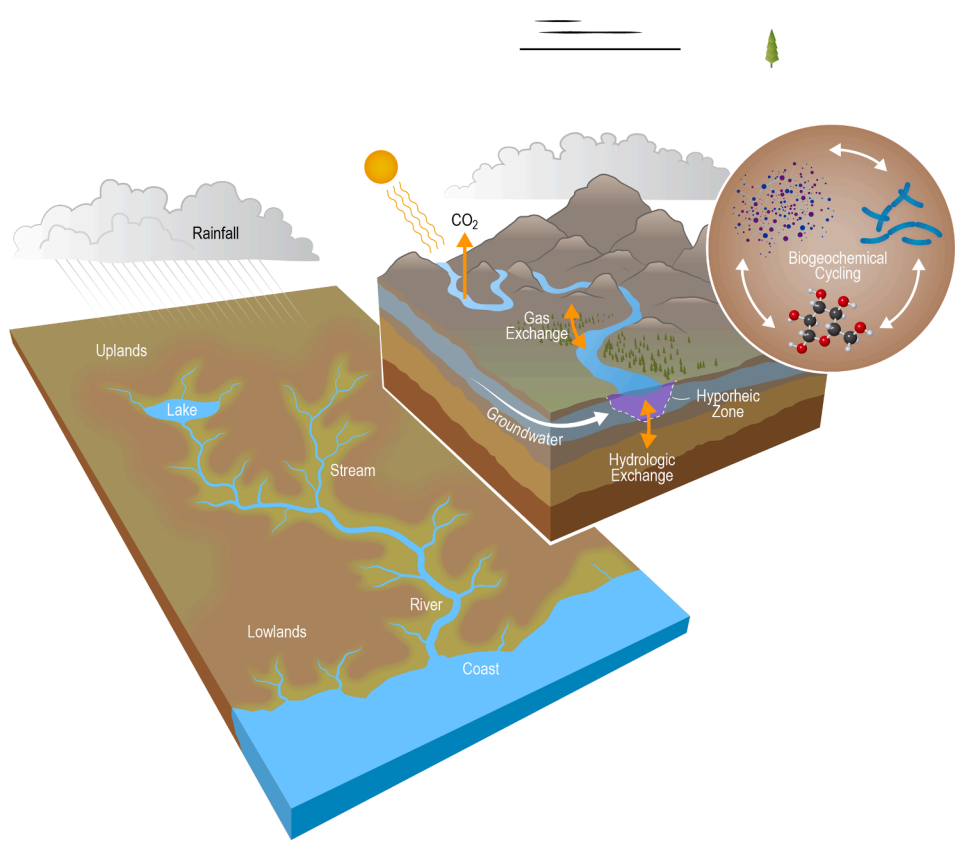

Fig. 1. Conceptual model of hydrologic and biogeochemical processes at the watershed scale.

Particulate loads (e.g., POC, particulate phosphorous, TSS) occurring during Irene and Lee accounted for more than 30% of the annual discharge concentration in many places (Paerl et al., 2018). Anthropogenic activities such as fertilizer applications, deforestation, urbanization and dam construction can exacerbate extreme responses and feedback. For example, deforestation significantly enhances runoff with associated increases in sediment, nutrient, and organic matter loadings (Heaney and Huber, 1984; Hawley and Vietz, 2016; Paul and Meyer, 2001). Impervious surfaces in urbanized areas limit groundwater recharge and direct stormwater into defined flowpaths that support flashier hydrograph responses to storms, facilitate erosion, and carry pollutants that impact stream biota and broader ecosystem health (Walsh et al., 2005; Walsh et al., 2007; Burns et al., 2012; Herlihy et al., 1998; Grimm et al., 2005; Kaye et al., 2006; Tsoi et al., 2011; Fletcher et al., 2013).

Improving the understanding of how extreme events impact watersheds has become increasingly more critical as the occurrence of these extreme events are projected to be more frequent and more intense (IPCC, 2012). Watershed models are key tools for understanding watershed functions and their responses to perturbations, and thereby for managing water resources (Weiler and McDonnell, 2004; Burt and Pinay, 2005; Beven, 1997; Jones et al., 1993). Mechanisms that well represent watershed hydro-biogeochemical responses to mild environmental stresses may not be extrapolated to represent responses to extreme events such as floods and droughts. Furthermore, the spectrum of environmental stresses that have been modeled is data sparse, especially with respect to extreme events. High variability in the relatively few end member observations, against which models are calibrated, results in high uncertainty in model conceptualization, which is ultimately translated into model structural error. Decreasing model structural uncertainty would better inform sustainable management of watershed systems under projected environmental stresses, which are critical for enhancing our economical and societal resilience (Srinivasan et al., 2017; McDonnell et al., 2018).

The objectives of this review paper are to: (1) review the current status of watershed modeling and monitoring in understanding watershed hydro-biogeochemical processes and predicting water quantity and quality under perturbations; (2) identify the key knowledge and capability gaps; and (3) present a path forward to integrate modeling and observations to advance predictive understanding of watershed hydro-biogeochemical responses to perturbations.

2. Current knowledge and gaps in understanding watershed responses

The response of water quality to extreme hydrologic events in a watershed is shaped by geology, topography, land use, and past environmental conditions (Kaushal et al., 2018a; Kaushal et al., 2018b). Interactions of hydrologic and biogeochemical processes in watersheds are inherently complex (Fig. 1). They are manifested over a variety of temporal scales and spatial scales from single microorganism to individual plants to landscape (Wang et al., 2015). Coupled hydrologic processes include precipitation, overland flow, evapotranspiration, variably saturated flow, and the movement and exchange of between the land surface, soil, and the underlying aquifers (Yu et al., 2018). Coupled biogeochemical processes include mineral weathering, cation exchange, photosynthesis, nutrient cycling within each hydrological compartments, sediment erosion, as well as transformation and exchange between those compartments. Understanding watershed biogeochemistry that controls key water quality signatures at broad spatial scales must account for not only how processes in different landscape patches (e.g., in upland, riparian zone, and wetlands) are regulated, but also how they interact as water travels across the watershed. Transport processes must be coupled with element-specific cycling across space and time to understand the contributions of landscape patchiness and hydrologic and biogeochemical connectivity (the connection and disconnection of disparate landscapes via surface and subsurface flows) in controlling stream and river water chemistry (Harvey and Gooseff, 2015). Research has just begun to connect transport mechanisms with element-specific releases to surface water (Bao et al., 2017; Kaushal et al., 2018a).

2.1. Watershed hydro-biogeochemical processes

The depth and length of groundwater flow paths strongly control C and N cycling and the delivery of below-ground biogeochemical reaction products to surface water (McDonnell et al., 2007). High DOC exports have typically been associated with near-surface hydrologic flow paths that intersect DOC rich forest floor and surficial soil layers in riparian or wetland locations (Frank et al., 2000; Inamdar and Mitchell, 2006). Rising groundwater tables also contribute to increased DOC concentrations in surface waters, known as the "flushing" effect (Creed et al., 2008). Nitrate ($NO3^-$) exports from watersheds occur along both shallow and deep groundwater flow paths (Laudon and Sponseller, 2018; Inamdar and Mitchell, 2006; McGlynn and McDonnell, 2003). These flowpaths are impacted by land use changes, such as urbanization which limits groundwater recharge (Brown et al., 2009). Therefore, understanding the subsurface routing of water through a watershed is fundamental for explaining hydro-biogeochemical responses in surface water. However, the role of subsurface biogeochemistry in watershed responses to extreme events and chronic changes remains poorly understood.

Subsurface flow depends on precipitation thresholds. In one example (Tromp-van Meerveld and McDonnell, 2006a), it was shown that precipitation events exceeding the threshold of 55 mm resulted in a hundred-fold increase in subsurface flow compared to subsurface flow changes that resulted from storms producing less than 55 mm of precipitation. Storm flow can be partitioned as moving slower through capillaries in the soil matrix or (generally) faster through preferential pathways. Traditionally, such preferential pathways were conceptualized as conduit macropore networks in the soil matrix that re-route water to arrive at the stream at rapid speeds (Beven and Germann, 1982). Preferential flows also occur at the interface between shallow surface soil and an impervious layer (e.g., bedrock; Freer et al., 2002; Graham et al., 2010; Hopp and McDonnell, 2009; Lehmann et al., 2007; McGlynn and McDonnell, 2003; Salve et al., 2012; Tani, 1997; Tromp-van Meerveld and McDonnell, 2006b). Soil pores and microtopography of the bottom impervious layer are hypothesized to fill, then water can spill over the bottom boundary layers and initiate preferential flow with a threshold response (Tromp-van Meerveld and McDonnell, 2006b). More recent studies have also shown that preferential flow paths through weathered and fractured bedrock may contribute significantly to watershed water balance (e.g., accounting for more than 30% of precipitation) (Kosugi et al., 2006; Graham et al., 2010; Aishlin and McNamara, 2011; Flinchum et al., 2018; Tromp-van Meerveld et al., 2007). Preferential subsurface flow influences the source, age, and timing of water, C, and N losses in many systems, with important implications to biogeochemical reactions, residence time, and routing to downstream ecosystems (Lohse et al., 2009). Changes in precipitation extremes will likely alter runoff pathways and groundwater recharge, which may in turn increase nitrate and DOC concentrations in both groundwater and other receiving waters. These impacts are likely to differ in areas experiencing anthropogenic alterations to landscapes that increase susceptibility to precipitation events (Walsh et al., 2005; Burns et al., 2012). However, it is extremely challenging to mechanistically capture such preferential flows across watersheds because there are few observations of such flow responses during extreme storm events, and subsurface domains, especially bedrock fractures, are not easily accessible. While isotopic signature and long-term mass balance experiments could provide valuable information for the mixture of flow paths, residence time, and contributions from various land use patterns, such measurements have not been acquired in many watersheds.

Plant canopy interception and root access to subsurface water for

transpiration can also impact the water balance by altering the soil storage of water and material, consequently on water and solute availability including location and timing across the landscape (Brauman, 2015). Under drought or water-limited conditions, plants modulate the transpiration demands by controlling the opening of their stomata to avoid catastrophic failure. Empirically-derived wilting parameters are crucial in connecting soil water conditions to plant transpiration (Fang et al., 2017; Chen et al., 2008). Eddy covariance flux tower measurements (Baldocchi et al., 2001) provide valuable datasets to identify the connections between the ecohydrologic fluxes and their driving forces and understand the feedback mechanisms between processes. An information theory-based approach (Goodwell et al., 2018) has been recently applied to understand how forcing and feedback mechanisms are linked to ecosystem responses (water, carbon, and heat fluxes at the land surface) to different types of disturbances (e.g., rainfall pulses and drought) using process connectivity between environmental variables. Based on analyses performed on two transects of eddy covariance towers across elevation and climatic gradients at the Critical Zone Observatories (CZOs) in Idaho and California, Goodwell et al. (2018) found that ecohydrologic fluxes along climate gradients respond differently to disturbances, with significant influence of heterogeneity in soil characteristics, topography, vegetation, and soil microbial activity. Accounting for deep groundwater dependence of ecosystems under water stress is especially important for managing dryland ecosystems to achieve water resources sustainability (McDonnell et al., 2018; Miller et al., 2010).

Knowledge of unprocessed atmospheric nitrate in waters is important to assess forest health and water quality in watersheds. A recent synthesis (Sebestyen et al., 2019) of nitrate isotope studies around the Northern Forest Region revealed that nitrate enters the forests from atmospheric deposition and sometimes rapidly moves to streams without being biologically processed. Especially during higher-flow events caused by either rainfall or snowmelt runoff, unexpectedly high levels of unprocessed nitrate flows to streams could occur over a brief time window. Too much nitrogen, termed “nitrogen saturation,” can change forest composition and mobilize calcium in soil, leading to declining forest health and water quality. The effect of nitrogen saturation could be amplified if extreme precipitation events continue to increase in frequency and magnitude. Understanding the fate of nitrogen produced in the air and transported to the land and river networks is currently lacking due to lack of long-term monitoring of nitrate isotopes (Schlesinger, 2009).

Hydrologic flow paths and runoff sources are critical for explaining the differences in dissolved organic matter (DOM). The concentration, composition, and sources of DOM were found to differ dramatically between base flow and storm event conditions during a three-year period (2008–2010) in a forested headwater catchment in the mid-Atlantic Piedmont region of the US (Inamdar et al., 2011). The aromatic and humic DOM constituents in river water increased significantly during storm events, attributed to the contributions from surficial sources such as throughfall, litter leachate, and soil water. Groundwater sources contributed a large fraction of the DOM constituents during base flow and were responsible for the high percentage of protein-like fluorescence observed in base flow conditions. By studying multiple storm events, this same study (Inamdar et al., 2011) also revealed that summer storm events produced the highest concentrations of humic and aromatic DOM, while such response was muted for winter storms. A large precipitation event following summer drought produced a complex DOM response; this was not observed for other similar storm events, confirming the dependence of response on past environmental conditions. Deforestation and urbanization also increase DOM loading to waterways, often with different chemical character than surface water DOM profiles (Williams et al., 2010; Wilson and Xenopoulos, 2009; Fu et al., 2007; McEnroe et al., 2013), and amplify the impacts of precipitation events through enhanced erosion and preferential flowpaths (Burns et al., 2012; Heaney and Huber, 1984; Paul and Meyer, 2001; Hawley and Vietz, 2016).

The composition of DOM has a large impact on the watershed biogeochemical processes, as revealed in recent studies (Stegen et al., 2018; Goldman et al., 2017; Graham et al., 2017; Graham et al., 2018). Laboratory experiments and field observations have revealed that microbial activities and organic carbon (OC) characteristics regulate the underlying mechanisms of biogeochemical cycling in surface water and subsurface systems, such as aerobic respiration and denitrification (Stegen et al., 2018; Goldman et al., 2017; Graham et al., 2017; Graham et al., 2018). Understanding of the input and fate of DOM in river networks has undergone dramatic transformation over the past decade with the availability of new measurement technologies such as high-resolution mass spectrometry. Challenges exist in translating information about the relative composition of different DOM components to masses to enable a better understanding of (1) the coupling between DOM composition and microbial uptake and nutrient cycling, and (2) the role of DOM at the watershed level (Inamdar et al., 2011). These challenges result in conceptual uncertainty in translating the knowledge into model representations. Methods are lacking to propagate that conceptual uncertainty through an integrated hydro-biogeochemical model framework and evaluate its importance, thus failing to take full advantage of the information potentially available through these transformative advances in characterizing molecular properties.

2.2. River corridor hydrology and biogeochemistry

Hydrologic exchanges between the surface water and groundwater creates hydrological, thermal, biological, and chemical gradients across the interface of these two water bodies, which have significant impact on human and environment health (Bobba, 2012; Conant et al., 2019). The interaction zone, broadly defined as the river corridor (Harvey and Gooseff, 2015), experiences bidirectional exchange of water, energy and nutrient driven by static and dynamic pressure variations over the streambed (Grant et al., 2018). However, quantifying the exchange of water and chemicals of interest across this interface at watershed scale is hampered by limited data availability and integrated models that are not sufficiently refined to account for heterogeneities in the stream channels and aquifers (Barthel and Banzhaf, 2016). As of today, the study of river corridor processes still faces the challenges identified in Harvey and Gooseff, 2015 five years ago: 1) how to transfer small scale process knowledge to larger scale water quality and ecological response that are cumulatively affected by these small processes; 2) how to resolve the effect of heterogeneities of multiple origins on hydrologic exchange flows and fate of nutrients and contaminants in rivers; 3) how to understand river corridor functions by quantifying “hot spots and hot moments” and reactant delivery effectiveness by hydrologic exchange flows for biogeochemical processing of nutrients and organic matter; and 4) how to avoid potential measurement bias of hydrologic exchange fluxes. These challenges have recently been reiterated in a review paper by Ward and Packman, 2019. For an improved understanding of biogeochemical transformation processes across this interface, high resolution monitoring is essential to determine the spatial and temporal variability of hydro-biogeochemical parameters (Gassen et al., 2017). On the other hand, hydrologic connectivity cannot be ignored when addressing watershed scale water quantity and quality (Freeman et al., 2007; Harvey et al., 2019). Low-frequency large precipitation and snow events under future climate change can contribute to a significant proportion of annual terrestrial dissolved organic matter input to drainage networks and to downstream, higher-order rivers, bypassing headwater streams due to higher stream velocities during these events (Raymond et al., 2016).

2.3. Linking with microbial and biogeochemcial processes

While it is often assumed that high resolution data generated by emerging molecular techniques can improve our understanding and

predictions of biogeochemical cycling (Rocca et al., 2015; Graham et al., 2016; Hall et al., 2018), we have a poor understanding of the environmental contexts as well as the spatial and temporal scales at which these data types truly provide added value for predictive power of watershed function. Recent meta-analyses have demonstrated weak relationships between microbial genes and biogeochemical processes, highlighting a falsehood in the common assumption that molecular data is spatially and temporally representative of broader ecosystem function (Rocca et al., 2015; Graham et al., 2016). Molecular information is typically extracted from a gram or less of sediment at sparse (or a single) time points and detect both active and residual constituents. In contrast, watershed functions of interest are over much larger spatial domains at daily or even finer resolution when evaluating rapid responses to intensive hydrologic disturbances. Therefore, questions remain regarding the spatial scales and domains at which molecular information is valuable for informing reactive transport processes at the watershed scale, and how the importance of molecular data varies over time when the perturbation progresses. For instance, Graham et al. (2014) demonstrated seasonal disparities in the power of microbiome genes to explain N cycling rates, and Blinn et al. (1995) demonstrated that benthic organisms can require four months of recovery time following subsequent 12-h disturbances. In such a situation, genetic information on microbial communities may provide significant insight into biogeochemical reaction rates. Good et al. (2018) have shown the utility of a genohydrology approach at monthly or longer timescales.

High resolution molecular data may be most useful for improving predictive models in systems with high spatiotemporal variability, wherein microorganisms integrate over the short-term hydrologic history of the system (days to weeks) and metabolomic data reflect biogeochemical processing in real-time. Examples of such situations include hyporheic zones, perturbation responses, and high-frequency stage variability (e.g., hydropeaking, coastal, storm-driven). Hyporheic zones are a nexus of hydrologic mixing and biogeochemical hot spots, with spatiotemporal variability in chemical constituents (Boulton et al., 1998; McClain et al., 2003; Harvey and Gooseff, 2015). Heightened heterogeneity in this zone can generate disconnects between microbial metabolism and ambient geochemistry, therefore deviating true biogeochemical rates from functional predictions that are based solely on hydrobiogeochemical data types. Perturbations may similarly decouple extant microbiomes from environmental conditions, therefore increasing the value of molecular insights on predictions of biogeochemical rates during perturbation. High-frequency stage variations can alter the spatial extent and mixing conditions of hyporheic zones as well as perturb multiple components of watersheds (Song et al., 2018; Shuai et al., 2019), creating an ideal system for maximal value in molecular data.

2.4. Watershed Functions under Mild and Extreme Perturbations

Interpretations of watershed modeling studies under mild and extreme perturbation forcing remain uncertain for several reasons. First, water quality responses to observed perturbations vary depending on the intensity, duration, and magnitude of an event. Various numerical modeling approaches simulate well the hydro-biogeochemical responses to most events in the subsurface and surface water domains, though simulations of responses to extreme events continue to contain high uncertainty due to the chaotic nature of large-scale atmospheric circulation (Shepherd, 2014). A study of 35 tropical cyclones over the past two decades found that watershed export of nutrients and carbon after major storms can be storm-specific, depending on the mechanisms that mobilize the nutrients and carbon (Paerl et al., 2018). For P, large storm flows may lead to its release from sediment in inundated wetlands that experience low-oxygen river water conditions that often occur after the passage of tropical cyclones. P concentrations increased as flow increased, which magnified the total impact of the storm. However, N concentrations had a non-monotonic and generally negative relationship with flow, suggesting non-point sources from unique land use were dominant, while dissolved and particulate organic nitrogen did not correlate significantly with flow (Paerl et al., 2018). Second, there are difficulties in obtaining field observations and doing process-based studies. Currently, watershed models under extreme perturbation forcing have been data sparse due to difficulties in obtaining field observations and performing process-based studies (Kaushal et al., 2018b; Vidon et al., 2018). Models calibrated against few end member observations may lead to large uncertainty. Some particular extreme events have been well-documented, though not all systems (e.g., riparian zones) in the watershed are well represented (Vidon et al., 2018). Third, there is uncertainty about future anthropogenic disturbance to the environment and how that impacts watershed hydro-biogeochemical processes. Nutrient and carbon flushing is largely dependent on previous accumulation, due in large part to changing land use (Paerl et al., 2018). Models show that flood magnitudes can decrease significantly in large rivers downstream of dams (Lu et al., 2017), impacting nutrient and carbon loads downstream. The capacity for stream and river ecosystems to retain and transform nutrient pollution from landscapes can become "saturated" during floods unless nutrient pollution sources are reduced at the watershed scale (Kaushal et al., 2018b). Fourth, there is a lack of a consistent strategy in terms of monitoring methods to fully assess the large-scale impact of extreme events (Vidon et al., 2018).

Climate change has increased the frequency and intensity of fires, which alter the watershed hydrobiogeochemical functions by reducing vegetation cover, and soil hydraulic/biogechemical conditions. Forest fire increases the surface flow rather than groundwater flow, resulting in higher stream temperature (Wagner et al., 2014) and increased nutrient exports to streams (Hanan et al., 2017). Also, increased solar radiance on the soil surface due to lower vegetation coverage may accelerate the decomposition of soil organic matters (Wagner et al., 2014). Post-fire precipitation increased hillslope/channel erosion and its rapid geomorphic change can alter the stream metabolism (Tuckett and Koetsier, 2016). However, the impact of forest fire can vary among different watersheds (Oda et al., 2018); for example, some watersheds with higher interaction between surface and groundwater tend to have less significant fire effect on stream temperature than the watersheds with lower surface–groundwater interaction (Wagner et al., 2014). Furthermore, vegetation in higher elevation area (energy-limited watershed) tend to take longer time to recover from fires, which could prolong the periods of impaired water quality as impacted by the fire (Wagner et al., 2014).

Anthropogenic activities such as land cover change (e.g.deforestation), and urbanization alter hydrologic fluxes and water qualities. Expanded agriculture lands play a major role of contaminating groundwater and stream water qualities through the intensive use of inputs such as pesticides, chemical fertilizers and manures of livestock, etc. In agriculture-dominated watersheds, subsurface flow via tile drainage and homogeneity of evaportranspriation by mono-cultural vegetation cover reduce the hydrologic variability. Urbanization increases the population density, consequently increasing the nutrient loads including waste water discharge. The urbanization increases the intensity and the frequency of flooding as the hydrologic response to precipitation is faster due to increased impervious area.

3. Watershed monitoring

Hydrologic and biogeochemical monitoring of watersheds is broadly dispersed across agencies and individual research teams. While an exhaustive review of all efforts across the globe is beyond the scope of this paper, we provide a summary of major infrastructure within the US with the goal of emphasizing strengths and weaknesses of current efforts. For example, the U.S. Geological Services (USGS) has developed and maintains an expansive monitoring network (https://waterdata.usgs.gov/nwis) focused on surface water quantity and quality using in situ sensors (e.g., stream gauges, water quality sondes) and field-collected

samples. A key attribute of the USGS network is that much of the data is freely available and is consistently structured and managed. This allows the USGS data to be used extensively for operational decision making, flood prediction/response, and basic research into watershed function. The USGS network is, however, biased towards larger rivers and the network is primarily above the head-of-tide. As such, there are gaps in the monitoring of low-order streams and tidal rivers. USGS has also established the National Ground-Water Monitoring Network (NGWMN) (https://cida.usgs.gov/ngwmn/index.jsp), which provides monitoring data from groundwater wells distributed across federal, state, and local agencies.

Recognizing a need for consistent monitoring data across environmental contexts, the U.S. National Science Foundation (NSF) has established the National Ecological Observatory Network (NEON) (https://www.neonscience.org/) as an observational platform across all biomes of the US. Similar to USGS, NEON data are consistently generated and structured, and are freely available. NEON includes both terrestrial and aquatic components, and their data span everything from ecosystem fluxes to soil microbes to plant/animal communities to stream discharge. The use of consistent methods to generate and openly provide data are not unique to the USGS and NEON, but they are also not necessarily common across other monitoring efforts. It is important to recognize that NEON was not established to monitor watersheds per se, but rather to monitor terrestrial and aquatic environments in localized field sites distributed across biomes of the US. NSF funds other major field efforts as well, such as the long term ecological research (LTER) network, which includes elements of ecosystem monitoring and experimentation. Like NEON, the LTER network is not necessarily focused on watershed monitoring. Other efforts funded by the NSF are more watershed-oriented, in particular the CZO network (http://criticalzone.org/national/) that spans a number of watersheds across the US. Efforts within CZO sites span a broad range of watershed attributes, though they often emphasize the geology and geochemistry of the deep subsurface. The NSF-funded CUASHI effort (https://www.cuahsi.org/) is another critical capability within watershed science. CUASHI is a consortium of universities that serves integrated watershed data (e.g., water discharge and quality) and provides access to models (e.g., the national water model) and training in watershed science methods.

In addition to the USGS and NSF, The US Environmental Protection Agency (EPA) has significant monitoring efforts, such as their National Streams and River Assessment (https://www.epa.gov/national-aquatic-resource-surveys/nrsa) that focuses on the ecological state and water quality of streams and rivers within the US. The EPA efforts have less emphasis, however, on watershed hydro-biogeochemistry. The US Department of Energy (DOE) funds a network of 5 watershed test beds distributed across the contiguous US. They collectively span much of the watershed continuum from low-order headwater streams in Colorado, to mid-order streams Tennessee, Wyoming, and Georgia, to a high-order river in Washington State. Research within these test beds is highly integrative that includes both monitoring and experimentation associated with surface and subsurface hydrology, (bio) geochemistry, microbiology, plant physiology, and ecosystem processes. In addition, data-generating efforts in these test beds often focused on informing mechanistic hydrobiogeochemical numerical models, such as subsurface reactive transport codes. Among agency-funded efforts, the DOE test beds are relatively unique in their level of focus on informing predictive models, which contrasts with other efforts (e.g., NEON) designed primarily as observatories with less emphasis on informing models.

Similar monitoring strategy and efforts exist across the globe to understand watershed functions. For example, Canada's Water Office provides real-time, nation-wide stream gauge data (https://wateroffice.ec.gc.ca/). Canada has also formed a watershed research consortium (http://cwn-rce.ca/project/canadian-watershed-research-consortium/) that aimed to develop consistent monitoring programs across watersheds to enable improved understanding and decision making. Recently, more community-driven networks are emerging, such as StreamPulse (http://pulseofstreams.weebly.com/) that includes hundreds of datasets from across watersheds to evaluate stream metabolism. The 'internet of water' (https://internetofwater.org/) that focuses on improving access to watershed data by linking data producers (e.g., USGS), data hubs (e.g., NGWMN), and data users (e.g., researchers and decision makers). Worldwide Hydrobiogeochemistry Observation Network for Dynamic River Systems (WHONDRS) (https://whondrs.pnnl.gov/) is another network initiated by the watershed science community to provide unique data resources with detailed molecular characterization, focusing in the river corridors impacted by dam operations.

Enhanced coordination and standardization in terms of data generating methods and data archive practices is a major need within watershed science. The USGS and similar efforts in Canada and other countries provide a model of coordination, consistency, and openness that all of watershed science should aspire to.

4. Watershed modeling approaches

Watershed models can be broadly thought of as being either empirical (data-driven) or process-based (mechanistic), although in practice many models employ a combination of the two approaches. Empirical models link inputs (e.g., geomorphic properties, land use, precipitation) and outputs (response/state of a watershed) through observationally-derived relationships. Because such models do not attempt to explicitly quantify the underlying physical, chemical and biological processes that connect inputs with outputs, they usually require a small numbers of parameters and are computationally inexpensive to implement. Some examples of empirical models include the unit hydrograph and curve number method (USDA, 1986) used to estimate runoff, and the Universal Soil Loss Equation (Hudson and Food, 1993) used to estimate soil erosion. Machine learning (ML)-based relationships are a form of empirical model, typically derived solely through analysis of large datasets without imposing physical constraints, and methods such as Artificial and Bayesian Neural Networks (Committee, 2000; Dawson and Wilby, 2001; Dawson and Wilby, 1998; Dwivedi et al., 2013) are increasingly being used to simulate hydrologic processes. Empirical models can be useful in ungauged watersheds, but they are valid only under conditions (i.e., high-level watershed characteristics) similar to those under which they were derived. Thus care must be exercised to ensure empirical models are not used outside their range of applicability. This may strongly limit their suitability for predicting responses to extreme events, which by definition are outside the range of "normal" events on which empirical relationships are based on and may also lead to fundamental changes in hydrologic connectivity and other features that control watershed responses.

Process-based models attempt to impose physical, biological, and chemical principles (e.g, conservation laws or laws of mass action) on the mathematical formulae relating model outputs to inputs (often using ordinary or partial differential equations). In practice it is not possible to resolve processes based on first principles alone. Closure approximations must be introduced (Wood, 2009), usually resulting in effective parameters or constitutive relationships that must be inferred from observational data, thus blurring the line between process-based and empirical models. Ubiquitous spatial heterogeneity in watershed processes commonly renders such parameters spatially variable and scale-dependent. Among process-based models, so-called lumped models use simplified governing equations without explicitly accounting for spatial variability in inputs and parameters. Examples include Stanford Watershed Model IV (SWM) (Crawford and Linsley, 1966), TOPography based hydrological MODEL (TOPMODEL) (Beven, 1997), Hydrologiska at Vattenbalansavdelning model (HBV) (Bergstrom, 1976), Hydrological Simulation Program FORTRAN (HSPF) (Bicknell et al., 1996; Duda et al., 2012). These models are easy to use and calibrate, computationally inexpensive, and most codes are open source. However, lumped watershed models can only simulate aggregated behaviors of a watershed system, for instance, the streamflow response at the watershed

outlet. Lumped models require long-term monitoring data for calibration, and their heavy reliance on calibration limits their applicability to extreme events that fall outside the range of historical observations.

Unlike the lumped models, process-based distributed models attempt to capture the spatial heterogeneity of system responses by using spatially-distributed parameters and inputs, while the set of governing laws/equations remain same for the entire domain, such as the shallow-water equations (Hirsch, 1988) and the Richards equation (Richards, 1931) for surface and subsurface flows, respectively. FLUX-PHIM-BGC (Shi et al., 2018) and RHESSys (Tague and Band, 2004) models are good examples for distributed watershed simulators that couple hydrologic process, surface energy flux, vegetation and nutrient dynamics. FLUX-PHIM-BGC was extended from PHIM (Qu, 2004), a distributed hydrologic model that simulates the water flux from surface and groundwater and its interaction and stream routing. Later, FLUX-PHIM (Shi et al., 2013) was developed to account for the spatial and temporal heterogeneity in surface energy balance. Finally, FLUX-PHIM-BGC was developed to account for vegetation dynamics and carbon/nitrogen cycling in soil and stream. In principle, a spatially discretized model of a system with spatially distributed parameters and inputs is expected to provide better predictions than its lumped counterpart. However, such distributed models also require significantly larger number of unknown model parameters to be specified or estimated. The parameter dimensionality could quickly become intractable when dealing with complex, coupled physical and biogeochemical processes over a large spatial domain. Consequently, the computational cost associated with parameter estimation for such high-dimensional, computationally expensive models has hampered the practical application of distributed watershed models (Pokhrel et al., 2008).

4.1. Watershed simulators

A number of watershed simulators have been developed for water quantity and quality modeling at the watershed scale (e.g. Daniel et al., 2011; Singh and Frevert, 2005; Wellen et al., 2015; Migliaccio and Srivastava, 2007; Moriasi et al., 2012; Devia et al., 2015; Elliot et al., 2010; Gao and Li, 2014). While it is beyond the scope of this review to provide detailed characterization of all available watershed models, readers are referred to previous review papers for more information (Wellen et al., 2015; Fatichi et al., 2016). Given the focus of this review on ecohydrological and biogeochemical processes, here we focus on watershed simulators that represent coupled vegetation, hydrology, and biogeochemistry in both land and river systems within a watershed context. Thus, some popular models are not included in our discussion because they do not simulate biogeochemical processes pertinent to water quality predictions, despite their wide use in watershed hydrologic modeling. Such examples include the Hydrologic Engineer Center's Hydrologic Modelling System (HEC–HMS), Topography Based Hydrological Model (TOPMODEL) (Beven, 1997), Variable Infiltration Capacity (VIC) model (Liang et al., 1994; Hamman et al., 2018), and the Distributed Hydrology Soil Vegetation Model (DHSVM) (Wigmosta et al., 1994) are not discussed.

Specifically, the watershed water quality models that are reviewed here include: the MIKE SHE (Système Hydrologique Européen) model (Ma et al., 2016; Jaber and Shukla, 2012), Hydrologic Modeling Fortran (HSPF) (Duda et al., 2012), Soil and Water Assessment Tool (SWAT) (Neitsch et al., 2011; Arnold et al., 1998; Gassman et al., 2007), Storm Water Management Model (SWMM) (Huber, 2003; Cambez et al., 2008; Rossman, 2010), Annualized AGricultural NonPoint Source model (AnnAGNPS) (Bingner et al., 2018; Yuan et al., 2001), Areal Non point Source Watershed Environment Response Simulation (ANSWERS) ANSWERS-2000 (Bouraoui and Dillaha, 1996), Watershed analysis risk management framework (WARMF) (Goldstein, 2001; Herr and Chen, 2012), Regional Hydro-Ecologic Simulation System(RHESSys) (Tague and Band, 2004), The Penn State Integrated Hydrologic model (PIHM) coupled with biogeochemcial processes (Flux-PIHM-BGC) (Shi et al., 2018). Based on the models reviewed in previous studies, as well as the models that have been identified as useful tools to support Total Maximum Daily Load (TMDL) analysis (Shoemaker et al., 2005; EPA, 2019), we summarize and compare key hydrological and biogeochemical processes represented by those simulators in Table 1.

As shown in Table 1, those popular watershed models vary widely in terms of process complexity and algorithms used to solve different processes. In general, all watershed models linked plant growth with hydrologic and water quality processes. Most of them used prescribed crop characters (e.g. Leaf Area Index – LAI), instead of explicitly simulating the dynamic plant growth processes. Simulators also have their unique development histories. Each simulator has distinct strengths in solving different problems owing to different assumptions that were made during the construction of various model architectures. Although SWAT dynamically simulates plant growth and development as regulated by climatic (e.g. temperature) and environmental (e.g. nutrients availability), its representation of forest growth processes are oversimplified (Yang and Zhang, 2016), making it unsuitable for simulating forest management. However, RHESSys (Tague and Band, 2004) included a carbon cycling model adapted from BioME-BGC (Thornton, 1998) with litter and soil organic matter decomposition and nitrogen cycling model (Parton et al., 1996) to simulate dynamic vegetation responses to climate, soil moisture and nitrogen conditions. Similarly, FLUX-PHIM-BGC (Shi et al., 2018) also can simulate the spatial and temporal variation of LAI across landscape by adapting carbon cycling module from BioME-BGC.

As to surface runoff, soil water, and ground water simulation, the existing models use very different approaches, ranging from empirical methods to physically based equations. Most models (except SWMM and MIKE-SHE and FLUX-PHIM-BGC) use Manning's equation or other simplified forms of the St. Venant equation rather than its dynamic wave version to improve computing efficiency. Among the 9 models, HSPF, SWAT, and WARMF explicitly represent soil N and P cycles and simulate reactive transport of N and P through channels, while other models use simplified approaches to simulate coupled land and channel cycling of water quality constituents.

We also review whether those simulators have been adapted to High Performance Computing (HPC) given the increasing complexity and computational demand of watershed models. Most of the simulators have not been adapted to HPC except for SWAT, RHESSys, FLUX-PHIM-BGC, and MIKE-SHE. RHESSys and FLUX-PHIM-BGC adopted the openMP library for paralell computing. MIKE-SHE, the only non-public domain simulator reviewed here, has implemented algorithms to leverage Graphical Processing Units (GPUs) in addition to central processing unit (CPU)-based parallelization. The channel routing component of SWMM has been parallelized to solve the Saint Venant equations. SWAT has multiple versions of parallization; for example, Wu et al. (2013) used Message Passing Interface (MPI) to parallelize the SWAT model, and Zhang et al. (2017) use OpenMP (Open Multi-Processing) to parallelize the gridded SWAT (SWATG) model. Although HSPF has not been parallelized yet, it can be run on linux clusters to facilitate parameter estimation in parallel mode. In general, models that offer a graphical user interface are not capable of code parallelization for shared and distributed memory platforms.

4.2. Emerging modeling trends, gaps, and challenges

Recently there has been growing emphasis on including integrated surface–subsurface flow, biogeochemistry, and land surface (including plants) processes to simulate watershed functions. To properly simulate the biogeochemical cycling of carbon, nutrients, and metals within the watershed systems, it is essential to couple integrated hydrological processes across the atmospheric upper boundaries to the bottom of bedrock with vegetation dynamics and mechanistic carbon/nitrogen cycling. Representing the increasing complexity of coupled processes using physics-based approaches are becoming more and more practical

Table 1
Key hydro-biogeochemical processes simulated in watershed water quality models.

Model	AnnAGNPS	ANSWERS-2000	HSPF	MIKE-SHE	SWAT	WARMF	SWMM	$RHESS_{ys}$	Flux-PIHM-BGC
Landuse (primary)	Agriculture	Agriculture	Multiple	Multiple	Multiple	Multiple	Urban	Multiple	Multiple
Vegetation	Crop growth	Crop growth	LAI	LAI and root depth	Biomass accumulation	Vegetation cover	Vegetation cover	Vegetation growth	Vegetation growth
Surface infiltration	SCS curve number	Green-Ampt equation	Philip equation	Richards equation	SCS curve number or Green-Ampt equation	SCS curve number	SCS curve number or Green-Ampt equation	Philip and Green-Ampt equations	Richards equation
Surface overland flow	SCS curve number	Manning and continuity equations	Chezy-Manning equation	Saint Venant equations	SCS curve number	SCS curve number	SCS curve number or Green-Ampt equation	Net detention storage	Saint Venant equations
Soil water infiltration/ drainage	Storage approach	Storage approach	Storage approach	Richards equation	Storage approach	Storage approach	Storage approach	Darcy equation	Richards equation
Subsurface flow	Darcy equation	Darcy equation	Empirical storage approach (lateral interflow and groundwater outflow)	Richards equation or linear storage approach	Kinematic wave storage model (lateral interflow) and linear storage approach (shallow groundwater)	Darcy equation	Darcy equation	Darcy equation (shallow groundwater) and linear storage approach (deep groundwater)	2D Dupuit approximation
Soil biogeochemistry	N, P, and C	N and P	N and P	User-defined pollutants	N, P, and C	N, P, and C	User-defined pollutants	N and C	N and C
Instream flow	Manning equation	Manning and continuity equations	Continuity equation and kinematic wave model	Saint Venant equations	Variable storage or Muskingum method	Manning and continuity equations	Saint Venant equations	Kinematic wave model	Saint Venant equations
Instream biochemical constituents	N, P, and pesticides	N and P	N, P, BOD, algae, and O_2	User-defined pollutants	N, P, BOD, algae, O_2, and pesticides	N, P, BOD, algae, and O_2	User-defined pollutants	N/A	N/A
Computing platforms	Windows	Windows	Linux[a,b] and Windows	Linux[a] and Windows[a,c]	Linux[a] and Windows[a,d,e]	Windows	Linux[a,f] and Windows	Linux[a] and Mac OS[a]	Linux,[a] Windows,[a] and Mac OS[a]

[a] Capable of high performance and parallel computing.
[b] Kim and Ryu (2019).
[c] Danish Hydrologic Institute (2019).
[d] Zhang et al. (2013).
[e] Rouholahnejad et al. (2012).
[f] Burger et al. (2014).

with dramatic advances in computing powers nowadays.

The response of water quality in receiving streams to any perturbation including extreme hydrologic events (perhaps occurring elsewhere in the watershed) and land use changes is shaped by many factors, including geology, topography, land use, and historic regimes of environmental conditions (e.g., climate and nutrient loading) in the watershed. These factors vary widely and nonlinearly across spatial and temporal scales, which make it difficult to model numerically. Hydrological events (Lu et al., 2017) and therefore reaction zones (McClain et al., 2003) can be highly localized in the watershed. An accurate characterization of watershed biogeochemistry must account for not only how hydro-biogeochemical processes are regulated within different localized landscape patches (e.g., in upland, riparian zone, and wetlands), but also how they interact as water travels through these often heterogenous patches (Laudon and Sponseller, 2018). Most existing watershed models do not dynamically link groundwater and surface water or consider the transition zones between these two water bodies. Moreover, the limited models to study hyporheic exchange and nutrient cycling often assume steady state and static pressure variations. However, anthropogenic activities are known to induce high-frequency variations that enhance the hydrologic exchange flows and the associated heat exchange and biogeochemical reactions (Shuai et al., 2019; Song et al., 2018), which have not been accounted for in existing watershed models.

Current-generation watershed water quality models do not fully incorporate emerging hydro-biogeochemical process understanding because of challenges associated with multi-scale heterogeneity, large spatial scale, and computational and characterization burdens. As a result, those models are of limited use for extrapolating from current environmental conditions to understand how watersheds will respond to land-use change and atmospheric perturbations. At the same time, there is still ongoing debate on how much complexity can be supported by data (Jackson-Blake et al., 2017). Most watershed water quality models (Kaushal et al., 2018a; Vidon et al., 2018) do not incorporate multi-component reactive transport, which limits their ability to accurately predict distinct mixtures of water quality constituents (Kaushal et al., 2018a) as a result of complex interactions between climate variability and human-dominated land use. The lack of biological and reactive transport processes in watershed models will likely lead to uncertainty and bias in predicting watershed C and N responses. The incorporation of fine-scale mechanistic understanding into a watershed biogeochemical model remains untested, but it has great potential predictive power to capture distinct water quality signatures and sources for multiple elements and chemical species across variations in land use, underlying geology, atmospheric deposition, and climate.

While hydrologic connectivity, flow path characteristics and distribution, and watershed transit times are key controls on watershed biogeochemical processes, suitable measures and model estimation procedures for these key variables, including the diagnosis of source area contributions (Hewlett and Hibbert, 1967), have not yet been devised and are lacking, especially regarding responses under extreme climate events. Subsurface flow and transport, a primary vector for water flow and material transformations in watersheds with long residence times, is often oversimplified in watershed models. It has been documented that no explicit representation of lateral flow, common in land-surface models, led to overly spiky behavior in watershed hydrographs (Clark et al., 2015a). Explicit representation of topology and subsurface transport pathways within models will lead to dramatic improvements in watershed-scale biogeochemical understanding and prediction.

Many existing watershed models are based on the assumption of stationary (Wagener et al., 2010); vegetation is static and the parameters of the model are constant over time, and the model parameters values calibrated with historical data are assumed to be valid under future climate conditions or altered watershed conditions. For example, rooting depth may change with climate conditions, but if vegetation parameters assumes to be static, the model may capture overestimate/underestimate of ET, depending on how rooting depth responds to the changing climate in reality. Another example is that fire may alter the hydraulic parameters with enhanced soil–water repellency and its changed magnitude may vary with the intensity of burn severity (Ebel and Mirus, 2014). The enhanced soil–water repellency may decrease with time. Therefore, the time stability of hydraulic parameters after fire events may not be valid. Since there are spatial variability of burn severity within the watershed, without explicitly accounting for the spatial–temporal variability of hydraulic variability, watershed model can not capture watershed responses to or after forest fires. Forest insect infestation may alter the flow paths (Ebel and Mirus, 2014); for example, decreasing of riparian forest with insect infestation may elevate the groundwater table in the riparian zone that results in generating more surface saturation excess flow, and increasing the nutrient exports (DOC and nitrate,etc) to stream. The challenge of modeling the impact of forest insect infestation is that there will be a time gap between response of elevated groundwater table and insect infestation. Therefore, in order to capture watershed responses to disturbance, model should explicitly incorporate the interacted processes (e.g. vegetation responses to warming or deficit of key nutrients (nitrate and phosphorus, etc.), and model should have capability of incorporating the altered processes after disturbance (fire, and insect infestation).

Scaling remains as a persistent challenge in watershed hydrology and biogeochemistry (Blöschl and Sivapalan, 1995; Scheibe and Yabusaki, 1998; Bras, 1999; Das and Mohanty, 2008; Li et al., 2008b; Crow et al., 2012; Gentine et al., 2012; Arora et al., 2015; Dwivedi et al., 2016a; Dwivedi et al., 2016b; Dwivedi et al., 2017; McDonnell et al., 2007), partially due to the intrinsic complex nature of the coupled processes and the computational tractability to capture enough complexity in reality. High-resolution watershed models are computationally expensive and require boundary conditions and forcings defined at the corresponding resolution to capture the nonlinear behavior. In contrast, coarse-resolution watershed models are computationally more affordable but do not adequately resolve finer-scale heterogeneity; thus, they are likely to misrepresent critical processes. Ideally, multi-scale process representation can be a way to demonstrate the ability of watershed models to reproduce processes across scales. Integrating multi-scale information into models will reproduce processes at their native resolutions, which can be a viable strategy for circumventing downscaling/upscaling needs. It is important to note that the term "scaling" has several uses, such as the estimation of intervening values from sparse data, aggregation or disaggregation of information by taking areal averages, and information transfer from small to larger areas (Western et al., 2002). Upscaling permeability presents such an example, where point scale measurements are used to infer effective permeability values at different scales. To illustrate further, the Richards equation was derived to represent the column-scale water movement, and it is used in several watershed simulators, as described in Section 4.1. Although these simulators are still useful at the watershed scale, scale-dependent parameters are required for acceptable functional behavior (Western et al., 2002).

The literature contains several different approaches to link parameters and state-variables across different scales (Blöschl and Sivapalan, 1995). In this context, the Miller–Miller similar media theory has been widely used to scale soil hydraulic properties as well as flow and transport equations (Miller and Miller, 1956; Sadeghi et al., 2016). Other researchers subsequently developed techniques to derive effective hydraulic properties using stochastic, fractal, or scaling invariant approaches (Russo, 1993; Mohanty et al., 2000; Rodriguez-Iturbe et al., 1998). These techniques have also been used to understand the scaling characteristics of other hydrologic aspects such as drainage patterns, stream networks, and topography (Gupta and Waymire, 1990; Sivapalan et al., 2011). The extension of the Miller–Miller similar media theory is the representative elementary area/watershed and Reynolds' averaging concepts, assuming that the physics are known at the smallest scale

considered. These concepts have primarily been used to define the physically meaningful control volumes at which hydrologic processes operate and give insights into understanding large-scale processes (Wood et al., 1988; Reggiani et al., 1998; Reggiani et al., 1999; Reggiani et al., 2001). The representative hillslope is an example of one such meaningful control volume in watershed science, which has been widely used to understand precipitation runoff, infiltration, and other key hydrologic processes (Troch et al., 2003; Troch et al., 2015; Hazenberg et al., 2015; Hazenberg et al., 2016). Biogeochemical scaling is still in its infancy. There are a few examples that have used dimensionless numbers (e.g., Damköhler numbers), Bayesian methods, and scale-dependent rates to upscale geochemical concentrations and fluxes (Gu et al., 2007; Li et al., 2008b; Arora et al., 2015; Dwivedi et al., 2016b). However, we will conclude here by mentioning that hydrologic processes mediate biogeochemical processes; therefore, resolving hydrologic scaling should be key in efforts to address biogeochemical scaling issues.

Despite of insights offered in the literature, the fundamental problem remains the limited predictive understanding of hydrobiogeochemical systems at the watershed scale due to the lack of a unifying theory of hydrologic scaling. In fact, there may not exist any single universal relationship of hydrologic processes, given the inexact nature of hydrologic science (Blöschl and Sivapalan, 1995; Beven, 2006). Notwithstanding these issues, it is possible to develop scaling laws or strategies to enhance predictive capabilities using watershed models. Here we want to identify key issues related to distributed parameter models and give directions for future research.

5. Watershed model and data integration

Extensive efforts have enhanced the mechanistic foundation of process-based watershed models in capturing interacting physical and biogeochemical processes while also making them spatially distributed to represent the spatial heterogeneity in parameters and inputs (Wellen et al., 2015). The development of increasingly mechanistic models is accompanied by concerns of overparameterization, equifinality (Jackson-Blake et al., 2017; Beven and Binley, 1992; Beven, 2006), and difficulties in estimating valid, spatially-distributed model parameters and driving forces (Kollet and Maxwell, 2008; Samaniego et al., 2010; Montanari and Koutsoyiannis, 2012; Raleigh et al., 2015; Raleigh et al., 2016). Some inputs (forcing and parameters) can be determined through direct observations in the field, whereas others are inversely estimated using the input–output records of the watershed. The best practices are recommended to include sensitivity analysis, optimization/calibration, validation, uncertainty analyses, and quantification of fit (Chapra, 2008). However, the increasing computational cost of high-resolution mechanistic watershed models inhibits the broad community from following the best practice to improve process-based models. It is an even bigger challenge for models targeting the watershed responses under extreme events (Wellen et al., 2015). Most model calibration practices often rely on single-point, sparse time-series observations (Wellen et al., 2015; Robson, 2014), which does not account for all the information that is contained in spatiotemporal observation data, and at the same time, it could lead to preference over simpler models. Considerable uncertainty exists in conceptualizing (i.e., selecting processes and their associated mechanisms for all the compartments and interfaces and parameterizing a process-based watershed model (McDonnell et al., 2007; Duncan et al., 2013). A multi-model approach called the Structure for Unifying Multiple Modeling Alternatives (SUMMA) (Clark et al., 2015a; Clark et al., 2015b) framework has been explored for hydrologic models (Clark et al., 2015a; Fenicia et al., 2011; Clark et al., 2008) to evaluate various conceptualization decisions in a systematic and controlled way. By doing so, modelers can select among multiple alternatives to improve model fidelity and pinpoint specific reasons for model weaknesses to prioritize research and development needs.

It is recently argued that the success of data-driven machine learning methods relative to process-based modeling indicates that there is unused information in observation data (Nearing et al., 2018). A more rigorous way of dealing with uncertainty is to pose it in terms of information, i.e., asking the questions of "how much information do we have and how well do we use it? (Nearing et al., 2018)" In this context, improving a model is about assimilating information (or learning) from both observations and models, thus establishing a theoretical linkage with the Bayesian learning based on the Bayes' theorem. Using a Bayesian learning framework, classical questions in watershed modeling such as scaling, heterogeneity, and complexity can all be posed in terms of information and learning.

Sensitivity analysis is a vital tool in numerical modeling for quantifying contribution of uncertainty from various sources to the overall uncertainty in model predictions (Dai et al., 2017a; Dai et al., 2017b; Razavi and Gupta, 2015; Gupta and Razavi, 2018). Conventional global sensitivity analysis methods (Saltelli et al., 2000; Chu-Agor et al., 2011; Song et al., 2015) focus on the importance of model parameters. They are insufficient for identifying dominant model processes, each of which usually consists of multiple parameters (Clark et al., 2015a; Clark et al., 2015b). Process-oriented sensitivity analysis has gained increasing attention for improving hydrological models and beyond (Dai et al., 2017b; Sivakumar, 2004; Sivakumar, 2008). A recent advancement in sensitivity analysis is to quantify uncertainty contribution from multiple, spatially-distributed model inputs using a simple, three-layer structure of uncertainty: model parameters, model structures, and forcing scenarios. Recognizing that a three-layer structure is too restrictive to describe the large number of uncertainty sources involved in multi-process environmental modeling and their complex relationships, a new sensitivity analysis method was developed based on the concepts of Bayesian networks (BNs) (Heckerman, 1997; Velikova et al., 2014; Pearl and Judea, 1988) to account for the complex hierarchical uncertainty structure of a model system (Dai et al., 2019). This BN-based sensitivity analysis method uses a graphical representation to propagate uncertainty with Bayesian inference, i.e., deriving joint probabilities. It affords substantial flexibility to quantify uncertainty contribution from a group of inputs, which is not possible without BN.

Transformational advances in watershed modeling capabilities are facilitated in part by dramatic increases in the amounts, quality, and coverage of relevant observational data, but new challenges exist in harnessing big data (Uddameri, 2018; Rosenberg and Madani, 2014). Importantly, coordinated efforts by many governmental agencies over the past few decades have resulted in widely available datasets with extensive or even seamless spatial coverage. In the United States, data availability and interoperability have been advanced through a number of initiatives. The U.S. Office of Management and Budget published Circular A-16 in 2002, which "provides direction for federal agencies that produce, maintain, or use spatial data either directly or indirectly in the fulfillment of their mission and provides for improvements in the coordination and use of spatial data." Further coordination was spurred by the U.S. Office of Science and Technology Policy (Subcommittee on Water Availability and Quality) through the Open Water Data Initiative started in 2014 (Bales, 2016; Maidment, 2016). These coordinated efforts over the past two decades have led to critical data products such as the National Hydrography Dataset (NHD), the Watershed Boundary Dataset (WBD), and NHDPlus (an enhanced version of NDH). Fatichi et al. (2016) describe several other sources of freely-available internet-accessible spatial datasets including soil survey, precipitation, meterological forcing, river morphology and hydrogeologic property data. Remotely-sensed data such as those provided by NASA's Earth Observing System (https://eospso.nasa.gov/content/nasas-earth-observing-system-project-science-office) further expand data types to include vegetation and land use/land cover, soil moisture, changes in groundwater levels, and many others.

Work is ongoing not only to increase data availability, but also to break down barriers to effective use of these data in model development.

A key challenge is posed by the diversity of data formats, locations, and modes of access, which often requires a large time investment in data compilation and formatting during model construction. Efforts to address this challenge include development of standardized data models (Hu et al., 2015; Abdallah and Rosenberg, 2019), open source tools for data retrieval and preprocessing such as HydroDesktop (Ames et al., 2012), HydroShare (Horsburgh et al., 2016) and the Observatory for Gridded Hydrometeorology (Phuong et al., 2019), and methods for linking Geographical Information Systems (GIS) with process-based models in loosely-coupled (Alcaraz et al., 2017), tightly-coupled (Bhatt et al., 2014), and seamlessly-coupled (Wang et al., 2016) approaches.

These advances not only enable better and more efficient development of process-based distributed hydrologic models, but also can lead to enhanced collaboration (Bandaragoda et al., 2019), improved reproducibility of published results (Stagge et al., 2019), and broader adoption of open science in practice (Yu et al., 2016). Automated model setup and execution based on open data, while necessarily subject to careful evaluation, could dramatically increase model accessibility and is moving from vision to reality (e.g., Starn and Belitz, 2018; Lewis et al., 2018).

6. Going forward: Systematic extraction of information from both observations and modeling for learning watershed systems to reduce uncertainty

Bayesian Networks possess great potential to unite data-driven and process-based modeling approaches to identify and extract the most useful information out of observational data and predictive models. The new BN development, combined with the wide adoption of Bayesian-based inverse modeling, parameter estimation, data assimilation, and model diagnosis (Rubin et al., 2010; Chen et al., 2013; Chen et al., 2012; Nearing et al., 2018; Liu and Gupta, 2007; Gupta et al., 2008; Over et al., 2003; Simmons et al., 2016; Ye et al., 2004; Joseph and Guillaume, 2013; Gelman et al., 2014; Nearing et al., 2016), suggests a new and potentially powerful Bayesian framework can be built to unite sensitivity analyses, data assimilation, inverse modeling, and model intercomparison/diagnosis under the Bayesian theory for systematic data-model fusion under both data and model uncertainty. BN will allow the integration of deep learning methods (Sun et al., 2019; Sun, 2018; Shen, 2018; Gentine et al., 2018; Reichstein et al., 2019) to discover unknown physics where process understanding is lacking. Such a framework for data-model fusion will advance the fundamental understanding of hydro-biogeochemistry in watershed systems by iteratively asking questions like "What do we know about the system; How well are we translating that knowledge into predictive power; and How can we be more predictive?" and answering them with integrated sensitivity analyses, data assimilation, and mutual information analyses. Such systematic learning from data and models will not only lead to a new modeling capability for forecasting water quality and quantity in watersheds of various scales and land use patterns; it can also guide design of monitoring networks and experiments to collect the most valuable information to reduce uncertainty in predictive models. Ultimately, the data-model integration will link best-in-class modeling capabilities with the multi-agency long-term monitoring efforts to meet society's needs under a changing environment, thus providing transferable scientific tools to help manage vital watershed systems for sustained water security and human and ecosystem health.

6.1. Opportunities for data-model co-design

There are many paths forward for future integration of more and better data into process-based numerical models. One is the collection and analysis of isotope data. Historically, isotope hydrologists utilized environmental and artificially labeled radioactive isotopes (e.g., Ra, ^{3}H, ^{14}C, ^{24}Na, ^{82}Br, and ^{32}P) to measure physical processes, such as stream discharge, groundwater direction, velocity, and age, and sediment loading at the reach or regional/aquifer scale (Joly, 1922; Agency, 1963; Agency, 1967) before broadly switching to utilizing conservative transport of stable isotopes (e.g., ^{2}H, ^{18}O, and ^{13}C) to infer other things, such as flow path characteristics (Klaus and McDonnell, 2013), water transit times (McGuire and McDonnell, 2006), weathering (Schulte et al., 2011), and water (Agency, 1970) and carbon (Dawson and Simonin, 2011) balances at the watershed scale. More recently, reactive transport of stable isotopes of nitrogen (^{15}N) and phosphorus (^{18}O in PO_4) have been utilized to identify non-point sources of anthropogenic N (Fry, 1999; Lake et al., 2001; Spoelstra et al., 2001; Robinson, 2001; Mayer et al., 2002; Zanden et al., 2005; Kendall et al., 2008; Savard et al., 2010; Nestler et al., 2011; Kaushal et al., 2011) and P loading (McLaughlin et al., 2006; Elsbury et al., 2009; Paytan and McLaughlin, 2012; Granger et al., 2017; Tonderski et al., 2017; Ishida et al., 2019), and, later, elucidate specific biogeochemical processes, such as dilution (Archana et al., 2018), nitrogen assimilation (Deutsch et al., 2009; Nikolenko et al., 2018), denitrification (Wexler et al., 2014), phosphorous release from anoxic sediments (Elsbury et al., 2009), and cellular metabolism in aquatic food webs (Davies et al., 2014) at various spatiotemporal scales.

Now, isotope data are increasingly coupled with or incorporated into numerical models, which further augment the ability of these models to simulate complex physical processes with high precision. Such processes include groundwater flow dispersion (Cornaton et al., 2011; Jiang et al., 2019), preferential flow partitioning (Van der Hoven et al., 2002; Dusek and Vogel, 2018), surface/subsurface water mixing (Turner and Townley, 2006), nitrification and denitrification (Choi et al., 2003; Chen and MacQuarrie, 2004; Rütting and Müller, 2007), and anammox (Granger and Wankel, 2016). The use of chemical and isotopic tracers has moved out of the field of chemi-hydrometry (Groat, 1915) to isotope hydrology (Agency, 1970) to hydrogeology and geochemistry (Agency, 1974), and now, to hydro-biogeochemistry and process-based numerical modeling. Watershed modelers will continue to require more isotope data to feed into their models and many current monitoring networks serve as suitable infrastructure for collecting such data.

On the other hand, remote sensing (RS)–in the context of watershed science–is the science and art of acquiring information about the land surface and subsurface or physical processes using remotely located sensors Ritchie and Rango, 1996. A diverse set of RS techniques exist to collect above- and below-ground data. RS relies on active and passive sensing technologies. Active sensors emit energy to examine part of the watershed (i.e., target), while passive sensors detect the radiation emitted from the target. After acquiring signals, various algorithms have been developed to translate them into surface and subsurface properties as well as hydrological and biogeochemical variables. The quality of RS data depends on its spatial, temporal, and spectral resolutions. More information about RS can be found in the literature Arora et al., 2019; Entekhabi et al., 2010; Fonstad et al., 2013; Li et al., 2008a; Turner et al., 2004; Zhang et al., 2003. RS provides a means to acquire spatial data and characterize their heterogeneity at the watershed scale. On the contrary, conventional methods are primarily limited to point measurements and incapable of providing adequate data to represent the heterogeneity of the land surface and subsurface properties reasonably. Therefore, the use of RS data has the potential to transition data-poor to data-rich environments needed for advancing watershed science. The use of RS in hydrology is not new, and its potential was revealed very early. In 1965, Walter Langbein, a pioneer of watershed science, advocated for the use of satellite platforms for acquiring hydrologic data, while RS techniques could measure soil temperatures, water vapor, and radiation using aircraft platforms (Langbein, 1965). Ragan and Jackson (1980) subsequently used curve numbers and land use mapping (Landsat product) to quantify runoff (Ragan and Jackson, 1980). More notably, Beven and Kirkby (1979) demonstrated the importance of topography in predicting runoff using digital elevation maps. Since then, numerous articles published in the literature have used RS products to

describe and characterize different aspects of watershed science, such as soil moisture, surface temperature, landcover/vegetation, precipitation, snow depths and cover, and groundwater (Fonstad et al., 2013; Hutengs and Vohland, 2016; Li et al., 2008a).

We can now see every component of the water cycle remotely: precipitation, snow, evapotranspiration, surface soil moisture, deep groundwater, and river discharge (e.g., Andreadis et al., 2017). For rainfall, the Tropical Rainfall Measuring Mission (TRMM) at the turn of the millennium (Kummerow et al., 1998) eventually evolved into the Global Precipitation Measurement (GPM) constellation (Smith et al., 2007); CloudSat has also provided complementary measurements of precipitation (Stephens et al., 2002). We have been able to see snow cover from the MODerate resolution Imaging Spectroradiometer (MODIS), with approaches to derive snow water equivalent (SWE; Hall et al., 2002); airborne capabilities such as the Airborne Snow Observatory (ASO) can assess SWE with high fidelity using LiDAR and can complement the snow depth measurement with albedo used for melt rates (Painter et al., 2016). Evapotranspiration has been derived from Landsat, the Advanced Very High Resolution Radiometer (AVHRR), and MODIS for decades (Fisher et al., 2017), and the ECOsystem Spaceborne Thermal Radiometer on Space Station (ECOSTRESS) on the International Space Station was designed specifically to focus on evapotranspiration at very high spatial and temporal resolutions (Fisher et al., 2019). A snapshot example of evapotranspiration over the Columbia River Basin in the US is shown in Fig. 2.

The Soil Moisture Observing System (SMOS) and Soil Moisture Active Passive (SMAP) missions have provided global coverage of surface soil moisture (Kerr et al., 2001; Entekhabi et al., 2010); airborne measurements provide increased depth and canopy penetration (Colliander et al., 2017). The change in deep groundwater storage can be derived through gravity-based measurements of total water storage from the Gravity Recovery and Climate Experiment (GRACE) and GRACE Follow-On (GRACE-FO) missions (Rodell and Famiglietti, 2002; Sheard et al., 2012); global positioning systems (Argus et al., 2014) and measurements of surface deformation (Farr and Liu, 2014) can also be used to derive changes in groundwater. Finally, LiDAR can be used to measure river (and lake, reservoir, and ocean) heights, which can be used to infer river discharge; the airborne Surface Water and Ocean Topography (AirSWOT) has established the foundation for the upcoming satellite SWOT mission (Durand et al., 2010). Space agencies throughout the world continue to develop new missions to advance remotely sensed hydrological measurements, and the future will contain an even richer assessment of the hydrological cycle from space (National Academies of Sciences, 2018).

Although RS products are currently primarily used to characterize watershed properties for hydrologic processes, efforts are underway to derive biogeochemical properties (e.g.leaf chemistry) based on geomorphology and vegetation characteristics using hyperspectral data (Falco et al., 2019) as well as to understand the subsurface physical properties of the watershed using airborne electromagnetic (AEM) survey (Hubbard et al., 2018). Overall, RS promises massive data on every aspect of watershed science. A fusion of distributed hydrologic models and RS will take watershed science to the next level in the future.

Additionally, US DOE's Biological and Environmental Research (BER) office manages unique user facilities that can generate genomics and molecular-level data that are highly relevant to understand watershed biogeochemical processes. For example, Joint Genome Institute (JGI) (https://jgi.doe.gov/) focuses on generating data from nucleic acid (DNA, RNA) sequencing and analysis that are used to support BER missions in biogeochemistry, carbon cycling, and bioenergy. Particularly relevant to watershed hydro-biogeochemistry is JGI's focus on using sequence-based data to understand biological mechanisms that influence biogeochemical processes, which in turn control the cycling of carbon and nutrients through environmental systems. JGI has a heavy

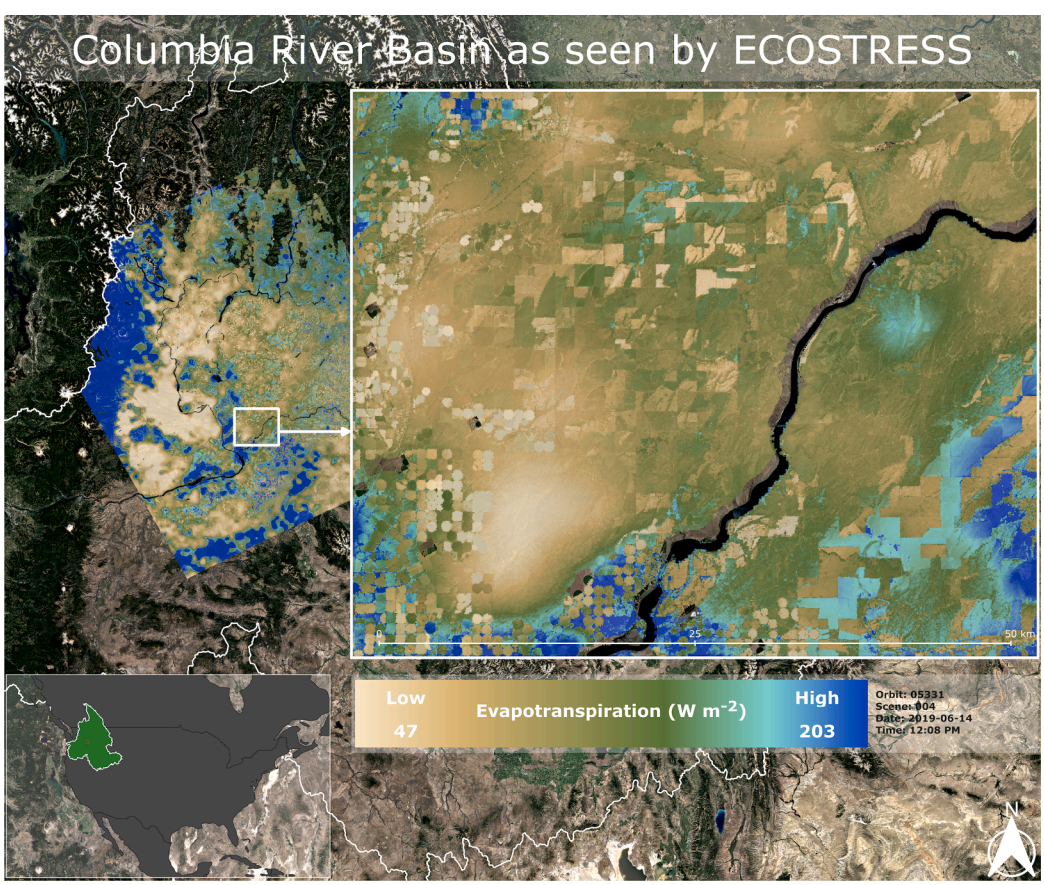

Fig. 2. Evapotranspiration over the Columbia River Basin in the US from ECOSTRESS. The data show variability across the basin as well as fine-scale heterogeneity (70 m resolution) associated with landscape fragmentation and agricultural water use. Blue colors indicate high evapotranspiration (W m^{-2}) at the time of overpass (12:08 PM local time on June 14, 2019), and beige colors indicate low evapotranspiration. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

emphasis on interrogating microbial communities from natural systems, in context of associated physical and chemical processes, due to microbes acting as essential catalysts driving C and nutrient cycling. Sequence data are generated from a broad range of environmental systems, spanning terrestrial, subsurface, and inter-facial components of watersheds. Ultimately, data generated by JGI are meant to help improve mechanistic models aimed at predicting the effects of environmental disturbances, such as hydrologic disturbance (e.g., drought, flood, altered snow pack) and increasing greenhouse gas concentrations. Similarly, Environmental Molecular Science (EMSL) user facility (urlhttps://www.emsl.pnnl.gov/) aims to lead the scientific community in gaining predictive understanding of molecular processes that control the flux of materials underpinning biological and ecosystem functions. Watershed biogeochemistry is an important aspect of this scientific vision. EMSL maintains relevant integrated research platforms in (1) plant, soil and subsurface transport; (2) Isotopic and chemical analysis; (3) proteomics, metabolomics and transcriptomics; and (4) theory and simulation, data analytics and visualization. As DOE user facilities, both JGI and EMSL provide no-cost access their extensive array of instrumentation and staff expertise through a competitive, peer-reviewed proposal process. At the same time, DOE-BER has also has invested substantially in building an open-source software and data platform, Systems Biology Knowledgebase (KBase, http://kbase.us), to enable data sharing, integration, and analysis of microbes, plants, and their communities (Arkin et al., 2018). KBase consolidates information from a variety of widely used external data repositories, including more than 30,000 reactions and compounds from KEGG (Kanehisa and Goto, 2000), BIGG (Schellenberger et al., 2010), and MetaCyc (Caspi et al., 2006). KBase provides a web-based user interface that allows users to easily link these diverse data types with a range of analytical functions. Thus, it serves as a much-needed community resource to foster open collaboration and enable large-scale analyses on scalable computing infrastructure and consequently accelerate scientific discovery with improved reproducibility.

While data generating capabilities continue to expand, as summarized above, the vast majority of these efforts do not use models to guide their design and implementation. There are significant opportunities to optimize additional data generation by explicitly using model-generated hypothesis and model-based uncertainty and sensitivity analyses to guide the types of data generated, their spatial distribution, and temporal resolution. This is the spirit of model-experiment iteration or 'ModEx.' For example, recent field and lab-based efforts pointed to important biogeochemical influences of organic matter thermodynamic properties within river corridors (Stegen et al., 2018; Graham et al., 2018; Graham et al., 2017; Garayburu-Caruso et al., 2020; Boye et al., 2017). Many of these studies were in aerobic systems, in which thermodynamics has not been considered to play a role (Jin and Bethke, 2003). That deviation from theoretical expectation prompted the development of new theory that mechanistically links thermodynamic aspects of organic matter to catabolism and anabolism (Song et al., 2020). These new theoretical developments point to a key parameter, referred to as lambda, that reflects the efficiency of converting the energy gained from organic matter oxidation into microbial biomass and, in turn, biogeochemical reaction rates (Song et al., 2020). The development of this 'lambda theory' has inspired the search for spatial and/or temporal patterns in lambda across river corridors. More specifically, data from a 2019 sampling campaign organized by the WHONDRS consortium (Stegen and Goldman, 2018; Consortium, 2020) and carried out by the community are currently being explored for continental- to global-scale spatial and/or environmental gradients in lambda. It is expected that resulting knowledge will be used to develop mechanistic models across river corridors using tools provided by KBase. Those models can then be used to generate new hypotheses about the drivers and influences of spatiotemporal variations in lambda and other aspects of organic matter chemistry, among other mechanisms such as microbial physiology. We are in the midst of what will likely be a long-term iteration between models and data in which one inspires the next step for the other. It is important that the watershed science community work together to find ways to expand the use of ModEx at a broad range of spatial and temporal scales.

6.2. Incorporating reactive transport capabilities in watershed models

The incorporation of fine-scale mechanistic understanding into a watershed biogeochemical model has the great potential to enhance model predictive power to capture distinct water quality signatures and sources for multiple elements and chemical species across variations in land use, underlying geology, atmospheric deposition, and climate. New capabilities are needed to couple the reactive transport codes with integrated hydrologic simulators, such as WRF-Hydro (Barlage et al., xxxx), Parflow-CLM (Maxwell et al., 2015; Maxwell and Condon, 2016), and CLM-PFLOTRAN (CP1.0) (Bisht et al., 2017). Subsurface reactive transport simulators have improved notably in capability and ease of use in the past decade (see Table 3 in (Steefel et al., 2015)). Most of them employ an operator splitting approach to solve reaction and transport terms, an approach in which a single time step consists of a transport step followed by a reaction step using the transported concentrations. This is in opposition to the global implicit approach in which reaction and transport are solved simultaneously. The global implicit approach is difficult for multicomponent and multispecies systems because the coupling of species via reactions increases the size of the coefficient matrix and also typically results in sets of nonlinear equations which must be solved. While reactive transport modeling is currently more prevalent in subsurface science, it is possible to couple the biogeochemistry engines, such as PFLOTRAN (Hammond et al., 2014) and CRUNCH (Steefel et al., 2015), with surface flow and transport. In addition, temperature is not only an important water quality parameter in itself, but also controls biogeochemical reactions in all compartments of the watershed system. Therefore, coupling thermal processes with reactive transport processes is also highly desirable.

One essential step in modern reactive transport modeling is to construct the reaction networks and the associated reaction kenetics. Metagenomic information can be used to generate metabolic pathways leveraging the community resources made available through the aforementioned KBase. High resolution molecular data (microbial and biogeochemical) are implicitly represented in many reactive transport and process-based models of watershed compartments but are rarely explicit. Such implementations rely on these data types to inform conceptualizations of model structures and/or to represent select biogeochemical reactions. Despite computational challenges in incorporating high resolution molecular data into watershed-scale models, the theoretical basis for doing so is strong. Many biogeochemical processes are catalyzed by microbial enzymes, and therefore molecular information on microbiome structure (i.e., species composition and distribution of enzyme-encoding genes) and metabolomes (i.e., reactants and products) should correspond to biogeochemical process rates (Rocca et al., 2015). Changes in microbiome in turn impact resource availability for food webs, therefore generating cascades effects at the watershed-scale (Graham et al., 2019). Additionally, ecological theory poses many circumstances under which molecular data types should be decoupled from prevailing environmental conditions (e.g., stochastic assembly, phenotypic plasticity, and priority effects; DeWitt et al., 1998; Hubbell, 2001; Fukami et al., 2010; Stegen et al., 2012; Nemergut et al., 2013; Graham et al., 2016), thereby providing predictive power to process-based models beyond hydrologic and chemical variables alone. Indeed, a recent metanalysis showed that statistical models of biogeochemical rates that were based solely on environmental parameters left 44% of variation unexplained on average, posing the opportunity for molecular data to improve predictive power (Graham et al., 2016).

Molecular data may also provide valuable insight for streams and rivers in which continuous monitoring of hydrobiogeochemical attributes is unfeasible (Seibert and McDonnell, 2013; Good et al., 2018).

Studies have coupled stream microbiomes to basin hydrogeomorphology (Read and Vogel, 2015), flow rate (Crump and Hobbie, 2005; Doherty et al., 2017), and other catchment characteristics (Savio et al., 2015). Good et al. (2018) recently introduced the concept of genohydrology, which proposes that microbial gene fragments can be used to gap fill for unmeasured variables in predicting river corridor hydrologic function. Thus, there is ample opportunity to improve predictive models by incorporating molecular data streams. Recent modelling advances have attempted to do so, but there has been no conclusive evaluation of the circumstances under which high resolution molecular data are needed to improve model predictions. Overall, high resolution molecular data can be extremely valuable in predictions of watershed function but only in certain environmental contexts and spatiotemporal scales. Coarser, less computationally intensive models may be suitable for a substantial portion of conditions. Therefore, new emerging modelling frameworks should provide flexibility in model structure to account for situational molecular data within watershed scale models.

The incorporation of high-resolution carbon (C) characterization into watershed models is an emerging field and deserving more attention. Carbon is the primary energy source for biogeochemical reactions and aquatic food webs in watersheds. Size and chemical speciation of C pools are coupled to watershed hydrology as well as C source (e.g., surface vs. groundwater, terrestrial vs. aquatic; Stegen et al., 2016; Graham et al., 2017; Maavara et al., 2017; Wohl et al., 2017; Graham et al., 2018; Stegen et al., 2018). Recent field-based observations have suggested that hyporheic zone respiration is tightly correlated to the presence of both thermodynamically-favorable C (Stegen et al., 2018) and organic N (Graham et al., 2017; Graham et al., 2018). Laboratory investigation further revealed that interactions between C thermodynamics, C stoichiometry, and whole sediment nutrient status regulate respiration rates. Similar dynamics have been observed in anaerobic redox conditions in wetlands (Boye et al., 2017; Boye et al., 2018). Carbon chemistry is spatiotemporally variable within watersheds and therefore is a prime candidate for enhanced predictive power from the inclusion of molecular data in watershed models. For instance, elevated river stage washes terrestrial C into surface waters (Golladay et al., 2000; Atkinson et al., 2009), changing the ratio of terrestrial-to-aquatic material and the associated C chemistry of aquatic C pools. Conversely, low stage creates patchy changes in biogeochemistry associated with groundwater discharge (Dent and Grimm, 1999; Dahm et al., 2003). While linkages between hydrology and C pool character have been studied extensively, subsequent impacts on watershed biogeochemistry are not well-understood. Given recent research demonstrating the impact of C chemistry on biogeochemistry across a range of oxygen concentrations and the heterogeneous nature of C pools through space and time, we highlight high resolution molecular data describing C chemistry as a promising avenue for watershed model development. We propose that molecular measurements and experiments need to be targeted in such a way that they are also useful for evaluating which types of data are useful and under what conditions.

To address complex multiscale watershed challenges, we need to integrate modeling advances that generally happen in parallel across a disconnected software ecosystem. Current approaches for hydrobiogeochemical modeling can involve a broad range of modeling platforms spanning from pore-scale reactive transport codes to reach-scale hydrobiogeochemistry models, particle tracking, and watershed- and hillslope-scale flow models. Unfortunately, the historical development of these tools has been siloed, with domain experts developing models that are focused on specific processes or spatial scales of interest. The result is our current disconnected ecosystem of modeling tools, which often have overlapping capacities but limited ability to communicate with one another or leverage each other's strengths. This landscape has evolved from lack of coordination between different modeling communities, which may have historically worked in isolation but are increasingly collaborating as we adopt an integrated approach to hydrobiogeochemical systems. Additionally, domain scientists are generally not trained in computer science and may have limited or no formal training in best practices for agile software development. Moving away from this paradigm will require software interfaces that facilitate process sharing between models without inhibiting the model-specific advances that are needed to improve process representation at every scale. Workflows are also needed that allow users to more efficiently learn new tools and leverage the results from existing models, which may be outside their domain specialty.

7. Summary and conclusion

The success of the aforementioned proposed advances in watershed science will depend critically on the utility of future models, which in turn will depend on their accessibility to other users. Given the inherent complexity of watershed models and the substantial effort required to learn how to use them, watershed models should be developed with the Earth science community, and perhaps beyond, in mind. In addition to providing source code and documentation of data, model developers are encouraged to work under the Open Science concept by following the "PLUS" guideline (Yu et al., 2016), making a model structure Persistent (i.e., data, software, and authors should be persistently identifiable through digital object identifiers, for example), Linked (i.e., data and software should be linked with figures and directions referring to each other, for example), User-friendly (i.e., software and documentation should be written with a broad audience in mind), and Sustainable (i.e., software should be maintained at repositories so that access and further development are possible) (PLUS). Additionally, model packages should include documentation of the workflow in order for a novice to use it completely (Yu et al., 2016). Tools for such documentation include Jupyter Notebooks, which provides a platform for written documentation, executable code, and data visualization (Fienen and Bakker, 2016; White et al., 2016).

Beyond model accessibility, there is a need to couple open science principles/methods across both data generation and modeling with coordinated research efforts that span multiple watersheds. Coordination across watersheds that vary in physical, chemical, and biological attributes is essential to elucidate transferable principles. Such principles can be used to develop simplified representations of governing processes to gain computational efficiency in larges-scale models. To identify challenges, opportunities, and solutions to achieve open, coordinated multi-watershed science, the DOE BER program has worked with the watershed science community to develop the concept of 'open watershed science by design.' The vision is captured in a recent workshop report (https://doesbr.org/documents/Open_Watersheds_By_Design_DRAFT.pdf) and is based on the purposeful design of watershed science efforts that ascribe to a set of key principles. In addition to the PLUS guidelines summarized above, open watershed science by design is based on ICON-FAIR principles. ICON research is (1) Integrated whereby data generation and modeling activities are designed from the beginning to link physical, chemical, and biological data and processes, (2) Coordinated using consistent protocols from field to lab to analysis/modeling, (3) Open such that data and codes are intentionally structured to be findable, accessible, interoperable, and reusable (FAIR) (Wilkinson et al., 2016), and (4) Networked whereby data generation and sample collection are designed with and done by the watershed science community such that resources (e.g., data and sensors) are provided to contributors that would otherwise be difficult to access.

Key to ICON-FAIR research is the use of design thinking methodologies to enable innovative solutions to challenges such as governance, protocol development, resource distribution, data-model integration, and the protection of individual researcher identity. Many of the challenges with open science in general and ICON-FAIR research in particular are technical, but others are cultural and institutional. There is a need for both top-down and bottom-up solutions. For example, some of the top-down solutions include (1) funding agency requirements for and

quantitative evaluation of making data FAIR and codes PLUS, (2) sustained investment in new cyberinfrastructure that streamlines the processes of making data FAIR and integrating those data with process-based and data-driven models, and (3) institutional change in how researchers are evaluated, with greater weight given to open data and code products. Bottom-up solutions to achieve broad adoption of open science and ICON-FAIR research are very diverse such as (1) education on the benefits to individuals of making their data open (e.g., more citations), (2) senior researchers that are relatively immune to being 'scooped' leading by example through extensive use of open science methods (e.g., FAIR data, study preregistration), (3) researcher-initiated opportunities for other researchers to engage in synthesis studies based on the FAIRness and PLUSness of their data and code, and (4) community-developed manuscripts or analyses that are open to all to contribute (e.g., developing manuscripts through social media as in Graham et al. in prep).

Combining open-science principles with design-thinking techniques has great potential to deliver new understanding and modeling/predictive capacity that are directly (e.g., improved predictions of water quality) and indirectly (e.g., informing Earth system models) relevant to society. Essential to open science and ICON-FAIR-PLUS research in a watershed context is leveraging and integrating capabilities, data, and expertise across agencies. This will reduce fragmentation across various watershed science efforts, thereby enabling an interoperable system of knowledge, data, capabilities, and models that can be used to enhance our ability to predict the response of watershed systems to ever-increasing disturbances. We point the reader to the workshop report on open watershed science by design for additional details (https://doesbr.org/documents/Open_Watersheds_By_Design_DRAFT.pdf).

Although interagency cooperation and the increasing practice of open science principles have already had dramatic impacts on availability of data, codes, and model results, there remains great opportunity for further advancements. Multiple federal government agencies have mission elements that address national needs related to water. These diverse mission needs have engendered a large base of water-related data and modeling capabilities that, while useful for their intended purposes, are not well integrated to address overarching national problems. To address this need, an informal multi-agency group has been formed to create and refine a vision for, and initiate action toward development of, a national capability on Integrated Hydro-Terrestrial Modeling (IHTM) including the related data infrastructure. A recent workshop provided a venue to bring together representatives of water-related agencies and their scientific partners (including university researchers) to initiate and refine the IHTM vision and promote it's development (https://dx.doi.org/10.25584/09102020/1659275). It is envisioned that more interoperable and integrated data and modeling capabilities will not only advance the water-related missions, collectively and individually, of the participating agencies, but will also enhance national capabilities for prediction and scenario-building in cross-cutting areas of high priority, including critical contemporary problems such as (1) nutrient loading in the Mississippi Basin, hypoxia in the Gulf of Mexico and the Great Lakes, including related sediment and contaminant transport; (2) water availability in the West, including groundwater depletion in the Southern Ogallala Aquifer and changes to water supply driven by changes in precipitation patterns and mountain snowpack; and (3) flooding, inundation, debris flow, and other water-related hazards during extreme events, including vulnerability of contaminated sites to flooding. Such interagency collaborations and partnerships, with supporting technical insights and perspectives provided by the research community, is indeed crucial for addressing our national and international water challenges.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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