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COMMENTARY

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A guideline for spatio-temporal consistency in water quality modelling in rural areas

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1 | SIX CHALLENGES FOR CONSISTENCY IN WATER QUALITY MODELLING

Several hydrological studies have expressed the need for consistency in hydrological modelling (Euser et al., 2013; Martinez & Gupta, 2011). Consistency means to match the simulated processes with knowledge and expectations from study catchments. In analysing consistency, hydrological processes are checked for accuracy in their spatio-temporal representation under consideration of available catchment observations. This includes innovative diagnostic methodologies to analyse the model assumptions and results in more detail (Gupta et al., 2008; Reusser et al., 2009; Yilmaz et al., 2008), and plausibility checks of input, internal and output variables based on catchment knowledge (Guse et al., 2016; Pfannerstill et al., 2017). In this commentary, we transfer the idea of consistency to water quality modelling at the catchment scale.

We focus on water quality modelling in rural mesoscale catchments and the interaction with agricultural production systems and their management. While it is acknowledged that urban areas contribute significantly to pollution and other harmful substances also affect water quality, the major focus here is on modelling the impact of agrochemicals. At the mesoscale, model studies are based on existing data, for example measurements of water quality variables at the catchment outlet. Representative data coverage (i.e. measurements) throughout the catchment is generally not possible. Model complexity is related to these conditions and includes a detailed representation of land use and land management. To handle models in terms of simulation time as well as due to data availability, simplifications of process representations are necessary. To capture the spatial heterogeneity and variability within the catchment, we focus our study on spatially distributed, integrated catchment models that are simulating both water quantity and water quality. The long-standing EGU-Session 'Water quality at the catchment scale: measuring and modelling of nutrients, sediment and eutrophication impacts' provides insights into recent advances in water quality modelling at the catchment scale. Based on this session, the literature and our own studies in the last years, we have developed a guideline for consistency in water quality modelling as visualized in Figure 1.

1.1 | Representation of rural landscapes

The main challenge in mesoscale, ecohydrological models is an accurate parametrization of rural landscapes. In comparison to water quantity studies, input data for water quality modelling are usually limited in time and space. Their measurement is often restricted to monthly grab samples at a few gauges. Only in the case of well-observed catchments are daily mixed samples or continuous sensor data available for model calibration and validation (Rode & Suhr, 2007; Wagner et al., 2018). Usually, nutrients are the focus of the chemical analysis. Data on sediments are usually restricted to suspended load, and pesticide data are only available in short measurement campaigns (Ulrich et al., 2022; Wagner et al., 2018). Thus, there is a mismatch between spatial and temporal scales in data availability and requirements for accurate process representations (Fu et al., 2020).

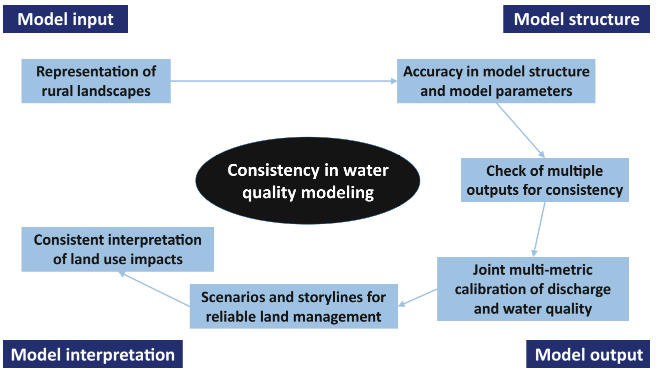

FIGURE 1 Six steps to achieve consistency in water quality modelling

Challenges arise from the need to interpolate, extrapolate or derive necessary input information from proxy data. Water bodies as well as storages in the landscape (e.g. concentrations in soil layers) must be initialized and transformation rates within the nutrient cycles need to be parameterized. These data are usually derived from literature and rarely represent the necessary spatial and temporal variability in the catchment correctly.

Agrochemical inputs to water bodies originate from point and diffuse sources. Most studies in rural areas focus on diffuse sources and consider entry pathways via surface runoff, drainage pipes and seepage through the soil, but they neglect contributions of point sources. In rural areas, wastewater entry can pose a considerable threat to water resources and human health, especially if untreated. While the load of harmful microorganisms is clearly minimized, this is not true for nutrient loads and other harmful substances throughout the year. Especially in cold periods or during low flows, the contribution of wastewater treatment efflux to water degradation can be considerable. Ignoring the point sources during calibration can lead to a distorted representation of landscape processes.

In addition, information on land use patterns and management is of major importance. While such details are often ignored in water quantity studies, in water quality modelling more detailed land use patterns (i.e. management practices, crop rotations, cropping systems and tillage practices) are necessary to represent the complexity of land use systems (Guse et al., 2015; Lei et al., 2022).

Even though dynamic representations of land use change are possible in many modelling frameworks (e.g. SWAT, mHM) and it has been shown that model outputs are affected by the temporal representation of land use (Guse et al., 2015; Wagner et al., 2019), static representations of land use are still common. In the context of water quality modelling, changes in agricultural areas are particularly important. Long-term changes in space and time can be assessed with the help of remote sensing data and land use classifications (Lei et al., 2021; Steinhausen et al., 2018) or field surveys in the case of smaller study areas (Lei et al., 2019).

Land management in space and time is important to initialize levels of nutrient pools in the soil, as well as to adequately depict legacy effects. Derivation of typical crop rotations includes data mining of agricultural yearbooks within administrative boundaries, surveys of agricultural areas for several years (Wilken et al., 2017), as well as expert interviews with local farmers. Information on the time of sowing, fertilization, tillage system, pesticide application and harvesting dates, for example, is usually unknown for mesoscale catchments but needed to adequately represent crop rotations (Guse et al., 2015; Lei et al., 2022). This information needs to be distributed in space and time to avoid a synchronization of measures over large areas resulting in artefacts in the simulation of pollutant loads. High variability in crop variety characteristics is well-known in agricultural sciences and even the position within the crop rotation has considerable effects on nutrient uptake and finally on crop yield. However, this level of detail in ecohydrological catchment modelling is not possible so far. Crop management can also include two crops on the same field (bi-cropping systems) with significant implications for soil protection, nutrient enrichment or competition in plant growth. Undersown crops or bi-cropping systems are implemented, for example, to protect the soil from erosion or to improve the nitrogen input through the combination of legume and cash crops (Conrad & Fohrer, 2016).

1.2 | Accuracy in model structure and model parameters

Hydrological models are characterized by specific structures, implemented processes and their degree of complexity. The model parameters selected to optimize the model for the catchment under study vary among different models. Water quality models include water quantity and water quality components and their interactions. While principles of quantitative hydrology are well-understood, how to implement nutrient cycles in models is often not sufficiently clear and rarely investigated in detail. The role of parameters in controlling the nutrient cycle in models is particularly challenging (Clark et al., 2015). Diagnostic model analysis to improve the understanding how well processes are represented in the model is well-established in quantitative hydrology, mainly in analysing discharge (Gupta et al., 2009; Reusser et al., 2009; Yilmaz et al., 2008). Using temporally resolved diagnostic methods, temporal variability of process behaviour in models is investigated knowing that process relevance varies under specific conditions, such as between wet and dry periods. Transferring diagnostic model analysis to water quality modelling is required to improve the understanding of water quality processes and the nutrient cycle. Until now, combined temporal diagnostic analyses to obtain a joint understanding of both water and pollutant cycle at the same time are rarely used (Schüerz et al., 2019).

Haas et al. (2015) used a temporal dynamics of parameter sensitivity approach (Reusser et al., 2011) to analyse temporal variability in the dominance of nitrate parameters. For each day, the dominant nitrate parameters were derived to detect their dominant phases. In comparing daily sensitivites of nitrate parameters with different runoff components and nitrate flow pathways, they determined which parameter controls which process at which time. The nitrate uptake parameter of the SWAT model was shown to be sensitive in phases of crop growth with a high nitrate demand at phases of low concentrations of nitrate in the soil. A joint interpretation of seasonal crop dynamics and agricultural management with water quality processes is needed to understand typical patterns of dominant processes and parameters in models. A comparison with the expected process behaviour shows whether all relevant processes and catchment features are well-represented.

1.3 | Check of multiple model outputs for consistency

Due to overarching interactions between agrochemicals with the environment, a consistent simulation of nutrients and agrochemicals requires correct representation of almost all ecohydrological model states and outputs. The spatio-temporal plant development has a decisive impact on the nutrient processes. Together with agricultural practices and soil characteristics, this governs the storage of nutrients in the soil matrix, concentrations in transport pathways and leaching from the soil. The consistency check for plant-related characteristics largely depends on the modelling scale and requires to consider the influence of each combination of plant–soil-climatic conditions on the simulated time series of leaf area index (Strauch et al., 2013), evaporation (Wagner et al., 2011) and biomass, as well as the timing of harvest and yield (Lautenbach et al., 2013). In addition, model outputs can be validated against spatial patterns (Bieger et al., 2015; Wagner et al., 2022). This requires the spatial representation of the remotely sensed or mapped variables in the model, for example evaporation or soil moisture (Odusanya et al., 2019; Rajib et al., 2016). Modelled nutrients at the subbasin scale can be compared with data available from spatially distributed field campaigns (Lei et al., 2021).

One strength of models lies in the separate representation of water flow pathways and their share in total streamflow. Nutrient concentrations in streamflow are an integrated signal of the individual transport pathways. Therefore, an evaluation of fluxes originating from surface runoff, tile drains, lateral flow and groundwater flow against observations are valuable to increase model consistency. In that regard, Fu et al. (2020) list isotopes, tracers and biomarkers (Pfister et al., 2017) as novel and useful approaches. If available, such data are valuable in validating a model's state variables and process representation (McMillan et al., 2012). If not available, the modelled share of transport pathways can be validated against the geophysical catchment characteristics and hydrogeological setting (Ala-aho et al., 2017).

Additional potential lies in novel data sources that can inform water quality studies, such as soft data information (Seibert & McDonnell, 2002), crowd-sourced data (Minkman et al., 2015) and social media data (Keeler et al., 2015; Venohr et al., 2018). While a direct comparison to model outputs or state variables for these data sources may not always be possible, such spatially distributed, qualitative information can constrain simulated water quality parameters in addition to, or in absence of, quantitative observations.

1.4 | Joint multi-metric calibration of discharge and water quality for all magnitudes

Model calibration and identification of suitable parameter values using a set of contrasting performance criteria is crucial for realistic model representations. It is still challenging to develop a suitable multi-metric method for water quality studies if the goal is to improve process representation and allow extrapolation for scenario analysis (Fu et al., 2020; Pohlert et al., 2007). The use of multiple performance criteria is an essential step in water quality modelling to cover different characteristics and dynamics of simulations (Ahmadi et al., 2014; Bekele & Nicklow, 2007). Pfannerstill et al. (2014) provided an overview of performance measures, including statistical performance measures such as Kling–Gupta-efficiency (Gupta et al., 2009), Ratio of root mean square error and standard deviation (Moriasi et al., 2007).

Signature measures that are directly related to catchment functions are recommended for hydrological modelling (Pokhrel et al., 2012; Yilmaz et al., 2008). Hydrographs and nitrographs are representations of different phases of the entire hydrological and nutrient behaviour over time in the catchment. The approach of constructing signature measures separately for different phases of the flow duration curve (FDC) (Pfannerstill et al., 2014) was further extended to the use of nitrate duration curves (NDC) for model optimization (Haas et al., 2016). FDC and NDC represent catchment functions of discharge and nitrate, respectively, and can be separated into different phases to analyse dynamics and magnitudes of stream flow and loads in detail. To obtain a plausible model simulation for water quality modelling, the performance measure is first applied separately for each defined segment, which composes both FDC and NDC (Haas et al., 2016; Pfannerstill et al., 2014). A combined metric for both variables and all considered performance and signature measures is calculated.

The use of different metrics made clear that a model run which is optimal for runoff is not necessarily optimal for nitrate simulation. A deeper look at nitrogen dynamics and relationships with hydrology is needed. The methodological approach was described exemplarily for nitrate in Haas et al. (2016), but it is suggested to transfer this approach to other agrochemicals.

1.5 | Scenarios and storylines for reliable land management

Decisions that affect water quality of river basins are made by multiple stakeholders and interest groups. One of the main challenges in sustainable river basin management is the integrated development of best management practice (BMP) options to improve water quality (Arabi et al., 2006; Chaubey et al., 2010). The simulation of BMPs requires that realistic agricultural practices are spatially and temporally arranged and implemented with different management and crop rotations (Lam et al., 2011; Strauch & Volk, 2013; Ullrich & Volk, 2009). The strong linkage between reliable simulation experiments in water quality modelling and interactions with stakeholders was emphasized in a review by Fu et al. (2020) to transfer the model outcomes to practical applications, good organization and capacity building.

Socio-environmental systems are highly complex, and all compartments are interconnected. Thus, making sustainable and integrated management decisions is challenging. Ecohydrological models have been used to make the impacts of management options more transparent (Haas et al., 2017; Lam et al., 2011); nevertheless, the usefulness of the results depends on the selection of realistic scenarios, storylines and the acceptance of these measures by stakeholders. Using models to analyse the impact of driving forces like climate, land use or other anthropogenic interventions has been a research focus for many years. Yet, the results of those studies rarely find their way to implementation due to the oversimplification of scenario compilation. One of the main obstacles in assessing potential future developments is the dialogue with stakeholders in an integrative manner of joint scenario development. This becomes even more obvious as soon as different environmental compartments or disciplines are involved. In recent years, scientists have tried to overcome this chasm by integrating not only the decision makers, but also all relevant stakeholders within a river basin (Nygaard et al., 2021).

The sub discipline of socio-hydrology has become more prominent and has helped to understand the underlying mechanisms for water distribution and water resources management (Kumar et al., 2020). The development of meaningful storylines helps insure that all parties are represented properly and inclusively and that complex socio-environmental processes are communicated with modern modelling and visualization techniques. The decision space should be adequately represented in space and time. Moreover, it is recommended that storylines and scenarios are developed in co-design with stakeholders. For example, land use change scenarios, land management (tillage practice, grazing) and crop rotations need to be implemented and spatially and temporally allocated within a river basin, and farmer dialogue should be employed to define the decision space and the framework for the scenario runs. Land use models are useful tools to run projections for different future scenarios and achieve a spatially distributed output (Palmate et al., 2022; Wagner & Fohrer, 2019). An adequate spatial and temporal distribution of BMPs, a suitable mix of measures as well as economic considerations are key to defining realistic scenarios (Haas et al., 2017).

1.6 | Consistent interpretation of impacts on water quality

Assessment and interpretation of the results of BMP scenario runs in terms of pollutant load reduction and cost effectiveness is crucial for their implementation. This means a search for a BMP that combines greater pollutant reduction and the lowest cost of implementation and/or loss of revenue due to reduced productivity. Most studies focus on the spatial patterns of individual BMPs, but their usefulness during different phases of the hydrograph and in relation to the magnitude of pollution is rarely considered.

For this purpose, diagnostic tools like duration curves are helpful to evaluate the impact of BMPs depending on the seasonality and the magnitude of, for example, nitrate loads in the catchment, to detect phases of better effectiveness (Haas et al., 2017). For the reduction of nitrate, for example, the model studies indicated the highest reduction by combining BMPs such as fertilizer reduction and buffer strips. However, both represent a loss of income due to a smaller crop area available as a result of buffer strip implementation and lower productivity when using less fertilizer (Haas et al., 2017).

The evaluation of BMPs should not only look at the agricultural sector (Chaubey et al., 2010; Lam et al., 2011). It is equally important to consider the valuation of ecosystem services and different agricultural productions and find a balance between environmental and economic sustainability. Water quality modelling in rural areas should be carried out considering the spatial and temporal distribution of nutrients in more detail seeking the most effective spatial location of measures to reduce pollution and, at the same time, improve biodiversity and system resilience.

2 | GUIDELINE FOR WATER QUALITY MODELLING

To summarize, we suggest a guideline for water quality modelling:

1. Spatial and temporal patterns of land use and land management are critical to adequately represent water quality in models. Remote sensing and land use models are very useful resources to be exploited.

2. The transfer of a model diagnostic analysis to water quality leads to a better understanding of how water quality variables are controlled by model structures and corresponding model parameters.

3. Assessing multiple model outputs regarding their temporal, spatial and process performance using observed time series, remotely sensed spatial patterns, knowledge about transport pathways and even soft data can significantly enhance model consistency.

4. Multi-metric calibration using performance metrics and signature measures both for discharge and water quality, such as FDC and NDC, leads to more balanced model simulations that represent all magnitudes of discharge and water quality accurately.

5. Scenarios and storylines should be co-developed with stakeholders in the river basin to make them more realistic and increase the acceptance of model results. They should be realistic in space and time, and provide a mix of available management options.

6. The interpretation of BMPs can be supported by diagnostic tools to show the effectiveness of measures and their combinations while considering their costs and impacts on ecosystem services.

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DATA AVAILABILITY STATEMENT

Data sharing not applicable to this article as no datasets were generated or analysed during the current study.

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