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Key Points:

- We assess four potential improvements in water quality modeling: environmental interfaces, in-stream processes, soil health, and urban areas
- Challenges include data quality control, model calibration, uncertainty management, scale mismatches, and model tool provision
- Modelers need to strengthen connections with experimentalists and stakeholders and cultivate procedural knowledge for modeling processes

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Modeling Water Quality in Watersheds: From Here to the Next Generation

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Abstract In this synthesis, we assess present research and anticipate future development needs in modeling water quality in watersheds. We first discuss areas of potential improvement in the representation of freshwater systems pertaining to water quality, including representation of environmental interfaces, in-stream water quality and process interactions, soil health and land management, and (peri-)urban areas. In addition, we provide insights into the contemporary challenges in the practices of watershed water quality modeling, including quality control of monitoring data, model parameterization and calibration, uncertainty management, scale mismatches, and provisioning of modeling tools. Finally, we make three recommendations to provide a path forward for improving watershed water quality modeling science, infrastructure, and practices. These include building stronger collaborations between experimentalists and modelers, bridging gaps between modelers and stakeholders, and cultivating and applying procedural knowledge to better govern and support water quality modeling processes within organizations.

1. Introduction

Water quality modeling has increasingly been used globally for water quality reporting, risk assessment, identifying and quantifying the sources of water quality constituents, and exploring potential outcomes of climate, hydrology, and management scenarios (Abbaspour et al., 2015; Whitehead et al., 2009). There has been substantial growth of water quality modeling related publications since the 1960s (O'Connor et al., 1973; Owens et al., 1964), with continuous publication of books (Chapra, 1997; Ji, 2017; Martin & McCutcheon, 2018; Thomann & Mueller, 1987) and many reviews on topics in the field. A synthesis of these can be found in Fu et al. (2019) who covered topics of watershed-scale water quality model use, development, and performance and discussed a range of challenges including “large-scale applications, model integration, model usability and communication, preliminary data analysis, modelling management practices, technology advancement, incorporating soft data, model identifiability, uncertainty analysis, good modelling practices, capacity building, and differentiating the effects of climate impacts from those associated with land use and management practices.”

However, it seems that progress in the science and practice of water quality modeling has somewhat stalled (Jakeman et al., 2018). This is evident in the increasing numbers of publications focusing on case studies and improvements of existing models and techniques, rather than addressing further fundamental research or challenging water quality issues that remain difficult to solve. A similar observation has been made

regarding modeling of cropping systems (Keating & Thorburn, 2018). Some watershed-scale models are criticized because of their overparameterization with respect to the problem context, data and prior knowledge available, and their tendency to be applied with insufficient rigor that objectively assesses the various sources of uncertainty (Jakeman et al., 2018; Pechlivanidis et al., 2011).

There may be several reasons why the progress has not advanced faster. First, water quality investigations that require modeling are often funded by government agencies who use models for policy making and planning. Such agencies generally have a stronger preference for investing in improvement of existing and established tools over commissions of new and potentially high-risk tools. The latter are addressed mainly by agencies whose charter is primarily research, but these have more limited resources, which are often leveraged to promote end user applications. The community of professionals who are applying water quality models in practical applications has built a level of acceptance and trust around some existing models that has provided continuity in their development, improvement, and maintenance. This is, in part, motivated by reducing costs, as there is generally a high overhead for an agency to move from one model to another. This can impede progress and the development of improved modeling capability. In addition, practitioners need reliable modeling tools that are accepted by their clients and that are credible in legal settings. In the context of models for policy development or implementation, the provenance, or track record, of the model is important, as previously completed modeling studies may lend credibility regarding the modeling to model users and potential critics. Thus, less investment typically is given to creating cutting-edge, experimental modeling and analyses, compared to improving existing, well-known, more accepted models that may be currently used or maintained by both research and action agencies, hindering new innovation in model development. In addition, many existing watershed water quality models are monolithic in structure. Thus, while an existing model can be enhanced by replacing parts of the model with new science module(s), modelers may be hesitant to make major changes because it is difficult to comprehend cascading effects of the changes.

Second, unlike the weather and climate community where the number of models is smaller because the community has reached some level of consensus on how modeling should be done, watershed water quality model development seems to be more fragmented with greater numbers of independent subdisciplines and special interest groups working on more customized, disparate models. This is, in part, due to the fact that water quality bridges across, and is influenced by, many aspects of disparate disciplines and knowledge domains across the community of water quality modeling experts. This diversity in the water quality domain can hamper the use of common language and development of scientific consensus in water quality modeling.

Third, water quality modeling development is still hindered by limited data availability and model parameter uncertainty (Arnold et al., 2015). This can make it difficult (or impossible) to develop or test a new model innovation. Water quality monitoring programs (including monitoring locations, observed variables, and sampling frequencies) are often not optimized for model population, testing, or for reducing model uncertainty. For example, in the United States, most water quality data are collected by states to assess whether water bodies are meeting designated water quality standards. Data collected for this purpose are rarely adequate to support development of a detailed water quality model. In addition, because each state generally uses their own laboratories for analyses, rarely are robust interlab comparisons performed, and thus, extensions of water quality model domains across political boundaries are often fraught with difficulties. Therefore, while monitoring information is required to support model development, calibration, and uncertainty estimation, available data rarely provide detailed information about the behavior of a system being modeled.

Fourth, modeling of complex, contested environmental issues where uncertainty is rife, such as with water quality management, requires a systematic, comprehensive, and engaging approach by modelers with clients and stakeholders. It requires that the modeling team be diverse so as to have a firm understanding of the phases and inherent steps of modeling and relevant practices to pursue. However, with every problem or project being different in many respects, appropriate practices to pursue depend on the contextual features of the problem at hand. Badham et al. (2019) attempted to demystify the modeling process in water resource management by indicating how one selects practices to follow by identifying a list of key questions to be addressed at each step. The lengthy list is indicative of the experience that must eventually be accrued by learning from a wide range of modeling projects. One essential challenge to accelerate improvements in the practice of water quality modeling would seem to be for modeling teams in the water resources

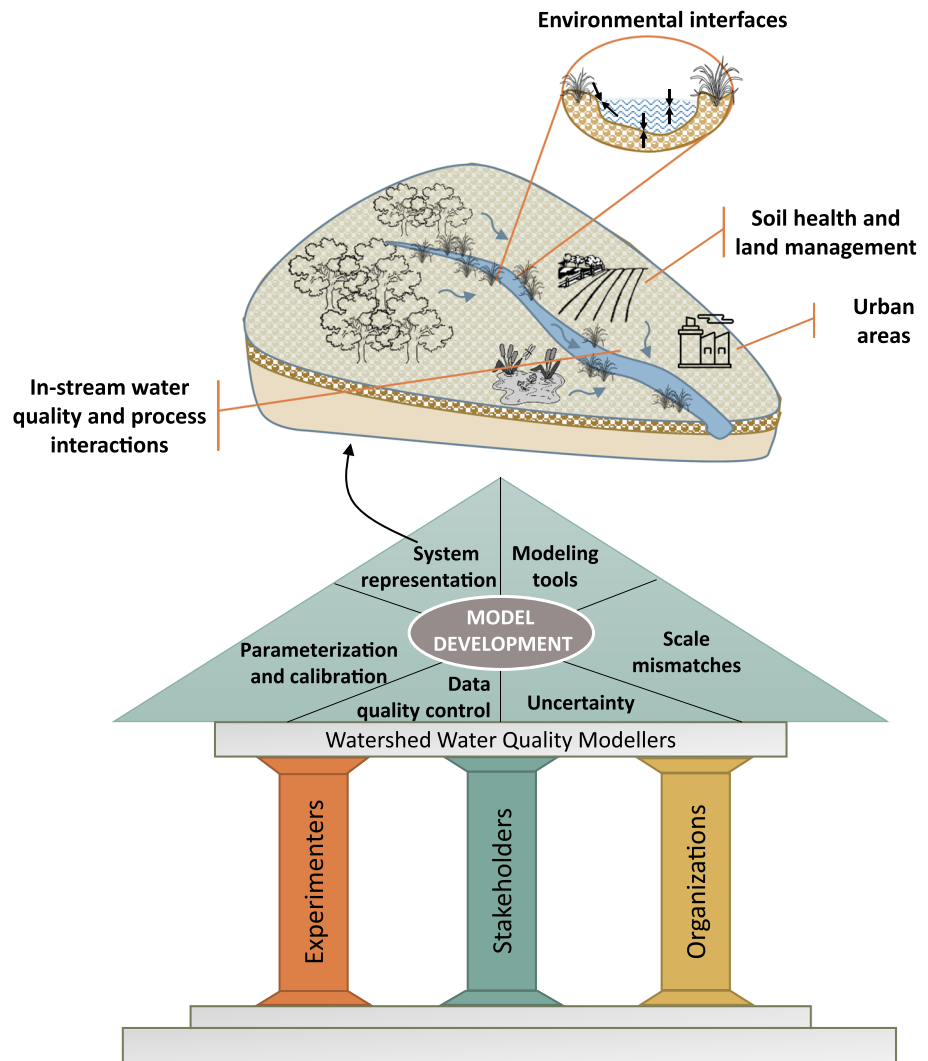


Figure 1. Topics discussed in this paper and their relationships.

management sector to contribute to the wider community their learnings and patterns of contextual practices from projects that they undertake. Another would be to evaluate the success and limitations of our model-based outcomes more holistically by adopting the paradigm that views modeling more as a social process and assesses our success by a wide range of criteria (Hamilton et al., 2019).

In June 2018 at the Ninth International Congress on Environmental Modeling and Software, about 30 water quality modeling experts and practitioners participated in a workshop on “Water quality modeling: A stocktake of needs and ways forward for supporting decision making.” The workshop aimed to identify potential for improvements in process and empirical representations that largely apply in key problem contexts, especially considering land and water management alternatives, and gaps in the process of developing and applying models. The workshop also aimed at identifying opportunities to further advance watershed-scale water quality modeling to support management and policy. The discussions at the workshop and afterward inspired the writing of this paper, which synthesizes the collective experience of workshop participants and authors on key challenges in and ways forward for water quality modeling in watersheds to support decision making.

The remainder of this article is organized as follows. Centered around watershed water quality model development are six key elements: system representation, parameterization and calibration, data quality control, uncertainty, scale mismatches, and provisioning of modeling tools (Figure 1). We devote section 2 to the

discussion of system representation as this underpins the core of watershed water quality model development. More specifically, four key potential areas for improvement in system representation are discussed: environmental interfaces, in-stream water quality and process interactions, soil health and land management, and urban areas. Then, the potential for improvements in other elements of model development are presented in section 3. Finally, we identify three pillars that can be strengthened as ways forward to advance the science of watershed water quality modeling: bridging gaps between modelers and experimentalists, bridging gaps between modelers and stakeholders, and cultivating and applying procedural knowledge to better govern and support water quality modeling processes within organizations (section 4). The intention of this paper is not to cover every aspect of water quality modeling but rather to provide a discussion piece and highlight what the authors have identified as gaps in the current science and practice of watershed water quality modeling along with areas for improvement.

2. Improvements in System Representation

In the following sections we describe the potential for improvements in the way the currently available suite of water quality models represents the aquatic system and those connected systems that affect it. These improvements, as summarized in Box 1, may manifest themselves in our limited understanding of particular environments or processes and/or limitations in our state-of-the-practice representations of them within the codes of existing water quality models.

2.1. Environmental Interfaces

Water quality can be significantly affected by the processes occurring at the environmental interfaces. These borders have been defined as a surface between two either abiotic or biotic systems that are in relative motion and exchange mass, heat, and momentum through biophysical and/or chemical processes (Cushman-Roisin et al., 2012). For example, the quality of water moving kilometers through an aquifer may change very slowly, but the quality of that same water may change rapidly when it discharges through chemically and biologically active bed sediments to a stream (Schindler & Krabbenhoft, 1998). The presence of environmental interfaces has been addressed in selected water quality studies (e.g., engineered remedial actions involving reactive barriers) but typically is not addressed in water quality assessments because the water quality effects of naturally occurring interfaces are difficult to characterize with typical sampling approaches (Hunt et al., 1997). As a result, our understanding and ability to simulate water quality changes at interfaces are not as advanced as our capabilities for noninterface portions of a flow path (e.g., the larger distance traveled in an aquifer). However, their lack of characterization can belie their importance (Björneholm et al., 2016). Understanding water quality at the point of use, which affects its suitability for ecological needs and human-intended purposes, requires an understanding of the sum of all salient upgradient processes, including those that may occur at interfaces representing a small increment of the total travel time and flow path.

Three main environmental interfaces may be considered in water quality modeling: air-water, water-sediment, and water-vegetation interfaces. The *air-water interface* of streams, rivers, lakes, and estuaries is subjected to momentum, heat, and mass transfer. Gas-transfer modeling (Gualtieri & Pulci Doria, 2012) or, if the transferred gas is oxygen, reaeration is most relevant in water quality modeling. However, to date, a universal equation to predict reaeration rate is still missing. Recent efforts have suggested that turbulence microscale could be assumed to be the most efficient transporting eddy near the air-water interface controlling gas transfer (Katul & Liu, 2017). Future research is needed to define a predictive equation valid in water quality modeling studies.

At the *water-sediment interface*, several exchange processes involve solids and solutes. Progress toward better understanding small-scale interactions between particles and turbulence could potentially lead to better identification of the drivers of sediment transport in surface waters and improvement of sediment transport models at the larger scale of water quality studies. Understanding the roles of surface and hyporheic hydraulics and biogeochemical reactions are key elements for upscaling results from the microchannel- and channel-unit scales to the channel-reach and watershed scales (Tonina, 2012). Future research should define common metadata to support interdisciplinary research, facilitate cross-site comparison, and quantify spatial and temporal heterogeneity in hyporheic functions to enable multiscale assessment and prediction of hyporheic processes in the framework of water quality models (Ward, 2016).

Potential improvements in system representation

Environmental interfaces – biological, chemical and physical processes of air-water, water-sediment and water-vegetation interfaces; linking importance of interfaces to model uses.

In-stream water quality and process interactions – examining appropriate dimensionality and model complexity; relationship between hydrodynamics and water quality; in-stream water quality data monitoring; combining empirical and physics-based models.

Soil health and land management – role and dynamics of soil biology and biochemistry on the water cycle; dynamics of soil hydraulic properties; impacts of agricultural practices on soil structure and biological properties in watershed water quality models.

Urban areas – mixed land-use interactions; monitoring and modeling highly variable intermittent contaminant discharges; integrated urban water quality monitoring and modeling practices.

Box 1. Major areas of potential improvement in system representation discussed in this section.

Finally, the interaction between the flowing waters and submerged and/or emerged vegetation occurs at the *water-vegetation interface* (Nepf, 2012). Despite great progress made in recent decades (Tinoco et al., 2020; Wang et al., 2019), additional research is needed to accurately reproduce the effects of natural vegetation on water flow, sediment transport, contaminant transformation, and contaminant mixing and to realistically implement these effects in water quality models. Proper parameterization of these effects at larger scales is a necessary step to reproduce and study the morphodynamic behavior of rivers, lakes, and estuaries at the different spatial and temporal scales considered in water quality modeling studies (Vargas-Luna et al., 2015).

The importance of an interface for water quality simulation will depend on the constituent (conservative or nonconservative), type of interface, kinetics of reaction, and flow rates through the interface. The effects of interfaces may be most pronounced when the constituents and interface are associated with microbially mediated reactions, because microbial communities affect the type, and commonly increase the rate, of reaction. Such microbially dominated interfaces can be expected at geochemical contrasts, such as oxic-anoxic interfaces, as these contrasts facilitate communities specialized for each setting and often are well suited to process the resultant products from the other. Close spatial proximity enhances the transfer between the two communities, which can, in turn, enhance biogeochemical processing. Our ability to characterize the type of microbiological community in the field has improved, but quantitative representations needed for water quality simulation still lag behind our ability to simulate abiotic reactions.

Knowing whether the effects of interfaces need to be simulated for a particular study will depend on the intended use of the results and societal concern. Assessing chemical reactions and geochemical gradients within an interface often requires highly refined resolution characterization spatially, and in some cases, temporally. To a large degree, existing water quality models lack detailed representations of the physical, chemical, and biological processes that may be accelerated within interfaces. Furthermore, although our ability to sample and analyze small volumes of water from interfaces is much improved, the level of specialization required for sampling programs to quantify processes within interfaces is rare and costly, making it difficult to test new model formulations. Thus, for the present, our ability to characterize water quality

changes within interfaces remains limited. Fortunately, many water quality issues can be identified and addressed at the point of withdrawal where the net effect of interfaces on solute fate and transport are most important. A focus on net effects, in turn, facilitates use of relatively straightforward water quality modeling approaches such as retardation and decay. Thus, detailed knowledge of interface reactions may be more important for small-scale simulations of how water develops its quality than larger system-scale questions such as if a water source in question can be made suitable for a given purpose.

2.2. In-Stream Water Quality and Process Interactions

In-stream water quality entails complex process interactions in space and time, which can be difficult to model. Complex stream geometry is typically simplified to one-dimensional transport to reduce development, simulation, and analysis costs, but criteria for examining the appropriate dimensionality and model complexity are generally lacking or poorly defined.

Anywhere water flow is concentrated into a channel may be considered a stream. Temporally, at a given point in a stream network, flow may be perennial or ephemeral, some with more regular seasonal patterns and some with very infrequent flows. The temporal variability alone makes sampling and estimation of water quality challenging. Spatially, in most water quality modeling, we conceptualize a stream as a single channel with well-defined banks. However, stream topology varies with geology and terrain, where channels vary in sinuosity and channel/bank morphology, which affects the dimensionality needed to capture transport. Anabranches (parallel flow paths) and braided streams present further complexity. In low-gradient landscape positions, where flow rates and Froude numbers (Detenbeck et al., 2005) are very low, transport processes may require higher-dimensional analyses. However, most models applied over seasonal/regional scales within large watersheds require an assumption of one-dimensional transport along a stream reach for simplicity. In addition to natural complexity, most streams are highly managed and regulated within a basin and even with transfer of water between basins. Flow control structures may be unmanaged or passive (e.g., weir or unregulated dam) or highly managed within a channel and via flow diversions. These unnatural flow paths and the human decisions that control them are poorly represented in most watershed-scale water quality models.

In-stream transport and transformation processes are important aspects of water quality modeling. Transport phenomena, such as advection, turbulent diffusion, dispersion, and boundary exchanges, are hydrodynamically based, while transformation processes, such as photolysis and chemically and biologically driven degradation, are kinetics based. Over the past decades, representations of these phenomena and their interactions have evolved from simplified 1-D, steady-state models, often based on the kinematic wave approach or on the Saint-Venant equations, to complex 3-D, time-dependent models of hydrodynamics, sediment, dissolved oxygen, eutrophication, microbes, and toxics. Meanwhile, the computational resources required to run these models have changed from high performance computers to desktop personal computers as personal computers have become more capable. Remote cloud computing using a model-as-a-service (David et al., 2014) is emerging in environmental modeling as an alternative to local computing.

Despite such progress, there is still an urgent need to improve our knowledge about the relationship between hydrodynamics and water quality, where the main difficulty lies in the treatment of turbulence. Turbulent flows are complex, three-dimensional, intrinsically irregular and chaotic and are characterized by intense mixing and dissipation, at a large range of spatiotemporal scales, and by the coexistence of coherent structures and random fluctuations (Basu, 2013; Pope, 2000). Turbulence strongly controls the transport of water and water quality constituents within the water column and across environmental interfaces. Hence, the equations governing hydrodynamic and constituent transport processes also reflect the effects of turbulence. However, in turbulent flow, these equations are extremely difficult to solve due to difficulties in resolving the temporal and spatial fluctuations of velocity, pressure, temperature, and concentration associated with turbulence (Kundu et al., 2015; Pope, 2000). Various approaches have been attempted to solve these fluctuations (Rodi et al., 2013; Sotiropoulos, 2005). Advances in turbulence modeling, especially using Large Eddy Simulation (LES) and hybrid Reynolds-Averaged Navier–Stokes (RANS)-LES methods (Stoesser, 2014), will help improve the modeling of constituent transport processes.

Other open questions and challenges in the hydrodynamics of water quality modeling relate to the parameterization of turbulent diffusion and dispersion processes and the effects from channel eco-morphological

features. Despite its importance in water quality modeling, transverse mixing rate estimation in natural channels is mostly based upon empirical equations as for the longitudinal dispersion coefficient, which is used in 1-D water quality models (Ji, 2017; Rutherford, 1994). Further research efforts are also needed to fully identify and accurately quantify the effects that channel vegetation, bends, islands, confluences, bedforms and macroroughnesses, and, more generally, bed friction have on river hydrodynamics and, in turn, on contaminants and sediment transport (Arfaie et al., 2018; Gualtieri et al., 2018; Kasvi et al., 2015; Liu et al., 2020; Vargas-Luna et al., 2015). Finally, other challenges in the integration between hydrodynamics and water quality modeling can be identified in the application of 3-D models to large rivers due to the need for large amounts of input data and huge computational power, as well in the definition of standards for the integration with hydrological models (Hodges, 2013).

Furthermore, in-stream processes and their related physical properties, such as flow velocity, depth, shear stress, turbulent features, and temperature, affect ecosystems. In turn, organism community affects the physical environment through hydrologic, geomorphologic, and hydraulic methods (Tonina & Jorde, 2013). Ecohydraulics studies connect flow properties with biological requirements to define habitat availability or to quantify flow-related ecological functions. These studies could be carried out at the microscale and at reach (10–50 m channel width) and segment (50–1,000 m channel width) scale as well as the sub-basin and basin scale (Tonina & Jorde, 2013). The relationship between ecohydraulics and water quality modeling of in-stream processes is complex. First, this relationship requires knowledge of the hydrodynamic processes in a water body and is subject to the same governing equations and solution methods/issues, including the treatment of turbulence (Rodi et al., 2013; Tonina & Jorde, 2013). Second, ecohydraulics and water quality modeling are mutually interacting. Hydrodynamic effects on the channel/riparian vegetation affect photosynthesis and respiration which, in turn, affects aquatic ecological communities (Ji, 2017). On the other hand, hydrodynamics and water quality jointly affect fish species abundance and richness (Gualtieri et al., 2020; Trinci et al., 2017). Hence, a closer integration between ecohydraulics studies and in-stream water quality modeling should be encouraged.

Conceptual understanding and quantification of dominant constituent transport and transformation processes are essential, regardless of the simulation methods used to estimate water quality variables. Important factors will vary depending upon the type of transport and biochemical reactions involved. For example, phosphorus (P) transport can be strongly related to sediment onto which P is sorbed. Important processes related to the flux of suspended sediment (e.g., sediment settling and resuspension and bedload interaction with suspended sediment, bank erosion, or deposition) may also control P transport and enrichment. Although such process interactions are complex, relatively simple conceptual mathematical models (e.g., Dietrich et al., 1999) can capture geochemical dynamics. In-stream geochemistry may also be important for liberating sediment bound chemicals (e.g., P_2O_5) into dissolved bioavailable forms (e.g., phosphate [PO_4]) in the water column. Under low-flow conditions and high water temperatures, anoxic conditions may allow biochemical transformations to occur that make P available to algae, often leading to toxic algal blooms. In addition, hyporheic exchange between shallow groundwater and the stream bed can supply nutrients such as nitrate to promote biological activity and eutrophication of water bodies. Thus, any model must be applied with adequate scientific understanding and expertise to avoid common pitfalls.

Estimation of water quality is highly dependent upon the in-stream water quality data collected by various government agencies. This has been an impediment to estimation, but data availability and access have improved with the advent of digital data storage and dissemination, as well as more standardized data protocols. Indeed, much data gathering and processing is now automated. Even so, a large portion of the effort in building a water quality model is data provisioning. There is also a growing disconnect between those who measure and understand data limitations and errors and those who model often without even visiting the field sites of concern.

Both statistical and machine learning methods provide ways of estimating temporal dynamics and patterns of variability in constituent concentrations and loads, assisting the identification of system stressors (Glendell et al., 2019), setting of regulatory targets (Jung et al., 2020), and model simplification (Jackson-Blake et al., 2017). However, extrapolation of fitted behavior beyond the ranges and environmental conditions of measured data requires extreme caution. Water quality is commonly measured in streams/rivers in efforts to quantify concentration (C , mg/L) and load ($L = C * Q$, where Q is average flow rate of water,

L/s, over a time interval) as a mass per time (e.g., kg/day) of the constituent of interest. In “well-behaved” streams where variations in Q and C are gradual, cross-correlations of $C(t) \sim Q(t)$, where t denotes time, may be great enough to estimate $C(Q)$ as a unique, monotonic function with high explanatory power; in such cases, L is estimated simply as $L = C(Q) * Q$. However, measured $Q(t)$ at a stream gauge more typically explains less than half of the temporal variability in $C(t)$ at the same location, even at regional scales (Guo et al., 2019). Empirical/statistical models may only be reliable over a range of measured conditions. For example, estimation of extreme values such as peak concentration may be estimated poorly, particularly when extrapolation of a correlation with surrogate data such as $Q(C)$ is erroneous. Errors may vary dramatically with the stream environment (spatially and temporally) and with the chemical or other constituent concentration being estimated. Even so, statistical models, such as SEAWAVE-QEX (Vecchia, 2018), that rely in part upon empirical $C(Q)$ relationships have become standard practice in estimating loads for regulatory purposes.

Machine learning is a growing field of exploration in many areas of earth science (Reichstein et al., 2019), including stream hydrology (Beck et al., 2016). Artificial neural networks, for example, often show high skill in fitting measured patterns, but overfitting is common and may lead to greater extrapolation errors than conventional multivariate statistical models. Similar caution is strictly true of more physically based models also, but some degree of extrapolation or “extension” of simulations beyond measured conditions may be less erroneous if the dominant transport processes have been captured. Biochemical and physical process models are often highly parameterized and also require extensive data to provide confidence in model responses to various environmental conditions. Hurdles to their application have been reduced with improved data accessibility and greater options for model calibration and evaluation. Even so, general application of process models remains beyond the capacity of most action agencies and practitioners. Opportunities are rapidly emerging to explore hybrid models by combining statistical methods, machine learning, and process models that may improve estimation of extremes and extension of models to unmeasured conditions in space and time. More work is needed to identify conditions where hydro-bio-chemical process models of in-stream transport can be used to extend statistical models beyond the range of measured concentrations or other conditions. Opportunities for hybrids of machine learning and process-based modeling deserve further exploration, particularly to identify deviations in behavior of machine learning and process model simulated results for extreme values and unmeasured conditions.

2.3. Soil Health and Land Management

Globally, agricultural soils make up about 40% of the entire terrestrial system (FAO, 2013) and in many watersheds more than 90% of land use, highlighting the necessity to adequately model the soil interface layer to understand and manage water quality at watershed scale. Yet, the structural role of soil microbiology on the water cycle—what practitioners call *soil health*—is poorly understood and modeled (Allen et al., 2011; Schoonover & Crim, 2015). Soil health fundamentally affects surface water's suspended load and its chemical properties. Models that treat soil characteristics as constant over time, invariant in the face of dynamic agricultural practices, and homogenous over large spatial areas neglect the central role of soil and soil management for water and mineral cycles.

Soil is the biologically active interface in the water cycle that determines the pathway that precipitation or irrigation water follows. The soil interface determines whether water infiltrates into the vadose zone or runs off at the surface, as well as the fraction of infiltrate that is retained in what some practitioners refer to as the “soil sponge.” Furthermore, it affects the amount of water that evaporates at the surface, transpires after plant uptake, or percolates into the groundwater. Researchers acknowledge that there is a deficit in our understanding of, and ability to model, the role that soil biology plays in the broader water infiltration process and resulting soil chemistry (Vereecken et al., 2019). In healthy soils, nutrients can be actively transported over tens of meters by mycorrhizal networks and “traded” with plants in exchange for carbon-rich sugars (Wipf et al., 2019). While soil carbon and infiltration rates are first indicators for microbial activity, multiple aspects (especially the history of plant cover, fertilizer application, and mechanical disturbance) determine how soil biology influences the physical and chemical characteristics of water flow (Baar, 2010; Gianinazzi et al., 2010; Lovelock et al., 2004). By changing its microbiology, soil management can determine the physical behavior of soil. For example, infiltration rates can easily vary by 1 order of magnitude depend-

ing on microbial richness (Franzluebbers, 2002), and the (biological) soil structure can either totally eliminate surface runoff or foster severe erosion (Zhang et al., 2007).

For water quality modeling, this means that soil is a dynamic ecosystem that may change its behavior in the water cycle depending on management, affecting both water quantity and water quality (Bonfante et al., 2019). Soil's physical and chemical characteristics vary with seasonal moisture (e.g., cracking in clay soil leads to strong infiltration until the clay swells and seals itself), affecting the depth of oxygen penetration (e.g., after spring ponding), micropore and macropore structure, and surface sealing after precipitation onto bare soil. Agricultural chemicals and amendments further affect the properties of soil, by either enhancing organic matter and biological activity (e.g., compost, grazing, and biochar) or reducing it via suppressing microbial life (e.g., by inhibiting plant root exudates via phosphorus fertilizer application or by oxidizing organic matter via nitrogen fertilizer application and tillage). As agricultural practices affect soil microbiology and soil structure, water cycles and mineral cycles change. Despite our conceptual models of how these processes work, quantitative understanding of microbial soil dynamics is not well represented in the current suite of water quality models and remains a limiting factor to effectively assess watershed intervention options for nonpoint pollutants.

Likewise in wetland soils, especially those managed as seasonal wetlands subject to a period of inundation during a rainy season and desiccation during drier months, water quality models do not typically account for annual variation in soil physical, chemical, and biological properties. During dry months, dense clay soils form cracks often extending approximately half a meter into the subsoil, creating a porous medium with extremely high infiltration rates during initial seasonal wetland flood-up as water fills up the open cracks and the soils regain moisture. Finally, at saturation, the soils swell and the cracks close, effectively sealing the soils and exhibiting very slow infiltration rates. In addition, rewetting of wetland soils often promotes strong pulses of microbial respiration and switching from aerobic to anaerobic condition. Very few water quality models allow changes to be made in soil hydraulic properties over the course of a simulation, impacting the performance of models that simulate these types of landscapes.

Scale matters. The spatial scale affects the factors that are important in setting the soil organic matter (Vos et al., 2019). Climate, vegetation, and soil texture are important at the global scale; but at the scale of watershed and smaller, agricultural practices also become important (Guo & Gifford, 2002). Changes in soil characteristics depend on the temporal assessment scale (Vos et al., 2019), with different directions of short-term impacts (e.g., tillage increases immediate infiltration) and long-term impacts (e.g., regular tillage reduces soil organic matter, infiltration, and water retention). A review of the literature (Blanco-Canqui, 2011) suggests that practices such as no-till cropping may have complex interacting effects such as increased soil water repellency, which will increase runoff, but also increased aggregate stability, which will reduce the erosive loss of soil via runoff. While some models include the effect of agricultural management on soil organic matter (Brilli et al., 2017; Holzworth et al., 2015), the flow-on effects to changes in other soil properties important to water quality modeling, such as soil water storage and surface roughness, are poorly captured (Palmer et al., 2017).

Soil biology creates macropores that are inherently difficult to model (Beven & Germann, 2013; Jarvis, 2007). Yet, the lack of representation of soil biology in many watershed water quality models may in part be because many watershed modelers are more likely to come from an engineering or water science background than from a soil or agricultural science background. Thus, they are more likely to have a better understanding of end-of-pipe solutions (e.g., erosion berms, drainage, sedimentation basins, and gully remediation) than solutions in managing soil biology (amendments, changes in tillage, fertilization, and chemical applications). In addition, soil biological solutions are highly uncertain. For example, farmers may or may not adopt recommended practices; there can be significant and variable time delays between implementation of a practice and beneficial effects (Volk et al., 2009); and even well-implemented practices are not guaranteed to produce the desired effects. However, soil biological solutions address the source of the water quality issues and, although they present challenges, contain the most likely broad-scale enduring solutions. Omission of soil biological solutions also excludes farmers and land managers from being part of the solution in improving watershed water quality.

Therefore, the authors advocate for a better representation of soil biology in water quality models. Geospatial digital soil mapping, paired with on-the-ground monitoring, promises to greatly improve our understanding

of water quality dynamics in watersheds. Satellite data have been routinely used for vegetation assessment (Huete et al., 1999), yield projections (Doraiswamy et al., 2003), and measurement (Deines et al., 2019). Recently, broad access to satellite data and cloud tools (e.g., the Google Earth Engine) has improved digital soil mapping (Minasny & McBratney, 2016; Zhang, Feng, et al., 2017), now enabling remote mapping of mycorrhizal activity in soils (Soudzilovskaia et al., 2019). Such tools may soon dramatically improve our spatial understanding of nonpoint contamination sources, visualizing how soil biology and soil management practices affect water cycles, erosion and water quality, and downstream conditions. Regenerative agricultural systems are emerging from this new paradigm of soil microbiology and especially mycorrhiza (Gosnell et al., 2019). Studies of how this revolution in agricultural production may affect water quality at watershed level are only emerging (e.g., Baffaut et al., 2019).

2.4. Urban Areas

Urban areas discharge a wide variety of pollutants, ranging from “traditional” parameters (e.g., sediment, organic matter, nutrients, and bacteria) to micropollutants (e.g., heavy metals and organic compounds) and other emerging contaminants (e.g., pharmaceuticals and endocrine disruptors). These discharges can be continuous (e.g., via the effluent from wastewater treatment plants) or intermittent (e.g., wet-weather induced via combined sewer overflows, separate storm sewer overflows [SSSOs], or wastewater treatment plant overloading). While the traditional parameters are relatively easier to monitor, the latter are characterized by a high inherent variability and pose logistical challenges in performing extensive monitoring, leading to a greater level of uncertainty in the pollution levels attributable to these sources.

Although urban discharges can be characterized as point sources from a watershed perspective, they can also be considered as diffuse sources when looking at single stretches of urban and peri-urban water bodies. For example, there might be hundreds of SSSOs delivering important pollutant loads (Brombach et al., 2005; Masoner et al., 2019) to a single river reach. The effects of wet-weather discharges on receiving water bodies are often site specific (Karlsen et al., 2019), with both chronic (often caused by the loads discharged from SSSOs) and acute impacts (often caused by combined sewer overflows resulting in oxygen depletion and/or ammonia toxicity). The latter can also depend on seasonal variations in the river conditions (e.g., oxygen solubility and baseflow), and they can be limited in space (House et al., 1993). Furthermore, existing monitoring protocols are often performed at a frequency that is not able to detect acute impacts from wet-weather discharges (Boënné et al., 2014; Halliday et al., 2015; Skeffington et al., 2015).

Effectively reducing water quality impacts associated with urban discharges thus requires holistic monitoring and modeling approaches that consider the dynamic interactions between the receiving water body and the variety of constant and intermittent urban discharges (Chapra, 2018). Since the 1980s, such awareness has led to the development of various integrated modeling tools, simulating the different elements of the integrated urban water systems (e.g., sewers, wastewater treatment plants, and rivers) (Achleitner et al., 2007; Erbe & Schütze, 2005; Rauch et al., 2002; Saagi et al., 2017). The International Water Association Task Group on River Water Quality Modeling (RWQM) specifically developed the RWQM1 model for such integration (Reichert et al., 2001; Shanahan et al., 2001; Vanrolleghem et al., 2001). Being contemporary to the European Union Water Framework Directive, which explicitly promotes holistic approaches in watershed management, RWQM1 still represents the state of the art in integrated urban water quality modeling. However, its applications are quite scarce both in practice and in the published literature, providing an archetype of the limitations in existing modeling tools. Model structure complexity and data availability are among the main reasons for such limited success: available models are often overparameterized (Reichert & Vanrolleghem, 2001) with respect to the spatial and temporal resolution needed to successfully simulate effects from wet-weather discharges. Indeed, in one of the most successful full-scale implementations of integrated urban water modeling (Benedetti et al., 2013), a simple model (Duflow) was preferred.

Another factor seldom considered by existing models is the high inherent variability in the quality of wet weather discharges, which are difficult to measure and thereby to model (Bertrand-Krajewski, 2007). This implies a strong need for resulting uncertainty assessment and its consequent increase in computational demands. When looking at micropollutant discharges, being one of the major impacts from urban areas (Dittmer et al., 2020), the need for resulting uncertainty assessment is further magnified. High variability in discharged concentrations, lack of data on the behavior of these substances, and oversimplified

representation of fate processes (particle settling, partitioning, etc.) are strongly limiting the application of existing models.

New monitoring approaches are becoming available, providing water quality data using advanced technologies for in situ, high-resolution (i.e., subhourly), point-scale monitoring (Blaen et al., 2016; Melcher & Horsburgh, 2017; Rode et al., 2016) or using unmanned aerial vehicles for rapid, on-demand, spatially distributed water quality measurements (Koparan et al., 2018; McDonald, 2019; Yigit Avdan et al., 2019). These create new opportunities for (automatic) parameter estimation, data assimilation, and reformulation of model structures that need to be incorporated into existing models.

Finally, urban water systems are increasingly recognized as complex socio-technical systems (Bach et al., 2014), as should more rural watershed systems. This requires more comprehensive understanding of urban water systems and their interactions with society. Economic valuation, energy considerations, and social dynamics are gradually being considered in urban water system models for the design of infrastructure management and adaptation strategies (e.g., Rauch et al., 2017). These types of integrated models often contain a high level of uncertainty and thus are generally recommended for exploratory modeling (i.e., testing different assumptions and possible strategies) rather than providing detailed descriptions of system dynamics and absolute predictions.

3. Improvements in the Modeling Process

Where the previous sections illustrated gaps in our knowledge of how to represent the aquatic environment to be simulated within a water quality model, the following sections illustrate areas of potential improvements in conducting modeling studies. These gaps, summarized in Box 2, represent our limited understanding of how to best apply models to achieve desired results, including arriving at actionable information derived from model output that can be used for decision making.

3.1. QC of Monitoring Data

Quality control (QC) of data refers to the application of methods or processes that determine whether data meet overall quality goals and defined quality criteria for individual values (McCarthy & Harmel, 2014; Mortimer & Mueller, 2014). Scientific and statistical evaluation of data is typically applied to determine if the data obtained are of the appropriate type, quality, and quantity to support their intended use. The data life cycle comprises planning, implementation, and assessment steps that are used to define quantitative and qualitative criteria for determining when, where, and how many samples (measurements) to collect and a desired level of confidence (EPA, 2006b). For the U.S. Environmental Protection Agency (EPA, 2006a, 2006b), the sampling methods, analytical procedures, and appropriate quality assurance (QA) and QC procedures are documented in a QA Project Plan (QAPP). Data are collected following QAPP specifications. The QAPP summarizes the sampling design and the manner by which samples are collected or measurements taken. This will place conditions and constraints on how the data should be used and interpreted. During the assessment phase, the data are validated and verified to ensure that the sampling and analysis protocols specified in the QAPP were followed and that the measurement systems performed in accordance with the criteria specified in the QAPP (EPA, 2006b).

Protocols for discrete data acquisition and assessment are well established and are described in many manuals and procedure documents (e.g., EPA, 2006a, 2006b). Protocols for real-time or continuous data QA/QC are not as well evolved, although vendors of hydrologic data management systems designed for continuous data acquisition and processing, such as Kisters Inc. WISKI and HYDSTRA and Aquatic Informatics AQUARIUS platforms, provide software used by enterprise-scale water management agencies. Flow and water quality data being reported at 15 min or hourly intervals from numerous monitoring platforms can easily overwhelm analysts and their ability to process the data and perform corrective actions. Automated features utilizing a high degree of customizable visualization allow importation of discrete QC data that can be used to tag records or sets of records that meet or fail to meet a particular criterion, build and update rating curves, derive statistics, and report in real time to meet stakeholder expectations for timely, accurate water information. Other features allow the annotation of actions to appear directly on the data time series plots while retaining the original unfiltered data record. QC is a partner to QA and, when errors are found, can reveal ways to prevent these errors via QA.

Potential improvements in modeling process

Monitoring data – sensor data acquisition protocols require standardization; greater adoption of quality assurance or quality control protocols needed for continuous data.

Parameterization and calibration – selection of data types for good representation of system functioning; selection of objective functions pertinent to modeling aims.

Uncertainty management – attribution of total uncertainty to its sources and their prioritization; exploratory modeling of risks; tractable and resources-efficient sensitivity and Bayesian methods.

Scale mismatches – scale-aware, temporal and spatial, data fusion techniques; coupling between 1D and multidimensional models.

Provisioning modeling tools – modern open source and flexible modeling systems should be more widely adopted.

Box 2. Major areas of potential improvement in the process of modeling watershed water quality.

A pertinent example in the San Joaquin River Basin of California, USA (Quinn, Hughes, et al., 2017; Quinn, Osti, et al., 2017), deals with the development of a water quality forecasting system for dissemination of real-time estimates of river salt load assimilative capacity. During periods when salt load assimilative capacity in the river is exceeded, the system would allow basin west-side agricultural and wetland stakeholders to manage and control salt loading to the river in order to match schedules of basin east-side reservoir releases of dilution flows. The lack of real-time data QA has limited the type of data sharing between stakeholders due to privacy and potential litigation concerns, even though data sharing is considered essential for basin-scale, real-time salinity management. The software solution sought by stakeholders needed to be a commercially available, off-the-shelf solution with the ability to apply business rules specific to the various water districts' needs, that is, for automatic validation, correction and presentation of data in graphical form, and visualization of information with web services. In terms of adaptation, a software QA solution that had previously been adopted and deployed by two of these water districts was preferred because districts that want to upgrade operations tend to more readily adopt technologies being used by neighboring districts. In addition, information exchange between district stakeholders was more easily facilitated when districts share the same software.

QA/QC of discrete monitoring data is a mature enterprise. Progress has been made over the past decade in standardizing procedures, providing easy web access to data and providing geographic information system-based search algorithms that simplify uploading and retrieval of data in secure, relational databases. The provision of analytical capability in geographic information system platforms and the ubiquity of high-level programming languages such as Python and R, which are now accessible to integrate with these platforms, have increased use of these discrete data resources. At the same time, it has increased the demand for more continuous data, especially for flow and water quality data that can show high variability.

Competition between vendors and the continual improvements both in quality and capability of both sensors and telemetered sensor networks have lowered costs and increased demand from customers. Standardization of data acquisition protocols around sensor output formats such as SDI-12, MODBUS, and 4-20 mA, which allowed the rapid expansion of environmental monitoring and accommodation of large numbers of vendors, has not been as successful in the domain of data QA/QC. This remaining technology transfer gap has stymied progress in data access and public agency sharing of data, especially in litigious states like California where data reporting errors can be used against agencies and water districts in the courts.

Public agencies in California have, in the past two years, mandated public access to certain data such as agricultural irrigation diversions from rivers and groundwater pumping records. The public demand for web accessible information and increased accountability was a driver for this legislative action. Although few members of the public will take the time and effort to scrutinize water district and other public agency records, the mere threat of access has been effective, both in diverting greater resources to Information Technology within these entities, and in having Information Technology employees devote more energy to visualization and other tools to make the information presented more understandable and easier to assimilate. Although state and federal government legislation and regulation are sometimes needed to “prime the pump” in these endeavors, much of the progress made to date, and that anticipated in the years ahead, has been driven by an increasingly interested public armed with easily accessible tools for processing data and demanding accountability.

3.2. Parameterization and Calibration

Model parameter estimation is critical to ensuring the reliability of models. While parameter estimation and model calibration remain formidable tasks given the dimensionality and nonidentifiability of many models (Guillaume et al., 2019), a variety of calibration approaches have been suggested and are routinely used. Several recent review papers highlight the state of practice (Daggupati et al., 2015; Moriasi et al., 2012, 2015), indicating the need for all models to be well calibrated and validated as far as possible, so that they can be used to extrapolate beyond previously observed scenarios by representing the system dynamics adequately. Despite well-established calibration schemes (e.g., Abbaspour et al., 2007), difficulties remain in properly reconciling models with field or laboratory observations. The central objective in model calibration is to ensure that the model parameters represent the system of interest adequately, usually for a predictive purpose and its water quality attribute(s) of interest; however, this task becomes complicated with limited data, high-dimensional models, and an overreliance on summary statistics that may not properly capture the functional properties (e.g., averages and extremes over appropriate time and spatial scales) of the water quality variables of interest. There remains significant difficulty in calibrating models so that they represent the variables of interest sufficiently in a way that the model is reliable (i.e., representative of the actual relevant processes in the system), as well as fit for purpose (so that the main variable or criteria of interest is modeled with confidence).

Freshwater quality parameters are often routinely measured by environmental regulators in many watersheds, but their typically low resolution will affect model calibration (Krueger, 2017). Often models must be reconciled with sparse data (in both space and time), or variables may be measured at a scale that is different to that represented by the model. The issue of scale for model parameterization can be exacerbated for parameters that are measured in the laboratory rather than the field and then translated to the model scale. Potential artifacts of such scaling are widely recognized in physical flow parameters such as hydraulic conductivity and dispersivity but are also expected in a model's geochemical representations, such as extrapolating lab-derived rates of reactions to the rates occurring in the field. In all, the frequent lack of data for model calibration at appropriate spatiotemporal scales highlights the need for new types of field and lab experiments (including on land and in water) and high-resolution monitoring that will help parameterize models and ultimately improve process understanding and system representation (Bol et al., 2018). Recent advances in sensor technologies (Meyer et al., 2019; Ross et al., 2019) and sediment tracing techniques using coupled isotopes and biomarkers (Glendell et al., 2018) provide one path to potentially improved parameter estimates and ultimately more reliable models.

Modern multiobjective calibration routines are well placed to estimate model parameters using multiple types of data. Less understood is how to develop multiobjective model calibration schemes that lead to

model parameters that better represent the system and will be more effectively extrapolated beyond the period of calibration. New field and laboratory experiments, soft data, and new observing technologies would all lead to increased information on system functioning, but calibration routines must ensure parameter estimates lead to greater confidence in model output, not just a reproduction of model residuals. While all automatic calibration routines require specification of a statistical objective function that summarizes the model fit to data, little focus has been placed on developing objective functions that ensure good representation of the system function or that properly capture the variables of interest. Recent research in hydrologic signatures may provide one source of inspiration for developing mathematical functions that properly capture the system function depending on the modeling scenario (McMillan, 2020).

More fundamentally, Bennett et al. (2013) argue the need to justify the selection of objective function for calibration in line with the model purpose. In examining model performance characterization adopted in various relevant fields, they review numerical, graphical, and qualitative methods. They also propose a five-step procedure for performance evaluation of models that includes “(i) (re)assessment of the model’s aim, scale and scope; (ii) characterization of the data for calibration and testing; (iii) visual and other analysis to detect under- or non-modelled behavior and to gain an overview of overall performance; (iv) selection of basic performance criteria; and (v) consideration of more advanced methods to handle problems such as systematic divergence between modelled and observed values.”

3.3. Uncertainty Management

The importance of addressing uncertainty in the modeling process, especially when involving complex systems as occurs with watershed water quality management, has become more widely recognized. It is clear that an understanding of uncertainty and its relative source strengths can support decision processes such as by estimating the risk associated with certain scenarios or model predictions. Uncertainty analysis can also help diagnose model weaknesses or suggest new experiments that will reduce critical uncertainties. Thus, discussion of simulations of water quality must also consider sources of uncertainty for the outputs of concern (Loucks & van Beek, 2017). There are two related challenges in regard to the uncertainty associated with water quality models: how best to characterize or quantify uncertainties and how to better constrain uncertainties.

The sources of model uncertainty can be largely grouped into two categories: that associated with the model (including its conceptualization, mathematical equations, and parameters) and that associated with the system observations used to drive the model and constrain parameters. Within these two broad categories, a multitude of model choices and types of data will contribute to uncertainty in the model itself. Typically, many water quality models can reproduce the observations (e.g., when they are nonidentifiable or mathematically ill posed), even more so than simulations of water quantity, because there are multiple reaction paths available and the water quality observations available for calibration are typically fewer.

It is also very rare in water quality modeling studies to report where uncertainty stems from and ranks among all the modeling sources. In the latter situation, only a subset of uncertainties tends to be considered with no justification as to why others were ignored. The attribution of the total model uncertainty to its sources remains a significant difficulty but is critical to improving the model and constraining uncertainty. On the other hand, sensitivity analysis can often be a valuable tool to apportion the relative influences of uncertainty in a model (Koo, Chen, et al., 2020; Koo, Iwanaga, et al., 2020). In particular, it can aid in establishing which model factors (largely parameters but also inputs) can be safely ignored and fixed at specific values so that calibration and uncertainty can proceed on a reduced order model with shorter runtimes.

The way forward in uncertainty quantification for water quality models therefore must first be an improved understanding of the potential sources of uncertainty and an assessment of their relative magnitudes or impacts. The uncertainty associated with the model itself is a function of the choices made by the modeler, including the implicit and explicit assumptions of the model hypotheses, the type of model calibration, and the model boundary conditions. Recent advances in computational tools aid this task, and the future of uncertainty analysis for water quality models requires further development of efficient and robust methods for uncertainty quantification. Bayesian and pseudo-Bayesian approaches have been well established to tackle uncertainty quantification for water quality models (Freni & Mannina, 2010; Liu et al., 2008; Malve et al., 2007; Zhao et al., 2014), but they may be difficult to apply for high-dimensional or expensive models.

It is similarly difficult to properly develop appropriate likelihoods or objective functions that represent model errors (Wu et al., 2019). Model emulation and model surrogates such as polynomial chaos expansions (Ghanem & Spanos, 1991; Xiu & Karniadakis, 2002), Gaussian processes (Williams & Rasmussen, 2006; Yang et al., 2018), and sparse grids (Bungartz & Griebel, 2004) are examples of powerful tools that can improve understanding of the model response surface and sensitivities, as well as for achieving faster running models for improving uncertainty analysis that tends to require large number of parameter samplings and hence model simulations.

Unfortunately, due to the computational expense of many water quality models (e.g., Buahin & Horsburgh, 2018), building an accurate surrogate can still be intractable. Recently, in other fields such as aerospace engineering, multifidelity methods (Gorodetsky et al., 2020; Jakeman et al., 2020; Peherstorfer et al., 2018) have been used to reduce the computational burden of uncertainty analysis. Multifidelity methods use an ensemble of models of varying complexity, speed, and accuracy (fidelity). A larger number of lower-fidelity simulations, which are faster but less accurate (e.g., models with reduced physics or coarse numerical discretizations), are used to explore the variability of a system and combined with simulations of a higher-fidelity (slower but more accurate) model to maintain predictive accuracy. These approaches enable more rapid convergence to high-fidelity statistics when such lower fidelity models provide predictive utility. In particular, multifidelity uncertainty quantification can converge more rapidly than single-fidelity uncertainty quantification in cases where there is a high-correlation between predictions of the models of varying fidelity (Jakeman & Jakeman, 2018). All these methods have potential to significantly shape uncertainty quantification studies of water quality models.

Effective uncertainty analyses also require closer connection between managers and modelers. The data, quantities, and performance measures submitted to the managers or policy makers may be prodigious, let alone failing to target the risk preferences of the stakeholders. For example, an uncertainty quantification study may be used to estimate the uncertainty in annual average constituent load predictions of a system, but the decision makers may only care about uncertainty in load predictions during large events or uncertainty in the change in constituent loads due to management intervention.

In addition, water quality modeling often comprises multiple component models. In addition to forbidding runtimes of any one or more components that constrain model uncertainty assessments, individual model components may also be managed by different groups, with varying computational software and hardware, which can hinder cohesive and automated modeling (Buahin et al., 2019). Water quality modeling efforts can benefit from leveraging recently developed methods in computational mathematics and engineering that decompose system uncertainty analysis into uncertainty analysis of individual model components that can be performed in parallel, thereby allowing those analyses to be combined resourcefully to assess system level uncertainties (Amaral et al., 2014; Guzzetti et al., 2020; Sankararaman & Mahadevan, 2012).

With the advances in efficient and robust methods for quantifying model uncertainty, uncertainty quantification and attribution itself then become a powerful tool for constraining uncertainty. By identifying the sources of uncertainty, modelers can prioritize improved model representations, consider the need for improving a priori parameter estimates from data, or develop an optimal monitoring network design that reduces parameter uncertainty. In the latter case, optimal experimental design uses models to select experiments that maximize information gain (e.g., change in estimated uncertainty). According to Jakeman and Jakeman et al. (2018), optimal experimental design has been shown in the computational mathematics literature to drastically improve the cost effectiveness of experimental designs for a variety of models based on ordinary differential equations (Bock et al., 2013), partial differential equations (Horesh et al., 2010), and differential algebraic equations (Bauer et al., 2000) and has been developed in both Bayesian and non-Bayesian settings (Atkinson et al., 2007; Chaloner & Verdinelli, 1995; Walsh et al., 2017).

Uncertainty in data requires special consideration when understanding the sources of total model uncertainty. As noted in section 3.2, water quality parameters are typically very difficult (if not impossible) to observe at the scale they are represented in the model. Observational data may be sparse and observed at a single point in space or time, then hard to reconcile with model simulations. Three major types of observational uncertainty are evident: measurement errors, representational errors (due to the unknown spatial and temporal variation of the variable), and proxy measurement errors when variables are inferred via a surrogate (e.g., turbidity as a proxy for total suspended solids, Jones et al., 2011; or total phosphorous

concentration, Lannergård et al., 2019). Proxy measurement is particularly important for water quality simulations because many water quality variables may be costly to measure or cannot be directly observed (Horsburgh et al., 2010). But proxy measurement introduces uncertainties on top of measurement and representational uncertainties that will affect any model parameterization. The uncertainty in observations can (at least in theory) be estimated independently of the model and then incorporated into uncertainty quantification frameworks. This requires understanding of how the data were collected, what factors might affect how accurately they represent reality, and the scale of measurement.

3.4. Scale Mismatches

Mostly because of concerns for cost and practicality, experimentalists often conduct studies and collect data at different scales and levels of detail than are represented in most available water quality models. Thus, there is a scale mismatch between the process formulations encoded within existing models and the data that are available to characterize and/or quantify them. Additionally, the data that experimentalists collect can be challenging to use for modeling because they require a high degree of domain knowledge to translate from what was observed (e.g., a decline in dissolved oxygen concentration in a chamber experiment) to information that is useful for modeling (e.g., an estimate of sediment oxygen demand that can be applied in a model).

Scale disparity between models and available data may be both spatial and temporal. Although remote sensing data sets are advancing rapidly, most water quality sampling programs rely on grab sampling at a limited number of carefully chosen locations and may be coupled with in situ sensors where budgets permit. Data fusion techniques that combine data from multiple sources and scales offer useful examples of how to resolve spatial mismatches (Zhang, 2010). But resolving temporal mismatches between data and models can still be difficult, given measurements for many important water quality constituents and variables must still be made in a laboratory setting on physical samples retrieved from the field. Grab samples rarely capture the temporal dynamics of natural systems. On the other hand, we can now collect data using in situ sensors at rates much higher than they are typically used in models. Thus, there are challenges in both using existing data and in designing new data collection efforts to satisfy modeling needs.

Scaling issues also arise when interfacing or coupling models. As an example, 1-D-2-D hydraulic model coupling is often implemented for simulating stormwater runoff, flooding, green infrastructure design, and assessment of the best management practices because these two types of models are complementary (Buahin & Horsburgh, 2018). 1-D models accurately and efficiently simulate flows in channels, pipes, and other conduits, while 2-D models are more suitable for landscape processes and overland flows. However, combining these two types of models requires decisions regarding how they should be coupled—that is, determining how water and constituent mass are transferred from a computational cell of the 2-D model to an element of the 1-D model in a way that satisfies the principles of conservation of mass and momentum. Time stepping may also be a significant issue because coupled models may not use the same time stepping routine. The HydroCouple framework (Buahin & Horsburgh, 2018) is an adaptation of the Open Modeling Interface model coupling framework and provides useful examples of how these challenges can be overcome. However, there is still much work to be done in testing these types of methods for model coupling, in terms of both effectiveness and computational efficiency (Buahin & Horsburgh, 2015).

3.5. Provisioning of Modeling Tools

Provisioning of modeling tools refers to the setting up of infrastructure within which models are executed. The assortment of model codes, the languages and environments in which they were developed, and the variety in computational environments in which they are executed have contributed to a diverse ecosystem of water quality modeling activities. Coding languages and environments used by modelers are still many and varied, with no consensus or standards across model development efforts. While the codes for many water quality models are open source and have grown a community of developers and users, others are proprietary. Proprietary codes can be a barrier to reproducibility of work completed using these models not just because one must have a license for the model software to run it. They also limit contributions to model advancement because there is no mechanism for potential contributors outside of the model development team to add to or modify the code. This is not necessarily an indictment of the performance or quality of proprietary models, some of which are very highly regarded and have been successfully used in many

applications. Rather, it is simply an observation that proprietary codes do not lend themselves to broad use, study, and advancement within the community of water quality modelers because they are not open.

Even where the model codes and data associated with model instances (i.e., the application of a particular model to a given area) are openly available, sharing and publication of modeling and analysis workflows for reproducibility of results are currently difficult. This type of reproducibility is important in establishing the credibility of models. Documenting which model was used for an analysis, which version of the model was used, and ensuring that the computational environment in which the model was executed is available or can be reproduced by others can be difficult (Morsy et al., 2017)—especially as time passes and popular/well-known/well-used computational environments change. Analysis workflows are often considered as a semistructured activity and are not well published in scientific literature. Furthermore, there is still a large gap between the skill set of most modelers and the skill set required to effectively use high-performance computing systems for robust experimental-type simulations (e.g., model intercomparison studies, calibrations, sensitivity analyses, and uncertainty analyses). Better tools are needed to support the development, sharing, and reuse of modeling and analysis workflows, supported by better publishing of the workflows (Fu et al., 2020). For example, the recently developed open source Mobius model building system provides a virtual environmental laboratory for practitioners with little programming experience to quickly develop and evaluate watershed water quality models, making uncertainty analysis more accessible to model users (Norling et al., 2020).

Finally, as we contemplate a next generation of water quality models, one paradigm that has emerged relatively recently to address the complexity of integrated assessment studies is that of loosely coupled or component-based modeling. As in other domains, the need for model integration in simulating water quality arises because there is rarely a single model that can simulate the needed processes at the different scales and complexities required (Argent et al., 1999; Beven et al., 1980; Buahin & Horsburgh, 2018). Several framework technologies are available that enable component-based modeling, including the Open Modeling Interface (Moore & Tindall, 2005), the Community Surface Dynamics Modeling System (Peckham et al., 2013), the Object Modeling System (David et al., 2002), and others. However, these coupled modeling frameworks are still not widely enough accepted or used within the water quality modeling community for there to be robust software implementations and a robust and extensive library of model components available for coupling in new model compositions.

4. Ways Forward

The authors' combined experience and perspective in developing and applying water quality models suggest that several recommendations related to the potential improvements discussed above can be proposed. It is hoped that these (see below) provide a path forward for improving water quality modeling science, its infrastructure, and practices, with the ultimate beneficiary being progress in water quality management and planning. The ways forward in the sections below and summarized in Box 3 are based on our experience over the past decades but also coalesced from the discussions and outcomes during and after the workshop that was held at the 2018 iEMSs conference.

4.1. Bridging Gaps Between Experimentalists and Modelers

Early model development was primarily for researchers' own use to better understand the systems in which they worked (Box, 1979). The model was likely only used by one person who had a deep understanding of the model's assumptions and limitations and who was primarily concerned with the model reflecting their understanding of how the system components interacted to result in system-level outcomes—so they were implicitly or explicitly testing hypotheses regarding the inner workings of the systems. This usage/purpose fell into the category of nomothetic research (Oquist, 1978), and the modeler was likely also the experimentalist.

With increasing specialization, a division has formed between the people collecting the data (experimentalists or observationists) and modelers. This has led to modelers being able to develop more comprehensive models and frameworks (e.g., the Soil and Water Assessment Tool [SWAT], Gassman et al., 2007; Source, eWater, 2019) that are well written and documented. But it has also led to a lack of understanding among many modelers of the issues associated with collecting data or characterizing systems. This can have two

Ways forward - building on the three pillars

With Experimentalists - build stronger collaborations between experimentalists and water quality modelers to improve:

- transfer of new system knowledge to modeling;
- understanding of uncertainty/limitations of both data and models.

With Stakeholders - bridge gaps between modelers and stakeholders to enhance our ability to improve modeling:

- to make it more fit-for-purpose;
- facilitate co-learning between scientists, policy makers and communities.

With Organizations - cultivate and apply procedural knowledge for improved governance of modeling within organizations, including building:

- human capacity and knowledge;
- operational frameworks around modeling activities and cyberinfrastructure.

Box 3. Ways forward to advance the next generation of water quality models and modelers.

results. One is a tendency for modelers to treat data as truth, disregarding or not understanding possible biases and uncertainties. The other is for modelers to regard the data, or even whole subsystems, as too unreliable to incorporate in models. The advent of such models has led to a third group appearing: model users. Model users apply existing models/platforms like SWAT and Source to particular problems without modifying the code. This third group focuses on applications of models to address particular problems and, consequently, are less engaged with the model algorithms as well as the data. They may have less understanding of the simplifications, omissions, and uncertainties in the model. They may also select models they are most familiar with, which may not be optimal for the problem.

While specialization is necessary to improve efficiency, in order to move forward, researchers in water quality modeling need to strive to overcome the divisions described above. This unification is essential to provide understanding of data uncertainty and data limitations that are important for development, calibration, and evaluation of models. This requires scientists who collect data to adequately report information about data collection procedures (i.e., metadata) so that data can be interpreted by others outside of the group who collected the data. It requires modelers to document the assumptions their models are built upon, along with limitations that may affect their suitability for use. It also requires that model users and data consumers use the metadata provided to understand the limitations of the models and data being used. Building capacity for water quality modeling includes increasing access to training, providing standards and documentation, and building thriving partnerships and networks, such as through user groups and communities of practice. These are all instrumental to propel the advancement of science in water quality modeling.

Furthermore, addressing known gaps in science with a next generation of water quality models and toolkits will also require bridging across experimentalists and modelers. Here we refer to well-known gaps in our current understanding of watershed and in-stream processes along with important scientific questions that have not yet been solved. These gaps manifest themselves as assumptions and simplifications in the

formulations of our current suite of models. As an example from the hydrology community, Blöschl et al. (2019) condensed a list of 260 questions submitted by more than 200 scientists down to a list of 23 unsolved problems in hydrology grouped around time variability and change, space variability and scaling, variability of extremes, interfaces in hydrology, measurements and data, modeling methods, and interfaces with society. Given the intimate relationships between hydrology and water quality, many of these questions and their groupings are well aligned with the gaps and opportunities we have identified in this paper. Solving them will require integrated studies that pair new observations with new model formulations to test alternative hypotheses. Like Blöschl et al. (2019), we believe that the diversity among experimentalists and modelers in the community is an asset that can be capitalized upon in addressing these unsolved problems in a holistic observation/modeling context.

4.2. Bridging Gaps Between Modelers and Stakeholders

Scale-appropriate simulation of contaminant fluxes and balances is necessary to avoid disparities for models versus management versus policy, because structures, functions, and processes change with scale (Heathwaite, 2003; Quinn, 2004; Volk et al., 2008). Volk et al. (2008) argue that three spatial scales (microscale, mesoscale, and macroscale) are required for adequately describing water balance and quality, conducting economic assessments, and determining the scale-specific applicability of different models and assessment systems. The need to simulate the multiple attributes of system function across a range of scales demands us to foster the integration of diverse perspectives (Hipsey et al., 2015). Enhancing our ability to combine different sources of data, knowledge, and modeling capabilities from different groups such as scientists, policy makers, and the general public has the potential to provide novel insights into the biophysical and social-economic dimensions that the models need to represent (Mackay et al., 2015).

To this end, there is a need to encourage participation in science by engaging stakeholders in the contribution of knowledge and modeling. Bridging gaps between modelers and stakeholders enables us to improve modeling (including making it more fit for purpose) and facilitate colearning among scientists, policy makers, and communities. For instance, Schönhart et al. (2018) reported that animated discussions among modelers and stakeholders on the topics of uncertainty and future scenarios motivated adaptations of model parameterizations and the interface to the nitrogen cycle between the models Positive Agricultural Sector Model Austria (PASMA) and Modelling Nutrient Emissions in River Systems (MONERIS).

For modelers interacting with stakeholders, many authors have emphasized the importance of integrity and openness, including maintaining communication, building trust, being transparent, making assumptions clear, and maintaining neutrality (Barnhart et al., 2018; Voinov & Gaddis, 2008). Stakeholder engagement should occur over the entire process of water quality modeling, from problem framing to model development, evaluation, and scenario analysis (Badham et al., 2019; Hamilton et al., 2015). It is critical that stakeholders understand and accept the model(s) selected for a particular water management study, including a recognition of the costs associated with maintaining the model(s) over time (Loucks & van Beek, 2017). Krueger et al. (2012) argued the importance of embracing a plurality of expertise and eventually models, and enhancing the legitimacy and transparency in the processes of engagement and information elicitation.

Another important element when working with stakeholders is communicating uncertainty. Barnhart et al. (2018) present best practices for communicating uncertainty throughout a stakeholder process, including selecting the methods for uncertainty analysis based on stakeholder knowledge and information gaps, providing clearly comprehensible graphs and depictions of uncertainty for all model outputs, and recognizing that certain stakeholder groups may be underrepresented or absent from discussions—which is a form of uncertainty—and providing a mechanism for these groups to become more active in the project. These best practices should be tested in water quality modeling. In addition, new technology developments related to web, social media, and visualization to support how models are built, packaged, and disseminated should be actively adopted by the modelers to communicate uncertainty (Voinov et al., 2016).

4.3. Cultivating and Applying Procedural Knowledge for Modeling Processes

Procedural knowledge encompasses operational guidelines that manage modeling workflows, as well as knowledge management strategies and supporting tools and cyberinfrastructure. It is an emerging issue related to how modeling processes can better be governed and supported within organizations (Arnold, 2013; Arnold et al., 2020). Organizations and the water quality modeling community as a whole

can focus on improving human capacity and the knowledge base, the operational framework surrounding modeling activities (e.g., guidelines, standards, model management, and technical support services), and the cyberinfrastructure and tools available for modeling (e.g., model codes, data management and analysis tools, workflow tools, and computational resources). The recently released literature review on nutrient-related rates, constants, and kinetics formulations in surface water quality modeling (Cope et al., 2020) is a good example of a knowledge base.

The preference for relying on well-established, legacy models has become a barrier to the development and adaptation of modern modeling frameworks, even though these models do not reflect the ongoing revolution in our understanding of the water quality processes. Therefore, development of new models and modeling frameworks should be encouraged as our knowledge and technology evolve. New model development will also serve as alternative conceptualizations which, when combined with the existing models, could become part of an ensemble approach to modeling water quality (much like we use multiple climate models for climate modeling). As a technology, “loosely” coupling models in a component-based modeling paradigm is one potential path forward, but the software tools to enable this still need to improve.

Rigorous model development and application require considerable model testing, preferably in a range of contrasting environments. In recent times, public repositories of data (e.g., www.hydroshare.org), along with flexible tools to customize data into the varying formats required by models, are becoming more available. However, work is still needed to curate data collections that could be used for model development and intercomparison studies as has been progressed in other domains (e.g., the Model Parameter Estimation Experiment data set in hydrology; Schaake et al., 2006). Data solutions for modeling, including consolidation of access to environmental data and facilitation of data transformation and processing, are being investigated (Laniak et al., 2013). Such repositories and services may provide a way for new or custom models to fast-track their testing. Further, if repositories and tools were expanded to show model outputs against measured data using interfaces suitable for nonmodelers, this may assist with the acceptance of custom models and ease the pathway for new developments.

The choice of software tools needs to be improved to meet operational goals of decision making and to bridge the gap between science and management (Argent et al., 2016). If existing models or tools are to be used, Van Voorn et al. (2016) provide a checklist for assessing model credibility, salience, and legitimacy, and Mateus et al. (2018) guide model managers in selecting tools and models that meet expectations in scope and experience. Real-time monitoring and analysis frameworks (Wong & Kerkez, 2016) and spatial workflow environments (Nielsen et al., 2017; Zhang, Bu, et al., 2017) demonstrate technical innovations that still need to be operationalized by agencies. Yet, these innovations in software tools should not distract from the need to build rigorous operational protocols that simplify technical procedures and ensure access to relevant knowledge in a timely manner (Argent et al., 2016; Arnold et al., 2020).

To ensure access to knowledge, ensure transparency, and enhance reproducibility, intellectual property rights to software tools must be managed appropriately (Arnold et al., 2020). Several open source codes are now available for water quality and aquatic ecosystem prediction (Fu et al., 2019; Hipsey et al., 2015). For instance, there is a substantial worldwide SWAT community, and there has been much investment in educational resources (e.g., videos, manuals, and handbooks), in updated SWAT literature databases and the development of supporting tools to aid the setup, evaluation, and assessment of SWAT. Future development should follow the development of flexible model libraries or even more granular model components (Buahin & Horsburgh, 2018), rather than the adoption of a single model of choice. Soundly constructed model libraries or interchangeable components may allow us to identify levels of process complexity and scale that are adequate to capture trends in observations (Hipsey et al., 2015) while enabling more flexibility in composing models that better meet project needs.

The authors advocate for a research structure that includes open sharing of all elements of the scientific process (ideas, models, tools, and data) as being essential to link theoretical developments and model infrastructure (Hipsey et al., 2015). This should also include assessment protocols for model performance for a rigorous validation of models (both quantitative and qualitative methods), to create standards, a common vocabulary supporting comparisons and synthesis between model applications (Harmel et al., 2014), as well as digital watershed observatories as platforms for engagement and knowledge exchange between watershed scientists, policy makers, and local communities (Mackay et al., 2015).

5. Conclusion

Progress in the science of water quality modeling has somewhat stalled. While there have been increasing numbers of publications on water quality modeling case studies and improvements to existing models and techniques, challenging water quality issues remain difficult to solve. This may in part be due to lower investments globally on the cutting edge of experimental modeling and analyses, fragmentation of subdisciplines and special interest groups on water quality model development, and limited data availability and characterization and quantification of uncertainty.

This review provides a synthesis of some major gaps in the current science and practice of watershed quality modeling along with positing areas in how we can do better. More specifically, we have discussed four key topics in system representation: environmental interfaces, in-stream water quality and process interactions, soil health and land management, and urban areas. While each topic has its own specific characteristics, common themes have also emerged across topics. The first theme is system complexity. This complexity is evident in every part of the land to water systems, from smaller scales at environmental interfaces and local system variations to watershed-scale water quality monitoring and modeling, to the complex interactions between the water systems and associated social-economic systems. Achieving a balance between representation of system complexity and model parsimony thus requires clarity in societal concerns and the intended use of the models, as well as the contextual knowledge and information content in the data available for the problem at hand.

The second theme involves a lack of understanding of certain parts of system behaviors that can be vital in representing water quality processes. Examples include: the processes occurring at environmental interfaces, which may represent a small increment of the total travel time and flow path, but can scientifically alter constituent concentrations; the relationships between hydrodynamics and water quality; and the role of soil biology dynamics and related soil biological solutions in changing surface water's suspended sediment and chemical properties.

The third theme is the potential for new sources of data to advance system understanding. Emerging data sources, such as satellite data for geospatial digital soil mapping, environmental tracers such as isotopes and biomarkers, and new sensor technologies and unmanned aerial vehicle for in situ high-resolution water quality monitoring, can dramatically improve our understanding of system behaviors.

In addition to system representation, we also discussed five topics related to the modeling process: QC of monitoring data, parameterization and calibration, uncertainty assessment and management, scale mismatches, and provisioning modeling tools. QC of discrete monitoring data is a mature enterprise, with standardized procedures in data acquisitions and assessment protocols. Future development should focus on development of tools to facilitate better visualization and presentation of the data so that the data (and its quality) are more understandable and accessible by the public.

In terms of model parameterization and calibration, while calibration schemes are generally well established, there remains significant difficulty in calibrating models so that they are representative of the relevant processes in the system, and so that the main variable or criteria of interest is modeled with sufficient confidence. Efforts to improve model parameterization and calibration should be directed to not only increase data and information on system functioning but also to development of more comprehensive suites of objective functions that properly capture the quantity of interest.

Uncertainty analysis is important in estimating risk associated with using certain model predictions, diagnosing model weaknesses, and suggesting new experiments to improve the accuracy and precision in model predictions. Significant improvement is still needed to enhance our ability to better identify the sources of uncertainty, advance uncertainty quantification and attribution techniques, combine these with qualitative techniques, and develop approaches to constrain uncertainty.

Issues in scale mismatch between most available water quality models and data collected by experimentalists, and at interfaces between coupled models, remain difficult to resolve. Better understanding of the uncertainty arising from the scale mismatch is warranted. Investigation of data fusion techniques can be useful in approaching the scaling issues. Additional barriers in advancing the water quality modeling process include proprietary codes for some water quality models, difficulties in sharing and publication of model workflows for reproducibility of results, a lack of skills in using high-performance computing systems for

robust experimental simulations, and the adaptation of loosely coupled or component-based modeling for more robust software implementations of integrated modeling frameworks.

To conclude our synthesis, we have provided three recommendations to move forward for water quality modeling science, infrastructure, and practices. First, we need to build stronger collaborations between experimentalists and water quality modelers, so that knowledge in system understanding can be adequately transferred to modeling, and uncertainty and limitations of the data and models are appropriately documented and interpreted. Bridging gaps between modelers and stakeholders is also vital to enhance our ability to improve modeling (including making it more fit for purpose) and facilitate colearning among scientists, policy makers, and communities. Finally, we advocate for cultivating and applying procedural knowledge to better govern and support water quality modeling processes within organizations, including human capacity and the knowledge base, the operational framework around modeling activities, and cyberinfrastructure.

Data Availability Statement

Data were not used nor created for this research.

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