Challenges for water-quality research in the new IAHS decade on: *Hydrology Under Societal and Environmental Change*

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Abstract Emerging water quality research challenges of the next decade are related to understanding how the function of complex catchment sub-systems interact and co-evolve in response to an unprecedented level of environmental change. Several high-level challenges are identified in this paper that relate to those of the new IAHS thematic decade ("*Panta Rhei*": 2013–2022), but explored within the specific context of water quality science. We review current research trends and outline the need for new approaches able to deal with complexity, non-stationarity and uncertainty in future scenarios. We then identify opportunities that exist for the community-driven integration of the diversity of models of hydrology, biogeochemistry and society, with environmental sensing approaches and cyber-infrastructure as a way to integrate process-driven and data-driven approaches for exploring river basin health and water quality dynamics. By embedding our collective efforts in development of a global network of catchment observatories, we believe we can support further knowledge discovery through facilitating comparative analyses and synthesis activities.

Key words water quality; river health; aquatic systems; new IAHS decade; network science; open source

INTRODUCTION

Sustainable river basin management in the face of global population growth and climate change is one of the most profound challenges confronting society (Ostrom, 2009; Vorosmarty *et al.*, 2010). Our freshwater systems have changed more rapidly in the past 50 years than at any other time in human history. Water quality degradation and issues of water security are driven by urban, agricultural and mining developments, and span both developed and developing nations. Great efforts have been made across the different regions of the world during the last few decades to monitor and describe freshwater quality problems and to reach more sustainable, holistic and integrated water management practices. However, the pace of contemporary environmental change is expected to amplify the drivers of water quality degradation that we already face.

As a result there is an urgent need for not only better overall knowledge about the water quality situation globally, but also a deeper understanding about processes and catchment dynamics involved in water quality degradation ranging from the point to the basin scale. While substantial progress in understanding how catchment condition relates to water quality response has occurred over the last two decades, we have surprisingly limited ability to predict water quality across a range of temporal and spatial scales relevant to decision making, making it difficult to clearly define long-term sustainable management approaches that satisfy the range of stakeholders.

For hydrological science to meaningfully contribute to decision making and policy development, we must seek new knowledge on the complex pathways of carbon, nutrients and pollutants through the diverse array of aquatic environments from catchment headwaters to the ocean. More efficient water management and remedial efforts need to be increasingly based on scientific knowledge that is well integrated across disciplinary and geographic boundaries. This requires the scientific community to embrace this challenge, and such impetus is being driven by the new IAHS scientific decade initiative (2013–2022) – *Panta Rhei* (Montanari *et al*., 2013). Here we attempt to define specific challenges facing the hydrological science community where research effort can be focused within the context of water quality science.

Scientific questions relevant to the new IAHS science initiative could be: What are the key natural and anthropogenic controls that shape the behaviours of changing catchment systems and their impacts on freshwater quality? How can we effectively bring together theoretical hydrology, experimental hydrology and new measurement techniques to advance our knowledge of water quality processes for the future? How can the typical time scales of change be identified? How do we estimate and predict the behaviours and patterns of freshwater quality, with a suitable level of uncertainty assessment, to support risk evaluation and decision making?

This paper further assesses these challenges and offers suggestions for a way forward. Note that our focus is not specifically on research associated with water quality treatment and supply, but rather has an environmental and source water focus. In particular, we explore the potential for advancing basin-scale water quality research through improved observation networks for collecting a wide array of environmental and societal data, in conjunction with multi-disciplinary, multi-scale predictive capacity suited to supporting both prediction of river basin systems and their management, whilst also facilitating the advancement of our fundamental understanding.

CHALLENGES IN WATER QUALITY RESEARCH WITHIN THE IAHS COMMUNITY

One of the major challenges in river basin science is understanding how the function of complex catchment sub-systems interact with each other and co-evolve in response to rapid and often unpredictable levels of environmental and societal change (Wagener *et al*., 2010). This challenge has been the focus of targeted research particularly with respect to water quantity for the past decade (e.g. Blöschl *et al*., 2013), and substantial advances have been made in describing catchment hydrological function. However, this challenge becomes significantly more complex as we broaden our scope to consider water quality. Here we align three high-level challenges we have identified with the three general themes outlined within Montanari *et al.* (2013).

Challenge 1 – Understanding controls on water quality dynamics

Our understanding of the effects of land-use change and catchment management practices on water quality outcomes has advanced considerably over the past decade. However, there remains a need to more deeply understand the spatio-temporal dynamics of nutrient and pollutant transport and transformation. These are explored briefly below as four specific challenges:

Quantifying pathways and processes that shape the spatial and temporal patterns of nutrients, sediment and pollutants, and links to new hydrological theory Numerous authors have explored how the degree of human influence manifests in nutrient export from landscapes, both in terms of the degree of land-use change and population expansion (e.g. Spargue & Gronberg, 2012). Similar studies have been done for looking at pathogen (Ferguson & Kay, 2012) and non-nutrient contaminants (Cook *et al*., 2011). Land-use changes are highly catchment specific, being a combination of deforestation or reforestation, urbanisation, etc. But in general terms, the question remains: how does the rate and extent of these changes manifest in water quality attributes over the local, sub-basin or basin scale? Sivapalan *et al.* (2012) pointed out a research challenge, in terms of nutrients, as being able to parsimoniously understand how uptake kinetics and stoichiometry are linked to hydrology and how the serial processing across uplands, riparian zones and stream networks mediates the export signature.

Ultimately, this requires the development of improved ability to assess how nutrients and contaminants interact with or depend upon basin geomorphology, soils, vegetation, land use and drainage systems. Central to this is our evolving understanding of the underpinning hydrological pathways (Hale, 2013; Klaus *et al*., 2013). Both nutrients and contaminants have phases that adsorb to suspended sediment, which implies that the soil condition and spatial and temporal patterns of erosion and sedimentation are also important aspects. Untangling these pathways and connections is critical and links to the broader challenges within the IAHS decade. This can be advanced through better landscape assessments and application of new experimental methodologies, for example, using isotopic data and inverse modelling (e.g. Yevenes & Mannaerts, 2012), or through use of biomarkers or other tracers to support source identification.

However, an important challenge is not simply identifying the source, but more deeply understanding how the biogeochemical transformations are superimposed on the underlying transport pathways. In particular, understanding the fate of redox sensitive compounds requires that hydrological pathways are well understood given variability in aerobic *vs* anaerobic processes and conditions in the surface and sub-surface (Hall *et al*., 2012). Sensitivity to redox dynamics also requires that we consider the varied geochemical controls and consider how these can regulate nutrient stoichiometry and contaminant availability across natural and modified landscapes (Salmon *et al*., 2010). Organic to inorganic (e.g. DOM:DIM) partitioning in surface *vs* sub-surface flows is also an area of research relevant to lake and river water quality that is often overlooked (Petrone *et al*., 2009; Miller, 2012).

The hyporheic zone has long been identified as an important hotspot (Gu *et al*., 2012) relevant to water quality since it links hillslope biogeochemical cycles to instream processes. The role of the hyporheic zone in regulating the passage of different forms of pollutants is an increasingly important area of research, particularly since riparian preservation, restoration and revegetation is a common management practice.

Finally, linking catchment hydrological change to water quality and aquatic system "health" is an area where more research effort should be focused. Whilst it is known that changing catchment condition will change patterns of sediment and nutrients in downstream lakes and waterways, clear links between catchment condition and actual biotic health remain elusive. A key challenge is therefore to develop approaches to link land-use change and catchment processes, waterway biogeochemistry and ecological health, across a range of scales (Hong *et al*., 2009).

Ecohydrological/biogeochemical feedbacks and controls on water quality Catchment systems are inherently changing and the extent of change is mediated by complex climate–soil–vegetation–society feedbacks. Whilst our process understanding has advanced considerably, subject to the challenges outlined in the previous section, our ability to understand future trajectories of water quality would greatly benefit from more detailed analysis and identification of feedbacks and controls. Well-documented feedbacks exist in some cases, e.g. temporal eutrophication, or erosion following clearing of natural vegetation. Other less obvious examples also exist, for example self-regulating connections within coupled physical-ecological systems (e.g. Ibisch *et al.*, 2006; Colleti *et al*., 2013).

As our analyses and models further account for human-systems our understanding of these controls on water quality should extend to include management practices. For example, the relationship between fertilizer application and downstream manifestations of water quality is subject to stoichiometric control during vegetation and soil nutrient metabolism along hillslopes. Similarly, the revegetation of riparian zones has been shown, paradoxically, to increase phosphate export as it also served to reduce stream turbidity and subsequent phosphate sedimentation following exclusion of livestock (McKergow *et al*., 2003), but is this generalizable? How do we balance these potential negative effects against positive effects on biodioversity (e.g. Davies, 2010)? Understanding these complexities is required for sustainable management solutions (Bunn *et al*., 2010).

Over longer time-scales, prolonged water quality degradation drives policy change in water abstraction, land management and pollution limits. As we tackle large integrated basin management problems, further research focus is required to resolve the non-linear dynamics across the range of scales from individual sites to the scale of the entire river basin. Ultimately, understanding the most important feedbacks and controls can help us evolve our thinking about land and water systems and target our management effort in the most efficient way.

Understanding the effect of non-stationarity in climate on catchment biogeochemical cycles Water balance modelling typically assumes catchment systems are in quasi-equilibrium over long-term time integrations, assuming stationarity in climate forcing, and periodic hydroclimatological modes (e.g. El Nino, etc.). In the case of non-stationary climate forcing, significant and non-linear changes in hydrological function have been reported to occur. Under these conditions, assumptions in our models about vegetation extent and function, and rainfall–runoff relationships, prevent us resolving the co-evolution of catchment dynamics in response to underlying climate shift. Advances in our models are improving our ability to predict changes in water balance and runoff; however, there is a paucity of literature on how climate non-stationarity may manifest in nutrient and pollutant pathways, and therefore the water quality of receiving waters. As a result, water quality models are conditioned on parameterizations that may not capture non-stationarity. Persistent shifts in climate may not only change nutrient export rates, but also the underlying pathways of nutrient transformations, since they are each uniquely sensitive to temperature and hydrological regimes, either directly or indirectly. They may therefore impact organic:inorganic nutrient partitioning and the underlying N:P stoichiometry of nutrient loads.

Resilience of biogeochemical pathways and aquatic systems to change In general, aquatic systems are vulnerable to deterioration when key system functions are pushed over thresholds, resulting in the loss of resilience and impacted states that lack integrity and diversity, and serve poorly in provision of ecosystem services. Freshwater systems are subject to direct pressures from pollutant loading, but this is also indirectly controlled through changes in soil health and climatic or anthropogenic induced changes in hydrological processes within the surrounding catchment. It is well established that nutrient loading leads to eutrophication and associated deterioration in water quality that is difficult to remediate (Smith, 2003). Similarly, altered patterns of hydrological forcing can alter the balance of nutrient cycling in some systems and induce changes and regime shifts (Sharip *et al.*, 2012).

However, understanding how changes in hydrology, nitrogen, phosphorus, pollutant loading and other factors interact to manifest in water quality condition still remains the subject of uncertainty (Brookes & Carey, 2011; Harpole *et al*., 2011), because the controlling factors for each can be highly variable in space and time, and the lag times between environmental change and changes in water condition are not well understood. Furthermore, it has been identified that some level of anthropogenic-induced nutrient enrichment may in fact lead to improved conditions until thresholds are reached (Gal *et al.*, 2009), though understanding when and why these points occur is complicated – the response of aquatic systems to positive or negative stressors is non-linear and subject to hysteresis (e.g. Scheffer *et al*., 2001; Jeppesen *et al*., 2005). Only conceptual models, idealised field experiments, and rudimentary numerical models have been used to tell us anything about these dynamics. Understanding how they manifest in diverse real-world systems is ultimately required, and this needs new integrated modelling approaches to holistically assess how land-use change, river-basin engineering and climate variability combine to affect water quality and biodiversity (Holling, 2001).

Challenge 2 – Predicting water quality dynamics from point to catchment scale

Bearing in mind the conceptual limitations outlined above, models of rivers, surface drainage systems, lakes, wetlands and estuaries form an increasingly important part of our water management analyses and for assessing scenarios of change. Their growing importance is evidenced in the sharp rise in the number of published applications in the literature (e.g. see the analysis of lake water quality model in Trolle *et al*., 2012). They are used as "virtual environmental laboratories" for developing ecological theory and to study feedbacks and sensitivities of particular sites in response to changes in natural forcing and through their interface with human systems (van Nes & Scheffer, 2005a).

Despite our substantial progress in model development and increased reliance on outputs of model scenarios for policy formulation, it is argued our best models remain unsuited to rigorously tackle these challenges (Mooij *et al.*, 2010; Rode *et al.*, 2010; Sivapalan *et al*., 2012). This is unlikely to change as we move further into higher dimensional prediction problems that integrate interactions between water quantity, water quality, ecological health and society. Below we highlight several key areas that could benefit from further research focus over the next decade:

Interdisciplinary model systems able to account for physical–chemical–biological interactions Several initiatives have emerged to allow prediction of water quality at the river basin scale (e.g. SWAT, HSPF, HYPE, MIKE-SHE), or at the scale of individual aquatic systems (e.g. FABM, CAEDYM, QUAL2K, MIKE11, DELFT3D). Whilst these have proved powerful to advance our understanding, they are heavily based on empirical relationships that do not fully cover the dynamic interactions between hydrology, hydrodynamics, geochemistry and biological systems across the required range of scales and environments.

A major barrier is the simple practical aspect that there are lots of highly-disciplinary models, which cover a wide variety of model approaches, but limited open-source codes and standards that bind the modelling community or facilitate integration efforts. This is necessary to promote adoption and enable us to avoid the problems of "reinventing the wheel" and "tunnel vision", which characterize the community (e.g. Mooij *et al.*, 2010). Given the highly inter-disciplinary nature of water quality science, a community approach for hydrological, biogeochemical and ecological models that goes beyond disciplinary boundaries is needed to focus research effort.

Reducing uncertainty Managing uncertainty in water quality models is difficult as they are usually highly over-parameterized (Arhonditsis *et al*., 2008) and significant uncertainty exists related to inputs, model structure, and parameter selection. Novel approaches such as Bayesian calibration frameworks are emerging as powerful, albeit computationally demanding, approaches for model assessment (Ramin *et al.*, 2010; Dietzal & Reichart, 2012). The adoption of these methodological advances routinely in our model studies will greatly improve our modelling practice; however, applications to date are limited to relatively simple models (Rode *et al.*, 2010).

One of the main challenges is that water quality models that resolve spatial heterogeneity are inherently multi-dimensional and contain extensive sets of linked equations that govern the interactions of key components (sediment, nutrients, primary producers, etc.) from the scale of a numerical "cell" or hydrological unit, to that of the entire domain. Modellers rely on testing model performance at point scale, and it therefore remains unclear whether the constitutive equations, which are mostly based on laboratory or plot-scale relationships, combine to successfully capture system-scale emergent dynamics, including stability and resilience, and the general response pathways to change – described here as "emergent uncertainty". New procedures are required to validate model performance against suitable metrics that characterise multi-scale catchment patterns and dynamics to give us confidence that the models are able to capture such behaviours.

Connectivity between catchment sub-systems The main challenge in exploring water quality dynamics in complex landscapes is the inherent spatial heterogeneity and highly dynamic nature of resource pathways (e.g. transport processes and biogeochemical pathways such as primary production, nitrogen fixation and denitrification, mineralisation). Spatial patterns and diversity in ecosystem attributes play a crucial role in shaping function and resilience, seen across the continuum from individual organisms up to whole landscapes (van Nes & Scheffer, 2005b; Kratz *et al*., 2007). We must also consider that real-world landscapes are comprised of networks of systems that link together (e.g. hillslopes, streams, rivers, wetlands, lakes, estuaries) – water flowing to the sea links upstream to downstream systems, stream channels to floodplains, and riparian wetlands and surface waters to groundwater. Connectivity is critical in shaping habitats and patterns of resource flow, by regulating the transfer of water, energy, organisms and elements. Each sub-system in a river basin network has a different ability to process carbon, nutrients and other contaminants and its own characteristic biogeochemical signatures (Harris, 1999).

If we consider that humans have influenced aquatic system connectivity more than almost any other system attribute through river-basin engineering (Nillson *et al*., 2005; Vörösmarty *et al*., 2010), we must therefore understand how these changes in connectivity manifest in system-scale dynamics, such as resilience and stability, and how they combine with other stressors to potentially lead to undesirable and persistent shifts in water quality condition.

Whilst we have some well-demonstrated model platforms for simulating individual sub-catchments or aquatic systems, to understand the role of connectivity in shaping water quality and ecosystem health we must be able to consider the interconnectedness of hillslopes, hyporheic zones, rivers, floodplains, lakes, estuaries and coastal lagoons to fully understand the extent of consequences of changes in land use – to date such studies linking the whole system have been rare. A major challenge here relates to the mismatch in resolution requirements between connected systems (Rode *et al.*, 2010). New approaches and software integration efforts are required to enable such investigations.

Regionalization and predictions in sites with no or limited monitoring The last IAHS scientific decade focused on Predictions in Ungauged Basins (PUB; Blöschl *et al.*, 2013) and resulted in a number of hydrological methods being put into practice. Yet, very few included a water quality aspect. Water quality predictions are often empirically based and involve compilation and exploratory analyses of geographically explicit predictor and response data, by non-linear regression techniques. Process-based water quality models used for regional analysis of ungauged basins are either: (a) based on *a priori* parameter values and poorly compared to monitoring data as they only cover part of the system and are difficult to validate (e.g. the soil leaching to groundwater), (b) using semi-distributed parameter sets with separate parameters for each gauged sub-basin, transferred to nearby ungauged basins, or (c) using homogenous parameter values based on simultaneous calibration of multi-basins in the whole region (Strömqvist *et al.*, 2012). Large-scale models, distributed and homogenous both in inputs and in calibration, have been widely discussed in the literature, but the success of calibrated parameters in independent basin validation depend on the processes represented by the parameter, with some processes better represented than others (e.g. Dunn & Lilly, 2001; Marachal & Holman, 2005).

Process-based water quality modelling is normally complex and dependent on many internal variables, which makes it difficult to apply new statistical methods developed in the PUB context for parameter constraints. Instead, methods have been suggested that fix parameters step-wise for parts of the flow paths by evaluating internal model parameters against observed data for multi-variables over large regions (e.g. Arheimer *et al.*, 2011). If variations in land use, soil type, lakes, river routing and emissions are explicitly accounted for in the calibration, a uniform set of parameters determined by calibrating the model once over the entire modelled region should yield a reasonable model validation. This, in turn, suggests the ability to make reasonable predictions also in ungauged basins within the modelled multi-basin region, but this is rarely evaluated systematically. For efficient water management it is important to identify problem areas and allocate measures where they are most effective and sources and sinks must be predicted for large regions, including where monitoring data is lacking and for non-stationary conditions, and there is still a challenge in developing regionalisation methods and suitable modelling frame-works.

Challenge 3 – Science into practice

The previous challenges implicitly consider anthropogenic drivers and socio-economic dynamics in their formulation. Yet, a further challenge that we must address as a science community, identified in Montanari *et al.* (2013), is the on-going engagement of science within management and planning frameworks. Whilst this in itself is not like the science-motivated challenges suggested above, there is a need for new integrated approaches to basin management and decision making which are able to simultaneously bring together scientists and stakeholders involved in catchment management, governance, and agricultural and urban development, with a focus on improving water quality as part of basin sustainability.

Linking water quality to societal health outcomes Aside from improving ecosystem conditions, the most important motivation to improve water quality is to ensure safe water for potable and recreational use. Yet, the highly distributed nature of water supply networks and dynamic nature of environmental and social systems has meant that connecting river basin condition with human health and epidemiological assessments has been particularly challenging.

Linking water quality data and disease caused by pathogenic organisms has seen the most attention, with other examples such as fluorosis in parts of India and nitrate toxicity. However, this is fairly limited and linking data about chemical contaminants, such as heavy metals, pesticides, endocrine-disrupting compounds and other pharmaceuticals, is still extremely difficult, particularly since for these contaminants the health effects tend to be chronic and integrate over long time exposures. Nonetheless, quantitative connections between water condition and human health (and associated economic costs) will ultimately provide essential baseline data with which management decisions can be confidently based on.

Catchment engineering and water quality At all scales a wide array of catchment engineering initiatives are routinely implemented either for the direct management of the water cycle and water quality, or for other reasons, with indirect effects on water quality. These initiatives are driven by the need to enhance water efficiency and improve water security as climate patterns change and populations expand. Examples include surface or sub-surface drainage engineering, stormwater harvesting and managed aquifer recharge, and in areas where water is scarce, increased reliance on desalination water. In cities, the increasing application of decentralised water supplies and Water Sensitive Urban Design (WSUD) practices (e.g. constructed wetlands, biofilters) can substantially improve water quality in urban waterways.

A substantial research investment is already being made in improving the efficiency of these practices, for example in the efficiency of aquifers, biofilters and/or wetlands for stripping nutrient and non-nutrient contaminants. However, research into quantification of the ecosystem services these activities provide is urgently required to ensure that the positive benefits of best practice are encouraged over less efficient alternatives (see Wong & Brown, 2009). Further, whilst individual engineering projects may have local impacts, there is a not always a clear understanding of how the individual projects sum to influence basin-scale water quality trends. To prevent the *ad hoc* re-engineering of catchment systems, project approvals need to be guided by a larger vision for overall river basin sustainability (Roy *et al.*, 2008), and this requires further research into areas of co-operative governance and participatory planning.

Participatory planning and management systems Public participation and involvement of stakeholder groups have been identified as important for successful implementation of pollutant reducing measures. It is argued that stakeholder interactions enhance the transfer of knowledge between stakeholder groups, developing a common perspective on the problems and their possible solutions, going beyond individual stakeholders' problem perception and solution space (Pahl-Wostl, 2007). In natural resource management, this is frequently referred to as social learning (Mostert *et al.*, 2007; Muro & Jeffrey, 2008) and facilitates more adaptive water management. In parallel with the demand for stakeholder involvement in natural resource management, there is a rising expectation that computer-based models may serve as a basis for these collaborative actions (Andersson *et al.*, 2008; Becu *et al.*, 2008; Rauch *et al.*, 2012). Success stories of collective development of management plans for eutrophication control based on participatory modelling of water quality have been reported recently (Arheimer *et al.*, 2007; Alcan Olsson *et al.*, 2011). However, such actions need reliable and transparent user-friendly tools. The development of socio-technical models, information systems and user-interfaces is large, and yet, the validation of results and explanation of assumptions is often lacking, which restricts the credibility and uptake among users. The challenge of making these tools scientifically sound still remains.

A WAY FORWARD – COMMUNITY DRIVEN KNOWLEDGE DISCOVERY

The scale of the challenges presently facing the research community requires a large and co-ordinated effort (Montanari *et al.*, 2013). Here we advocate several areas of research priority and community-level initiatives targeted at helping us tackle the complexity around catchment interconnectedness, non-stationarity in climate and socio-economic drivers, and our uncertainty in future scenarios. A key focus is to explore approaches that facilitate the integration of the diversity of models of hydrology, hydrodynamics, biogeochemistry, ecology and society, with the rapid developments in environmental sensing systems and cyber-infrastructure.

Open source model communities

Nowadays, many hydrological models are open source (e.g. HYPE, SWAT, PIHM, QUAL-2K) and many now simulate water quality. Attempts are made to create active communities collaborating on code development and sharing experiences with the ambition of speeding up the development and testing procedure by involving more people and not reinventing established algorithms. Moreover, the transparency involved will help for quality assurance and facilitate the reviewing process of scientific work, as documentation is open with easy access.

Beyond these individual community model initiatives, the advanced analysis and more widespread uptake of water quality models for decision support requires flexibility to join a range of coupled models of hydrology, water body hydrodynamics, biogeochemistry, aquatic ecology and socio-economic interactions. In the face of increasingly complex questions being asked of models, flexibility in models and model coupling is essential. To this end, efforts to develop a model typology and flexible numerical frameworks are required and can be achieved by defining the architecture of the key numerical and software elements to facilitate and harmonize development efforts. Initiatives such as OpenMI are working towards this for model coupling.

Importantly, the approach we should be advocating when considering model development should not mandate a particular model or approach, but rather a community library that serves as a collection of flexible model objects that can be used within custom system idealisations based on the modellers own scientific reasoning. This will support modellers by providing standards and a common vocabulary where hypotheses and experiments with model structures and integration of different methods can be explored and better scrutinized (Schmolke *et al*., 2010).

Complex models require a suitable level of observational data for validation, which is often not available to provide a high level of validation. Instead, approaches must be cognisant that ecosystem complexity is often paramount in shaping dynamics, but that we are constrained by the need for testable models. Therefore, a structured approach to gauge the complexity requirement is necessary, and flexibility in model formulation and integration of approaches must be factored in. To this end multiple model comparisons and ensemble model predictions should be encouraged.

Spatial dimensionality and system compartmentalisation will increasingly be simulated via a diverse array of physical drivers (e.g. hillslope model, wetland/floodplain model, river model, lake model, estuary model) and new generic and flexible frameworks for simulation of biogeochemical/ ecological "components" are required. Improved coupling interfaces to physical drivers are required to accommodate this diversity. Since there are multiple physical models necessary to cover the diverse scales of interest, we must accommodate a generic approach where processes are split to separate the components dealing with transport and mixing, and those dealing with reactions, transformations, growth, etc. This approach has been reported in various contexts; however, to deal with the complexity of networks of aquatic environments and the terrestrial–aquatic interface, a deeper consideration of integration of model approaches is necessary.

Sharing data

Investing in the development of large-scale datasets is a major undertaking for management agencies though it is routinely underutilised. Through sharing these datasets agencies can (a) see their data more thoroughly interrogated and (b) contribute to regionalisation and synthesis efforts. Many of the challenges described in the earlier section cannot be resolved at the scale of an individual catchment, and only through comparative analyses of many catchments that span many different climatic and land-use contexts can we develop a generalised understanding. Within hydrological science this has been well exemplified through initiatives such as MOPEX, and through synthesis activities where the power of comparative analysis has been demonstrated (e.g. Blöschl *et al*., 2013). However, to date these initiatives have generally been difficult to undertake between countries, and have generally not included water quality attributes.

At the national level, however, successful initiatives of data and knowledge sharing between scientists can be found. For instance, the Consortium of Universities for the Advancement of Hydrologic Science, Inc. (CUAHSI) was founded in 2001 in the USA, and includes 501 research organizations representing more than 130 USA universities and international water science-related organizations. CUAHSI develops infrastructure and services for the advancement of water science and the data sharing platform (EarthCube). The Critical Zone Observatory (CZO) initiative similarly collects and hosts information on hydrological variables and landscape processes.

Grass-roots initiatives on specific issues have also been successful, such as the Global Lake Ecological Observatory Network (GLEON), whose databases collect real-time sensor data from a variety of lacustrine environments from around the world. This data is publically accessible and has been used to conduct numerous comparative studies (Hanson, 2007).

Standards and improved validation metrics

Attempts have been made to develop standards in catchment and aquatic system models (e.g. the OGC suite of services, WaterML, Open Geospatial Consortium, WMO), but to date they have received limited uptake (Schmolke *et al.*, 2010). This is especially the case for models of water quality. To facilitate cross-site comparisons – as is required for regionalisation of predictions and synthesis – it is necessary for similarities in approach (Jakeman *et al.*, 2006), and also a requirement to develop a common nomenclature and controlled vocabularies.

The encouragement of standards in reporting model form and performance can further advance the quality of our models. General practice encourages us to test model skill at predicting changes in biogeochemical and water quality variables at scales that do not fully capture the range of those predicted by the model. Decisions about validation approach are also often *ad hoc*, based on the specific data and experience of the modeller, and a general desire to report on the suitable performance of the model. This site-specific and disciplinary focus of validation approach ultimately limits synthesis and transferability of knowledge between sites and applications.

As more data streams for model assessment are being considered there is an opportunity to review current approaches that can be used to assess model performance, and to devise general strategies to improve our confidence in model predictions. The widely agreed upon assessment protocols for model performance that encourage a more rigorous, multi-scale, validation of models, will serve to create standards and a common vocabulary to support comparisons and synthesis between model applications. Such assessments must extend to include a range of metrics and characteristic signatures relevant to water quality condition, including not just validation of key state variables, but also validation against process data, and comparison against system-level emergent properties, patterns and relationships (where possible). It is envisioned that the community–driven adoption of standards and model validation metrics will lead to more rigorously assessed models and this will accelerate advances in model accuracy.

Embracing new technology

Whilst we have seen an explosion in the diversity of sensors relevant to hydrology in the past decade, the next decade holds great promise for new measurement technologies able to provide *in situ* water quality data. Real-time measurement of water quality properties including DOC, chlorophyll-a, nitrate and turbidity are more frequently being reported and advanced measurements such as stable isotope measurements (Herbstritt *et al.*, 2012), heavy metals by DGT (Warnken *et al.*, 2012), and biosensors. Biotechnological advances are also opening up opportunities for real-time microbiological measurements, for example of pathogens (Lopez-Roldan *et al.*, 2012). To complement these data-streams with high temporal resolution, satellite products for high spatial resolution of water quality in wetlands, large rivers and lakes are also creating new opportunities for understanding controls on water quality (e.g. Ng *et al.*, 2012).

Importantly, our increasing emphasis on understanding the intertwining dynamics of humans with catchment systems means that novel approaches to collect non-traditional data sets are also required. The use of unstructured data, for example qualitative data on catchment use and public perception derived from automatic web searching, or data collected through citizen science initiatives driven by catchment management groups, can be integrated with tradition data streams.

Integration of models with observing systems

Developments in advanced sensing technologies, outlined above, and the accompanied progress in cyber-infrastructure and computational techniques for data analysis and hydroinformatics have created new opportunities for understanding how environmental systems respond to change (Hanson, 2007; Solomatine & Ostfeld, 2008; Porter *et al.*, 2009). Since our process models are highly over-parameterized and rarely validated across the breadth of model states relevant to the characteristic scales of change we are interested in, many have pointed to the emerging opportunities associated with sensor networks as a means to improve models, for example by reducing model uncertainty through data assimilation. Ultimately, the on-going interaction of models with observations can allow us to capture the systematic feedbacks between observation, prediction and management, under continuously changing conditions (Reed *et al.*, 2006).

Yet to date there are limited examples of model–data integration in the context of water quality prediction. This is most likely due to the difficulty and expense in collecting sufficient water quality data and since data assimilation to reduce error in complex water quality models remains impractical from a computational point of view. Nonetheless, further research focus in this area is likely as novel *in situ* sensors enter the market and spatial assessments of water quality variables from remote sensing increase. As computational ability continues to improve, innovative methods for integration of water quality data with model assessments will be required.

Such advances also provide new opportunities to deal with issues of uncertainty in forecast predictions. The integration of models within observing systems can be based on a learning framework that supports adaptation of model structure and function and potentially the subsequent adaptation of the observing system in response to model shortcomings. However, targeted research and innovation is needed in this area to define advanced diagnostic metrics for assessing catchment function and model performance (also discussed above), thereby extending our focus from assessment of state variable predictions to include characteristic hydrological signatures and system-scale emergent relationships. By iteratively adapting models of different scale and complexity to the observational data within a near-real time framework, as guided by the theoretically-based catchment metrics and signatures, lessons from observational data may be gradually incorporated into our model systems and predictive ability (Fig. 1).

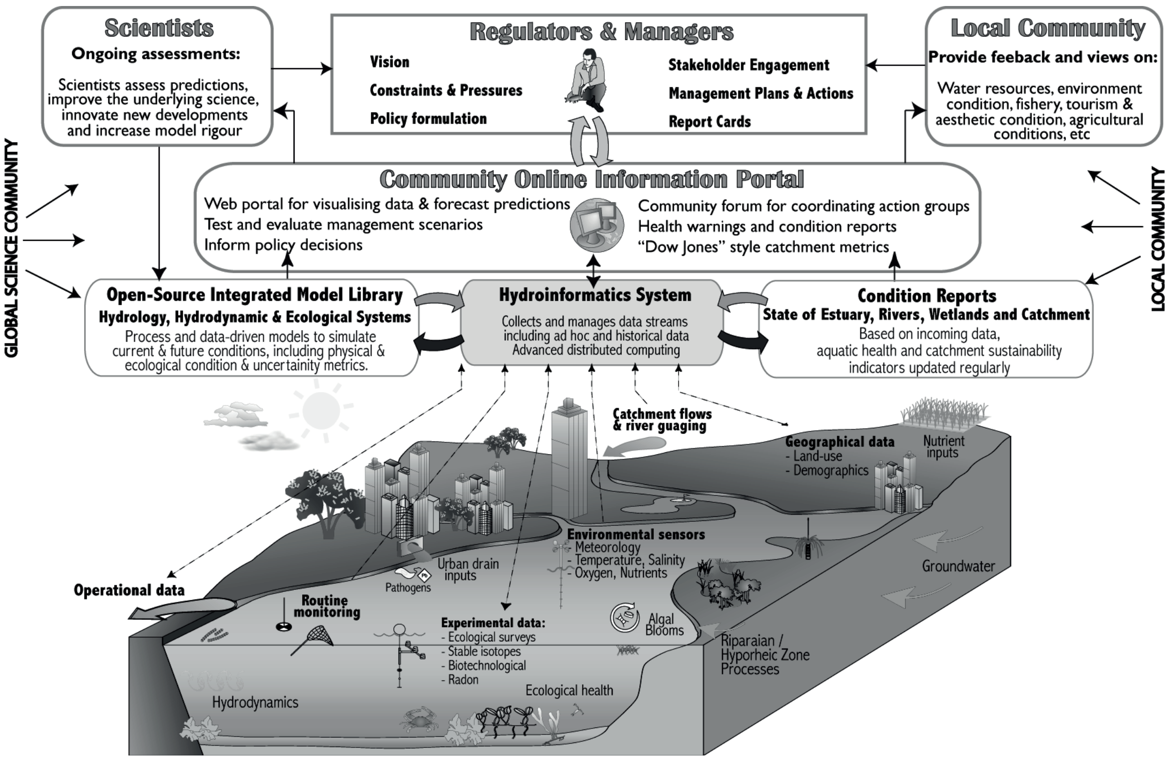

Fig. 1 A vision for an integrative scheme of water quality research during the next decade.

Synthesis and comparative hydrology

Synthesis activities help us search for "universal" descriptors of process, similarity in catchment emergent behaviours, and how patterns in water quality and in nutrient and contaminant pathways vary across geomorphologic and climate gradients (Sivapalan *et al.*, 2012). Quantitative and/or Bayesian analyses of pattern and process information relevant to water quality from diverse model applications should be extracted over different scales of integration to support multi-basin comparative analyses. Examples of embedding model systems within a global lake observatory network (cdi.gleon.org) further demonstrate how large-scale comparative analyses can be coordinated. Whilst simple in theory, in practice this is a challenge due to lack of standards and common approaches. The emergence of "network science" through initiatives like the PUB decade, is able to foster the community approach and facilitate cross-site comparisons and this needs to be further encouraged over the next decade to support synthesis of water quality.

CONCLUSION

Whilst technological advances in water treatment will increasingly allow us to use or avoid poor quality water for consumption, general efforts towards river basin sustainability and restoration of catchment systems demands we better understand and manage our nutrient and contaminant problems. To this end, we must take advantage of improved measurement and information technology to improve our ability to quantify nutrient and contaminant flux pathways from catchment to coast, better understand ecological and societal response to changes in water quality. This requires coordinated research effort from the IAHS community that can facilitate model development and data sharing activities. Combined with new management approaches that are built around a robust, science-based governance framework, and underpinned by suitable hydrological–water quality models and adaptive decision support systems (Fig. 1), we can achieve more sustainable outcomes across the range of basin landscapes and scales.

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