HYDROLOGIC AND WATER QUALITY MODELING: SPATIAL AND TEMPORAL CONSIDERATIONS

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ABSTRACT. *Hydrologic and water quality models are used to help manage water resources by investigating the effects of climate, land use, land management, and water management on water resources. Water-related issues are investigated over a range of scales, i.e., the extent and resolution of the spatial and temporal contexts, which can vary spatially from point to watershed and temporally from seconds to centuries. In addition, models' formulations may place scale restrictions on their use. In 2012, ASABE published a collection of 22 articles on the calibration, validation, and use of 25 hydrologic and water quality models. Each article detailed the process to follow and the issues that could arise during calibration or application of a specific model. The objective of this article is to synthesize those articles with regard to common spatial and temporal scale principles that should guide selecting, parameterizing, and calibrating a hydrologic model. This article describes how the spatio-temporal extent and resolution of a model application should relate to the modeling objectives, the processes simulated, the parameterization and calibration process, data available for parameterization and calibration, and interpretation of results. Overall, the intended scale of the model should match the scale of the processes that need to be simulated given the modeling objectives, the scale of input and calibration data should be compatible with the scale of the model and with the objectives of the study, and the model should be calibrated at the scale at which the results will be analyzed and interpreted.*

Keywords. *Calibration, Hydrologic modeling, Scale, Spatial, Temporal.*

Hydrologic and water quality models are fundamental scientific tools used to predict, forecast, and explain phenomena at different spatio-temporal scales in which direct observation or experimentation is not possible, not economical, or ethically prohibited. Models are used to assess the impact of stressors in multiple scenarios such as climate variability and change, population growth, policies and economics to help policy-makers define actions ensuring local to regional sustainability of water resources, and societal interactions including agricultural production systems. Hydrologic and water quality models are used for investigating a wide range of issues related to water resources, including contamination of aquifers, conservation of water resources, and design of best management practices for ground and surface water quality protection. Each water-related issue is best investigated at a specific scale, which can vary in the spatial context from point to watershed and in the temporal context from seconds to centuries. The spatial and temporal scales of the model are defined by the extent of the study area, the duration of the simulation period, and the spatial and temporal resolution of the calculations. Spatial resolution is determined by the smallest spatial element being simulated, and temporal resolution is represented by the time step of the simulation.

When the spatial extent is a point or a plot, models are used primarily to verify our understanding of physical and biological processes, such as reactive pollutant transport through a soil profile. For example, Silliman et al. (2002) used HYDRUS to verify results experimentally obtained in a soil column. When the spatial extent is the size of a field, field-scale models may be used to assess the productivity or agronomic risk of cropping or grazing systems, assess their environmental risk (Pierson et al., 2001), predict the evolu-

Submitted for review in April 2014 as manuscript number NRES 10714; approved for publication by the Natural Resources & Environmental Systems Community of ASABE in December 2014.

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tion of a state variable (e.g., soil moisture; Jensen et al., 1997), or plan soil conservation or irrigation and drainage management systems. Models that simulate large spatial extents such as watersheds may be used to assess the quantity and quality of water resources in streams, aquifers, and reservoirs (Wang et al., 2009) and their linkage with ecosystem responses. Models have also been used for regulatory purposes, such as the development of total maximum daily loads (TMDL; Benham et al., 2006). For larger spatial extents, river basin models are increasingly used to investigate global problems, such as water availability at continental scale (Trambauer et al., 2013) or nutrient discharge into Chesapeake Bay (Shenk et al., 2012) or the Gulf of Mexico (Jha et al., 2013). Spatial and temporal extents and resolution are not independent, as phenomena simulated over a small spatial extent (point) are frequently associated with shorter time steps than processes simulated over a river basin (Renschler and Harbor, 2002).

Moriasi et al. (2012) summarized the spatio-temporal scales of 25 models presented in the special collection of articles that focused on each model's calibration, validation, and use. The models fall into three categories: models that represent a one, two, or three dimensional representation of the soil profile; surface and subsurface plot and field scale models; and surface and subsurface watershed models.

All models require definition of a spatial extent, spatial resolution, temporal extent, and temporal resolution to represent natural processes and for model calculations. The spatial extent of a model relates to the size of the space simulated: soil profile, hillslope, field, or watershed (Zeckoski et al., 2014). The spatial resolution defines how this space is discretized, which defines the extent of channels and the size of spatial elements for which properties are considered homogeneous, with the smallest spatial element being a soil layer, a grid cell, a subarea, or a hydrologic response unit (HRU, a spatial unit characterized by a slope, soil type, and land use). Similarly, the temporal extent relates to the duration of the simulation period (from minutes to centuries), and the temporal resolution is defined by the time step used to perform the calculations or analyze the results (fraction of a second to years). The selection of both the spatial and temporal resolutions is a function of the resolution of the available input data, the nature of the simulated hydrologic and biogeochemical processes, and the modeling objectives.

The time step and the smallest spatial element used in the calculations affect the model's parameterization, its calibration, and how the model predictions are interpreted and used. The size of the simulated space and that of a representative element are linked for multiple reasons: time and resources needed to parameterize the model, data availability, computational time to run the model, and processes that need to be represented over small areas to explain model outputs that represent large areas. The duration and the time step of the simulation are similarly related. For physically based models solving differential equations governing the simulated processes, the time step and the spatial representative elements are also linked to the convergence and accuracy of the computational methods.

New resources available to model users allow the linkages between spatial and temporal frames to become more flexible. The current availability of high-resolution spatial maps from satellite, radar, and other sources and the development of tools to process, visualize, verify, evaluate, and translate these data in a seamless manner, allow simulation of increasingly larger areas for longer durations at higher temporal and spatial resolutions. With these additional resources, the elements of the spatial and temporal scales of a model can technically become decoupled from each other even though they should remain linked. For example, high-resolution land use and soil maps that feature areas with high runoff potential (e.g., urban areas) will not improve peak runoff predictions if the temporal resolution of the weather data is not sufficient to represent high-intensity rainfall events. The selection of spatial and temporal scales (extent and resolution) becomes the responsibility of the model users, who need to be aware of the impact that their choice will ultimately have on the complexity of the model, the accuracy of model predictions, and whether the modeling objectives will be met.

Few guidelines have been offered to help users in this selection process, yet mismatches between the scale of the processes, the scale of the data used to parameterize and calibrate the model, and the objectives of the modeling study can produce misleading conclusions or waste valuable resources. This article describes how the spatio-temporal scale of a model relates to the modeling objectives, the processes simulated, the data available to parameterize and calibrate the model, the efforts and procedures to parameterize and calibrate the model, and the interpretation of the results. Companion articles address other topics related to the calibration, validation, and use of hydrologic and water quality models: Zeckoski et al. (2015) define the terminology, Arnold et al. (2015) discuss how active hydrologic processes affect model calibration, Malone et al. (2015) focus on model parameterization, Daggupati et al. (2015) review calibration strategies, Moriasi et al. (2015) present performance measures, Guzman et al. (2015) concentrate on uncertainty issues, Saraswat et al. (2015) propose documentation and reporting procedures, and Yuan et al. (2015) examine model sensitivity to input parameters. The overall goal of this article is to highlight principles that will guide selecting the spatial and temporal scales for parameterizing and calibrating a hydrologic model. In the following section, we review how scales and processes are interconnected. The subsequent section discusses the scale of the data used to parameterize and calibrate a model. The final section provides a synthesis of how hydrologic processes, data, and modeling objectives affect the choice of spatial and temporal scales. We conclude with a list of guiding principles.

SPATIO-TEMPORAL SCALES AND HYDROLOGIC, BIO-GEOCHEMICAL, AND ECOLOGICAL PROCESSES

RELATIONSHIPS BETWEEN PROCESSES AND SPATIAL AND TEMPORAL SCALES

Different natural watershed processes can be modeled at several possible spatial and temporal scales (table 1; Gentine et al., 2012). For example, infiltration, excess runoff, splash sediment detachment, adsorption/desorption, and biochemical transformations may be considered point-scale processes because they take place at a point or uniformly over a small area. The area of application for a point-scale process could be a specific soil pedon at a particular location in a landscape. Point-scale processes might be evaluated experimentally using a soil column in the laboratory (Silliman et al., 2002) or a lysimeter in the field with small 2D or 3D elements (commonly in the order of centimeters to meters and within the validity of the continuum) considered to be isotropic (i.e., having similar properties in any direction of the element). HYDRUS and TOUGH2 are examples of models that can be applied to this spatial extent.

Plot-scale models represent a larger area, with properties assumed to be uniform. Plot-scale models are particularly suited for simulating conditions under which specific hypotheses are tested using replicated experimental treatments; plot-scale models serve to further indicate that these hypotheses are valid. Examples of models well suited to plots include EPIC, RZWQM, and Daisy. Point and plot scale models include processes associated with runoff generation, plant growth, infiltration, and nutrient cycling (table 1), which are described in detail by Arnold et al. (2014).

A hillslope model consists of a series of elements from the top to the bottom of a hill, with different slopes, soil profiles, and possibly management. For this spatial extent, additional processes become active, including those associated with subsurface flow and transport of sediment and pollutants. KINEROS and WEPP are models developed specifically for this extent. In some cases, plot-scale models can be applied to a field by lumping the parameter values over the field area and representing that field with a unique and homogeneous soil, slope, and management. In this case, effective parameters are used (Hansen et al., 2012; Malone et al., 2014), ignoring heterogeneity that could affect the hydrologic response. Field-scale models are appropriate for more complex units, with processes involving both diffuse and concentrated flow. Fields may be represented by multiple units, giving the ability to represent the existing spatial and temporal variability, as can be done in models such as APEX. Field-scale models are generally used to simulate processes such as infiltration, drainage, overland flow, buffers, ponds, or ephemeral gully erosion rather than channel and reservoir processes (table 1). Some of the models well suited for the field extent can also handle small to medium-size watersheds (APEX, WEPP, DRAINMOD, and MODFLOW/MT3DMS). For larger areas (i.e., watersheds and river basins), models with the capacity to represent spatio-temporal heterogeneity through distributed or semi-distributed spatial discretization are more appropriate. SWAT, WARMF, HSPF, MIKE-SHE, or WAM were specifically developed for these simulations.

The temporal extent and resolution of a model are influenced by the time over which hydrologic processes are active and changing (table 2). Processes can occur over times that range from a fraction of a day (e.g., precipitation, infiltration, streamflow) to years, decades, or centuries (e.g., biogeochemical cycles, landscape processes). Generally, the spatial and temporal resolution and extent vary together such that large watersheds are simulated and calibrated at coarser temporal and spatial resolution, and smaller catchments or fields are simulated with smaller time steps and higher spatial resolution. Developing the appropriate input data may require spatial and temporal aggregation or interpolation of measured data to match the spatial and temporal extent and resolution of the model.

SPATIAL SCALE AND SIMULATED PROCESSES

The potential for inappropriate representation of dominant processes and incorrectly accounted process interaction increases with the size of the simulated area because of more complex interactions, poor assumptions, and lack of spatio-temporal data. Recognition of process interaction may result in uncertainty about what processes should be targeted during calibration, uncertainty in the calibrated parameter values, and ultimately uncertainty in the results.

Table 1. Water, sediment, and nutrient processes active over a range of spatial scales ("+" indicates that the processes simulated at smaller scales remain active at the current scale.)

Process Category	Point) (<1 m^2)	Plot or Hillslope (1 to 100 m^2)	Field or Small Catchment (100 m^2 to 50 ha)	Watershed (50 ha to 50 km^2)	River Basin (>50 km^2)
Water movement	Runoff generation, infiltration, evapotranspiration, perched water table, and preferential flow.	+ Runoff routing	+ Concentrated flow, subsurface flow, drainage, buffers, ponds, wetlands, variable source areas, exfiltration, and interflow.	+ Streamflow, bank storage, riparian areas, groundwater flow, aquifer recharge, flood plain, point discharges, and water withdrawals.	+ Reservoirs and major hydraulic structures.
Erosion and sediment movement	Detachment and sheet erosion.	+ Rill erosion	+ Ephemeral gully erosion, deposition, and sediment trapping in buffers, waterways, filter strips, and ponds.	+ Streambank erosion, stream sediment transport, and sediment deposition in flood plain.	+ Sediment trapping in major hydraulic structures.
Nutrients and other agrochemicals	Soil/plant interactions; leaching to perched, shallow, and deep aquifers; sorption, transformation, and degradation in vadose zone and shallow aquifers.	+ Transport by surface runoff and sediment	+ Transport with drainage and subsurface flow, transformations and degradations in ponds and wetlands.	+ Stream transport, water/air and water/streambed exchanges, in-stream transformations and degradation, riparian area, algae and aquatic plants, and point discharges.	+ Cycling in major hydraulic structures.

Table 2. Water, sediment, and nutrient processes active over a range of temporal scales.

Processes	Relevant Time Scale: Seconds	Minutes	Hours	Days	Weeks	Months	Years	Decades	Centuries
Hydrologic processes									
Infiltration	✓	✓	✓	✓	-	-	-	-	-
Evapotranspiration	-	✓	✓	✓	-	-	-	-	-
Preferential flow	✓	✓	✓	✓	-	-	-	-	-
Soil moisture redistribution	-	✓	✓	✓	✓	-	-	-	-
Runoff/overland	-	✓	✓	✓	-	-	-	-	-
Quick return flow	-	✓	✓	✓	-	-	-	-	-
Field drainage	-	-	✓	✓	✓	-	-	-	-
Groundwater recharge/deep percolation	-	-	✓	✓	✓	✓	✓	✓	✓
Groundwater discharge/depletion	-	-	-	✓	✓	✓	✓	✓	-
Channel flow (small watershed, <0.5 km^2)	-	✓	✓	✓	-	-	-	-	-
Channel flow (large watershed, 0.5 to 50 km^2)	-	-	✓	✓	✓	-	-	-	-
River flow (basin, >50 km^2)	-	-	✓	✓	✓	✓	-	-	-
Biological processes									
Plant (row crops, grasses, trees) growth	-	-	✓	✓	✓	✓	✓	✓	-
Carbon cycle:									
Decomposition of fresh organic materials (crop residues, manure)	-	-	-	✓	✓	✓	✓	-	-
Accumulation and decomposition of soil organic matter	-	-	-	-	-	✓	✓	✓	✓
Bacterial growth and die-off	-	✓	✓	✓	-	-	-	-	-
Nutrients and pesticides:									
Nitrification, denitrification, urea hydrolysis	-	✓	✓	✓	✓	✓		-	-
N and P mineralization	-	-	✓	✓	✓	✓	✓	✓	✓
Degradation	-	-	✓	✓	✓	✓	✓	✓	-
Mixing by earthworms	-	-	-	-	✓	✓	✓	-	-
Algae growth/eutrophication	-	-	✓	✓	✓	✓	-	-	-
Erosion and sedimentation processes									
Detachment (rill/interrill)	✓	✓	✓	-	-	-	-	-	-
Gully erosion	✓	✓	✓	✓	-	-	-	-	-
River channel bed and bank erosion	-	-	✓	✓	-	-	-	-	-
Sediment Transport	✓	✓	✓	✓	✓	✓	✓	✓	-
Landscape/stream deposition	-	✓	✓	✓	✓	✓	✓	✓	✓
Lake sedimentation	-	-	-	✓	✓	✓	✓	✓	✓
Geomorphologic adjustment	-	-	-	-	-	✓	✓	✓	✓
Physical and chemical processes									
Adsorption/desorption	✓	✓	✓	✓	✓	-	-	-	-
Solute transport, including leaching	✓	✓	✓	✓	-	-	-	-	-
Oxygen depletion	-	✓	✓	✓	-	-	-	-	-
Groundwater chemistry (mineral dissolution and chemical precipitation)	-	-	-	✓	✓	✓	✓	✓	-

However, non-recognition of process interaction may result in incorrect conclusions. For example, erosion rate and sediment delivery estimates, and associated calibration parameters, may be altered during spatial aggregation because the relative lengths of hillslopes and channels are altered (Canfield and Goodrich, 2006). At small scales (areas less than a few m^2), soil detachment and transport are controlled by rainfall impact energy and shallow flow processes. As scale increases to the size of typical erosion plots (tens of m^2), runoff concentration, rill detachment, and transport processes may dominate. At still larger scales (hundreds to thousands of m^2), gully erosion and deposition may determine sediment yield; at watershed scales, stream channel processes and the connection to flood plains may overwhelm the entire sediment and hydrologic system.

Another example of the effect of spatial scale on simulated processes is the scale-dependence of denitrification, a key biochemical transformation influencing the fate and transport of nitrate-nitrogen in agricultural landscapes. At small scales (point to plot), denitrification mostly occurs in anaerobic microsites within the biologically active root zone (the top portion of the vadose zone). Denitrification also occurs in the shallow groundwater, where denitrifying bacteria use dissolved organic carbon leached from the root zone. At watershed scale, denitrification in aquifers becomes important as groundwater passes through “hot spots” in the hyporeic zone and floodplains in wetlands and streams (Groffman et al., 2009). When models are parameterized at a smaller scale and then scaled up to a larger scale, it is important that the critical processes are adequately represented and parameterized within the model structure. Additional calibration of parameters associated with the large-scale processes (e.g., algae growth in streams or lakes), and thus additional data, may be needed. Scaling up from a field scale to a larger scale is discussed later in this article.

Glymph and Holtan (1969) show a classic graph of the highly variable effects of spatial scaling on mean annual runoff for watersheds in different climates and physiographic areas (fig. 1). Arid lands (Arizona) show an inverse log-log relationship, while watersheds in unglaciated hill lands in humid eastern Ohio exhibit a more direct relationship that plateaus at about 100 km^2. A third site in Texas is also inversely proportional, but mean annual runoff is much less sensitive to watershed area. The forms of these relationships are in part due to the subsurface characteristics of

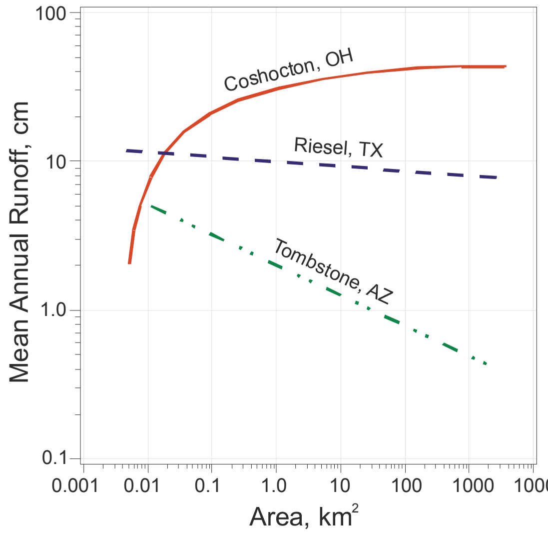

Figure 1. Spatial variation of annual runoff for three different climatological and physiographical areas in the U.S. (adapted from Glymph and Holtan, 1969).

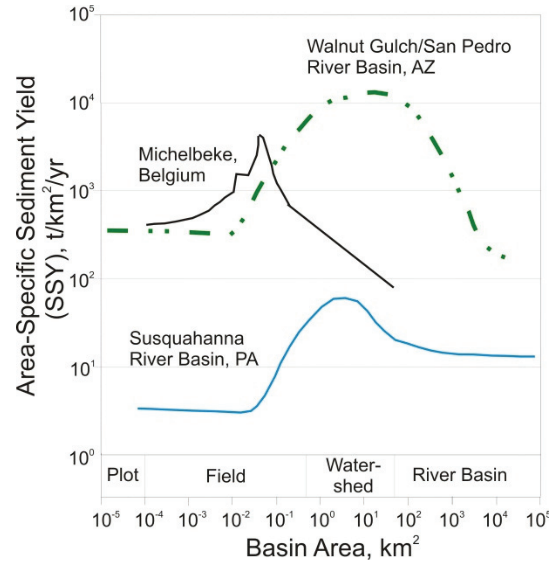

Figure 2. Specific sediment yield as a function of drainage area for three catchments: Arizona (AZ) and Pennsylvania (PA) after Osterkamp and Toy (1997) and Belgium after Vanwalleghem et al. (2005).

the regions. In arid lands, channel transmission losses and highly spatially varying precipitation cause a decrease in annual water yield with increasing area. At the other extreme, the area in Ohio is affected by subsurface flow percolating from the fields to form water tables perched on geological strata at a larger scale that drain to incised channels. For the Riesel, Texas, curve, the small watersheds are characterized as relatively flat (1% to 3%) with high clay content soils (55% clay; Harmel et al., 2006). These soils are expansive clays that produce large deep cracks during dry periods that limit lateral subsurface flow. The Riesel curve suggests a more uniform generation of runoff due to the clay soil and a mix of processes found in humid and arid lands. The graphs highlight the varying importance of subsurface flow processes in different climatological and physiographic areas.

It is commonly believed that unit-area sediment yield (t km^{-2} $year^{-1}$) declines as watershed size increases; as a result, many hydrologic and water quality models apply a sediment delivery ratio of less than one when extrapolating hillslope or hydrologic response unit erosion to watershed levels (e.g., Wang et al., 2011). However, figure 2 demonstrates that, for smaller watersheds, sediment delivery actually increases as contributing area increases because of contributions from new processes, including ephemeral gully and streambank erosion. Only after some threshold catchment size is reached does sediment yield decrease as watershed gradient decreases downstream. The relationship between catchment size and sediment delivery depends on many factors, including climate, geomorphology, and land management. Indeed, multiple maxima can be observed where these factors vary substantially within large basins (de Vente et al., 2007). Effective sediment size distribution also varies in complex ways as a function of watershed size (Walling and Moorehead, 1989).

An apparently good calibration (match between observations and predictions) at a watershed outlet does not ensure that the critical physical, chemical, and biological processes are properly simulated nor that the critical areas requiring treatment to meet watershed water quality goals are correctly identified. This is in part because there may be alternative upland and channel process combinations that result in predictions of flow, sediment, or nutrients at the watershed outlet that are consistent with measured data (Arnold et al., 2014). This can result in a phenomenon known as equifinality, a situation in which several parameter sets can meet the calibration criteria at the watershed outlet (Beven, 2006; Zeckoski et al., 2014). However, of the calibrated sets, fewer would be expected to represent the hydrologic processes accurately at all scales. For example, if critical processes such as gully or stream channel erosion and floodplain and impoundment deposition are not represented properly in the model structure, the model may not correctly reflect the effects of current or future conservation practices. To address the variability of spatial scales at which specific hydrologic processes occur, Goodrich et al. (2012) recommend calibrating KINEROS using a stepwise procedure by successively adjusting the sets of parameters that affect distinct processes and output variables at increasing spatial scales. By this recommendation, overland flow parameters are calibrated first using data collected at plot scale. Then data collected at the landscape scale (hillslope) are used to calibrate sediment transport parameters associated with concentrated flow. Finally, data collected at the outlet of the watershed are used to calibrate the parameters that characterize the channels draining the hillslope elements.

Temporal Scale and Simulated Processes

The previous discussion on spatial scale is also relevant for temporal scale. Uncertainty of model results increases when simulation over a longer period introduces conditions that trigger additional processes. For example, droughts may cause soil cracking and appearance of preferential flow paths, while periods of heavy rains may cause soil saturation and increased denitrification. Typically, calibration and validation periods span only a few events or years and may not include extreme events or infrequent sequences of events. On the other hand, management scenario analyses can span 20 to 50 years, and climate change analyses span 50 to 100 years or more, periods during which extreme events are likely to occur. If the simulation period is long, the calibration period needs to be long enough to include events of a magnitude that is likely to occur, from droughts to floods. If not, an additional uncertainty of the projected results needs to be recognized.

In addition to the random variability, temporal variability also includes a cyclical component associated with seasons and cycles of land management. For example, it is expected that temperatures will be warmer in the summer than in the winter. Some models may consider cyclical variability in predicting the mean response by using monthly climatic inputs instead of explicitly considering the random variations present in a rainfall and temperature sequence (e.g., RUSLE2; Dabney et al., 2012). This may be appropriate when the cyclical component of climatic variation is stronger than random variations (e.g., monsoon pattern) and when the modeling objectives require accurate long-term averages but place less importance on short-term variations. Consideration of cyclical patterns is critical when a response depends on the joint occurrence of critical conditions or events, such as bare soil or agrochemical application coincident with the expected seasonal occurrence of intense rainfall. The effects of both cyclical patterns and random variability within a population of events must be properly reflected in both long-term average and dynamic responses. Quantification of the model uncertainties or inaccuracies when increasing temporal extent is critical to reaching valid conclusions (Beven, 2006).

Another source of uncertainty in the model results when the temporal extent of a simulation is significantly longer than the calibration period is that the time dependence of critical processes needs to be well represented in the model structure. Watershed-scale responses to changes in management or climate variation typically lag responses observable in a plot or a field. For example, sediment and turbidity in streams of the southeastern U.S. may reflect the persistent influence of accelerated erosion during the first 200 years of European settlement, obscuring the effect of contemporary management. In this way, the otherwise pristine headwaters of trunk streams in glaciated British Columbia, Canada, are expected to carry high sediment loads for thousands more years due to geomorphic adjustment to massive glacial valley fill deposits (Church and Slaymaker, 1989). In addition, the subject of investigation (and the associated parameters) may be changing over time because of processes not simulated in the model. In that case, extrapolation of outcomes using the model would lead to greater uncertainty of projected results as the simulation and calibration periods become more remote from each other. For example, if stream erosion significantly alters channel dimensions over time, the hydrologic response of the system may not be stationary. The connectivity between the stream and its flood plain may be increased or decreased by sedimentation or erosion processes. Similarly, infiltration, drainage, erosivity, and other soil properties may change due to accumulation of organic matter or the cumulative impact of erosion and deposition. Human-induced soil disturbances such as tillage of agricultural land and tree harvest, site preparation, and planting of management forest plantations are known to alter soil hydraulic properties, soil organic matter decomposition, and nutrient cycling (e.g., Skaggs et al., 2008). Dabney et al. (2013) similarly showed that topographic changes over 50 years could alter future patterns of erosion.

In some studies, impacts of changing topography or soil properties are addressed by modifying these model inputs in a stepwise manner, adjusting for expected changes, and running the model under these modified conditions. Knisel and Douglas-Mankin (2012) cite an application of GLEAMS that accounts for long-term (50 years) changes in topography due to deposition of eroded sediment on field margins. Process-based models could track some parameter changes (e.g., soil properties, channel sizes) in critical state variables as feedback from predicted biomass accumulation or erosion. This would be similar to how models update other state variables at each time step. For example, the APEX model (Wang et al., 2012) provides the ability to update field capacity and wilting point water contents dynamically as a function of soil texture and organic carbon content. These parameters are subject to change as the surface layer erodes and biological processes affect the quantity and quality of residue. Similarly, the soil profile is updated as erosion decreases the depth of the top soil layer. These changes in the soil profile and properties typically occur on the scale of decades to centuries and are frequently not significant at temporal scales less than a couple of decades. However, long-term (>50 years) simulations can assess how these factors would affect productivity, erosion, and environmental losses. Other changes, (e.g., changing flow direction as a result of deposition; Dabney et al., 2013) are more difficult to implement gradually, as they require a different representation of the subject of investigation.

Spatial and Temporal Resolutions of Input and Calibration Data

Spatial and Temporal Resolutions of Calibration Data

Investigation of hydrologic phenomena is linked to observations in which translation of data to information is related to the spatio-temporal properties of the observations. The spatial and temporal resolutions of the observations are mutually dependent and cannot be separated (Hiebeler and Michaud, 2012). For example, capturing true peak flow values requires higher-frequency flow sampling than assessing base flow. In addition, smaller catchments require higher-frequency sampling than larger ones because of their more dynamic response. When used for model calibration, poor-quality observations caused by a mismatch between the spatio-temporal resolution and the spatial extent affect the identification of dominant processes simulated and the calibration of the associated parameters, which ultimately leads to greater uncertainty of the results (Beven, 1989). Thus, accurate representation of the spatial and temporal variability of phenomena (e.g., patterns) is related to the sampling frequency (e.g., temporal resolution) and density (spatial resolution) as well as the data quality (Van Rompaey and Govers, 2002).

Observations used during parameterization and calibration of hydrologic and water quality models need to be translated from the real world into the digital domain of the model at two different levels: (1) spatial and temporal discretization (i.e., geographical representation and temporal data aggregation/disaggregation), and (2) spatial and temporal definitions for numerical solution of algorithms embedded in the model code. An example of the first level is that data measured at the outlet of replicated plots may consist of stage collected at 1 min intervals along with analyte concentrations in individual or composite runoff samples collected at defined flow intervals. To be useful in calibrating a model, stage needs to be converted into flow rate, flow rates may need to be aggregated to volumes at a selected time step, and concentration values need to be converted to constituent loads for that same time step. In these translations, data may be transformed through direct mathematical operators (e.g., summation) or spatial/temporal interpolation (e.g., centroid of a square cell, mean values). Either the modeling or the monitoring teams perform these actions, which should be documented, and the selection of the needed resolution needs to consider the modeling objectives. For example, averaging flow data over a time step that is too long relative to the catchment area hides the temporal dynamics of the event hydrograph and may result in a model that does not simulate flow dynamics properly. Transformation of calibration data has an impact on how the processes the data describe will be interpreted, and these transformations must be considered in light of the objectives of the modeling study.

The second level of discretization is more subtle because it is internal to the model. Some models (e.g., MIKE-SHE, HYDRUS, RZWQM, MODFLOW) allow and automatically set a computational spatial and temporal resolution that can be different from that specified in the input and calibration data sets. Because space and time in the digital domain can be represented to an infinitesimal level, a spatial and temporal resolution must be assigned (e.g., 10 m^2, 60 min), and data are transformed within the model to match these resolutions, possibly using linear interpolations or other algorithms. However, these data transformations may result in a different representation of a phenomenon and thus affect the simulation results by misrepresenting hydrologic processes or causing numerical instabilities. For example, a daily rainfall amount may not be equivalent to a 24-hour amount, and the interpolated hourly value is generally not equal to 1/24 of a daily amount. Similarly, model interfaces such as ARC-SWAT automatically assign one precipitation gauge per subbasin, even if more are supplied as inputs. The loss of information due to interpolation or accumulation can result in severe misrepresentation of the spatial pattern.

The spatial and temporal extents of calibration data sets must be considered as well. As discussed earlier and by Arnold et al. (2012), it is recognized that calibration sets need to be long enough to include a variety of weather patterns with dry and wet spells and extreme events. Spatially, calibration of hydrologic processes at several locations throughout a drainage area can improve overall model performance. For example, in a watershed, calibration of the water balance at upstream stream gauges can improve the overall temporal performance at a downstream gauge (Arnold et al., 2012). In addition to in-stream data at multiple gauges, the use of which has been documented for model calibration (Santhi et al., 2008; White and Chaubey, 2005), estimates of variables derived from remote sensing data (snow cover, ET, LAI, soil moisture) can provide useful information (Moran et al., 1994; Sandholt et al., 2002). For example, calibration of hydrologic models has been successfully attempted in data-scarce regions using snow cover extent estimates derived from satellite data (Boudhar et al., 2009; Chaponnière et al., 2008; Stehr et al., 2009). However, algorithms that derive evaporative demand or soil moisture from vegetation indices and procedures are still being developed for use in calibration processes.

At plot or small field scale where experiments can be conducted with several replicates, additional challenges appear because some of the variability between plots remains unexplained and thus is not taken into account by the model. A strategy used by some modelers is to average the observed temporal and spatial variability between the replicated plots (Phong et al., 2011; Plotkin et al., 2013). Alternatively, Nearing (2000) and Harmel et al. (2010) proposed including the unexplained variability and the measurement uncertainty into the comparison criterion used to assess model performance.

SPATIAL AND TEMPORAL RESOLUTIONS OF SOIL, LAND USE, AND TOPOGRAPHIC DATA

Selection of input data resolution depends primarily on the size of the simulated area, whether it is a watershed or a 3D space including a streambed, the surrounding soil and the connected aquifer, and the variables of interest in the simulation (Mukundan et al., 2010). However, the resolution of input data has been found to impact model calibration, performance, and results. The sensitivity of a model to the spatial resolution of input data depends on the underlying assumptions of spatial uniformity and the equations used for simulating various processes. For example, if a process simulation is based on input parameters that remain constant over different spatial extents, then this process parameterization tends to be insensitive to the spatial resolution. For example, herbicide properties are often assumed to be independent of the area to which they are applied and thus independent of the spatial resolution. However, in most cases, model parameters vary across short distances, and their value depends on the scale at which they are assessed. For modeling purposes, their value is derived by generalizing spatial data over the smallest spatial element in the model. Finsterle et al. (2012) explained how this parameterization process makes these parameters model-dependent, i.e., their value depends on the model, the resolution of the parameterization, and the parameterization process. For example, hydraulic conductivity is affected by several factors that are not uniform across a field (e.g., compaction, spatially non-uniform historical management of the field, macroporosity; Mankin et al., 1996). When values for these soil parameters are derived from observations at a scale smaller than the simulated spatial unit, (e.g., soil sample versus cell size, hydrologic response unit, or subarea), the representative value for that simulated area may be very different from the measured values. The range of calibrated parameter values for the simulated areas is also likely to be smaller than the range of measured values. Conversely, as Healy and Essaid (2012) point out, the scale associated with a parameter measurement is sometimes larger than the size of the simulated areas. In this case, the range of calibrated values is likely to be larger than that of measured values. This would be the case with VS2DI when the grid cell size is only a few square centimeters.

At watershed extent, the method of parameterization, rather than model structure, may determine how the model responds to the spatial resolution of input data. For example, parameters from small areas of land use or soil type may be included specifically, averaged, or neglected. In SWAT (Arnold et al., 2012), the HRU parameters may be those of the most common soil types or land uses in a subbasin, neglecting minor soils or land uses. For maximum utilization of the spatial resolution of soil and land use data layers, an HRU may be defined for each combination of land use and soil in the subbasin. In HSPF (Duda et al., 2012), a subunit may be assigned an average value from the same input data. In the first case, input data spatial resolution has less impact on parameterization since minor soils or land uses are ignored, while in the second and third cases, all soils and land uses are either taken into account specifically (second case) or averaged (third case).

Soils Input Data

Soils input data in most models primarily refer to physical and chemical properties of soils. Physical properties are required for modeling the movement of water and air through the soil profile. Chemical properties are used to define initial levels of different chemicals in the soil and to control chemical transformations and leaching processes in the soil profile. Soil properties used with point and plot scale models are usually based on laboratory and/or field measurements for the modeled soil column or field plot. Larger-scale (field and watershed) hydrologic and water quality models in the U.S. use data mainly derived from one of two soils databases: STATSGO and SSURGO. The State Soil Geographic (STATSGO) database is available at 1:250,000 scale and is mainly used for multi-county and regional planning (USDA-NRCS, 2014b). The smallest mapping unit in the STATSGO database is approximately 625 ha. The Soil Survey Geographic (SSURGO) database, on the other hand, is available at 1:12,000 to 1:63,000 scales. The database was developed by the USDA-NRCS based on detailed soil surveys and is updated on a regular basis (USDA-NRCS, 2014a). The smallest mapping unit of SSURGO is approximately 2 ha. Thus, this database is appropriate for use in small to medium scale watershed simulations.

In most hydrologic models, soil map scale becomes less significant as watershed area increases (Juracek and Wolock, 2002). Some studies show that irrespective of the resolution of the soil data, the models performed similarly for certain outputs, such as flows (Di Luzio et al., 2005; Gowda and Mulla, 2005; Mukundan et al., 2010; Wang and Melesse, 2006) and sediment (Mukundan et al., 2010). On the other hand, in watersheds dominated by agriculture (Romanowicz et al., 2005) and those with flat topography or poorly drained soils (Chaplot, 2005), higher-resolution soil maps improved model performance with respect to water quality. Some studies reported contrasting findings; for example, some reported higher water yields with SSURGO and higher sediment yields with STATSGO (Geza and McCray, 2008, in Colorado; Peschel et al., 2006, in Texas).

Vertical discretization of soil profiles is a different form of spatial discretization and also affects model results. Downer and Ogden (2004) showed that with a coarse vertical discretization of soil profiles, infiltration processes were not correctly initiated and simulated, which caused a shift from hydraulic conductivity to initial soil moisture being a sensitive parameter. This shift subsequently caused difficulties during model calibration.

Topographic Data

Topographic data are essential for field and watershed scale modeling. Digital elevation model (DEM) resolution directly affects watershed delineation, stream network, and subbasin classification. These DEM-derived parameters affect estimation of runoff, sediment, nutrient, and pollutant loads. The topography of an area has a direct impact on the resolution of the DEM necessary to accurately delineate the watershed. In flat areas, a low-resolution DEM is likely to produce steeper slope gradients than exist in reality (Thompson et al., 2001). In areas with more relief, coarser DEMs generally result in decreased slopes and increased contributing areas (Wu et al., 2008). The larger grid cell of a coarser DEM will have an elevation that is the average elevation of the smaller cells of a higher-resolution DEM. Thus, elevations from the coarser DEM, and slopes calculated from these elevations, will cover a smaller range of values than those from a higher-resolution DEM. In spite of results by Vieux et al. (1993) showing decreased flow path lengths of the main channel with coarser DEM and results by Di Luzio et al. (2005) showing an underestimation of the watershed area, Wu et al. (2008) suggested that these effects are variable and depend on the shape of the flow path for flow path length and on the shape of the watershed boundary for watershed area. As a consequence, coarser DEMs can result in errors in the estimation of watershed area, slopes, and flow path lengths, which affect water yields at the watershed outlet as well as sediment loads, nitrate-nitrogen (NO_3-N), total nitrogen, and total phosphorus loads (Chaplot, 2005; Di Luzio et al., 2005; Lin et al., 2013). Vertical resolution of DEMs affects the terrain attributes particularly in flatter areas, and its effects are more pronounced for a finer horizontal resolution. Low vertical resolution can result in more zero-slope flat areas and a misplacement of the channel network (Gyasi-Agyei et al., 1995; Thompson et al., 2001).

In connection with the resolution of the DEM, the size of the modeled area directly affects watershed delineation. Generally, as the size of the simulation domain increases, so does the definition of the "minimum contributing area" required to keep the number of channel simulation units, and the run time of the simulation, within reasonable bounds. However, the ability to spatially identify the source areas of water and pollutants depends on the extent to which the channel network is explicitly elaborated. Dabney et al. (2013) modeled a 6.6 ha catchment and found that delineating channels with a minimum contributing area of 600 m^2 resulted in the best match between predicted channels and observed locations of ephemeral gullies in an Iowa field. At the other extreme, in simulating the Upper Mississippi River Basin with SWAT/APEX, channels were defined onto the outlet of 8-digit hydrologic unit code (HUC8) basins (Wang et al., 2011), i.e., areas greater than 2000 km^2. Figure 2 indicates that sediment contributions from concentrated flow in gullies and larger channels can greatly increase sediment delivered from areas of 10^{-3} to 1000 km^2. Modeling at the HUC8 scale must address these processes for the results and conclusions to be robust. In practice, the minimum contributing area is often selected as a function of the size of the area being simulated and of the topographic, land use, and soil data resolution more than as a function of the processes that need to be represented. Depending on the area being simulated, the selected minimum contributing area probably falls between the two extremes cited above and is rarely reported even though results are affected by that decision (Baffaut et al., 1997).

New approaches have been proposed to represent watershed spatial structure and to account for hydrologic connectivity between hydrologic response units, such as the catena approach (Arnold et al., 2010) and the variable source area approach (Easton et al., 2011) implemented within SWAT. Each of these approaches yields a very different pattern of source pollutant contributing areas compared to classical HRU discretization or fully distributed grid approaches. However, all the resulting patterns are very dependent on the extent of channel definition. This aspect is not associated with any particular model and is seldom given the explicit attention that it deserves despite recognition previously noted that a more detailed channel description results in a longer total channel length, smaller contributing source areas, and shorter hillslope lengths. Thus, it shifts the computed source area sediment contributions from hillslopes to channels (Baffaut et al., 1997, for WEPP; Canfield and Goodrich, 2006, for KINEROS).

Land Uses

Land uses within a watershed affect water yield as well as sediment and chemical pollutant loads at the watershed outlet. Type of vegetation significantly influences plant water use and evapotranspiration, surface runoff, soil erosion, input of chemicals and organic sources of nutrients to the soil-water-plant system, and nutrient plant uptake. These processes have a large effect on the watershed hydrology and the fate and transport of sediment and chemical pollutants within the watershed. Land use input data are used to parameterize watershed models for simulating hydrologic and biogeochemical processes influenced by the type of land use. Land use map resolution affects the relative amounts of land in each land use category and thus the effect of management associated with each land use, e.g., the amount of agricultural inputs applied or tillage occurring in a watershed. Di Luzio et al. (2002) showed that coarser land use maps resulted in higher average curve numbers, and hence caused higher water and sediment yields. However, these results cannot be generalized, as the effects of DEM, soil, and land use resolutions are interconnected and may depend on slope and land use distribution in the watershed and possibly on the size of the watershed. Coarser maps tend to emphasize dominant land use and soil classes, and average slope. Extremes disappear from the range of values present in the model. For land use and soils, small pockets of a specific land use or soil may disappear from the map because of the coarse resolution even though they may be significant source areas. For example, small polygons of urban or sludge-irrigated land may disproportionally affect flow or contribute to nutrient loads, yet they may not appear in a coarse-resolution land use map. Consequently, as the spatial extent increases and the spatial resolution decreases, the model progressively becomes a representation of the average or dominant conditions in the watershed and excludes the extreme conditions (Gentine et al., 2012). While this might be valid for long-term studies of water resources, eliminating areas or events that cause extreme behavior is clearly not recommended when the modeling objective is to identify areas or events that contribute most to water quality impairment. The objectives of the modeling study should determine the appropriate data resolution.

An additional factor that affects how the spatial input resolution impacts model results is the extent of the simulated area and model objectives. Di Luzio et al. (2005) and Heathman et al. (2009) discussed the hierarchy of spatial inputs with respect to their resolution effects on SWAT predictions. For any watershed, high-resolution land use maps substantiated by local surveys of management practices may aid in deriving more accurate parameters for prediction of surface hydrology and water quality. The resolution of soil spatial inputs may be less important for larger watersheds (Heathman et al., 2009). On the other hand, high-resolution soil maps, associated with a combination of topography and land use, are important when prediction accuracies are required at small spatial simulation units (e.g., HRU; Daggupati et al., 2011) or when the spatial extent of the simulated area decreases, as in field-scale studies using APEX (Mudgal et al., 2012) or RZWQM (Thorp et al., 2008). Bonta (1998) showed that annual runoff from a small agricultural watershed (0.26 ha) was more than twice the annual runoff from another adjacent watershed (0.51 ha) that was in similar land use and mapped in the same soil type on the NRCS county-level soil map available at that time. Runoff differences were explained by additional site-specific soil characterization (Kelley et al., 1975) and soil moisture data, first-order soil surveys, geological characteristics, and field observations of wet areas. However, these would not necessarily be known to a modeler trying to model small ungauged watersheds using readily available data.

Spatially distributed and temporally varying land use parameters are generally considered constant throughout a simulation. This assumption may be valid for larger watersheds and for distinctly different land uses (e.g., urban versus agricultural land), but subtle changes in land use may also be important. For example, changes from one crop to another, from cool to warm season grasses, or changes in the timing of activities such as planting, spraying, or plowing may vary spatially across the simulated area and temporally during the simulation period. For small simulated areas, it is critical that these changes be represented, and field-scale models such as DRAINMOD, APEX, and RZWQM incorporate these aspects. Similarly, watershed models such as SWAT and HSPF have detailed vegetation components that can simulate different vegetation types (trees, row crops, grasses), crop rotations, and farming practices. However, one easily envisions that model complexity would grow exponentially if, for example, the actual succession of crops was simulated for each field of a large watershed in a continuous simulation model. A temporal and spatial threshold below which simulating temporal and spatial changes in land use and land management is critical has not been defined and will depend on the variables of interest. For example, atrazine transport studies have shown that for 50 to 100 km^2 watersheds, it is important to know and distribute the application dates throughout the watershed (Bockhold et al., 2006; Heathman et al., 2008; Neitsch et al., 2002). Tools are available in some models to incorporate the spatial and temporal variability of management practices or temporal changes in land uses over the simulation period. For example, the automatic heat unit scheduling in EPIC, APEX, and SWAT gives the ability to schedule management practices across large areas as a function of climatic variability and the crops grown (Wang et al., 2012), temporal land use changes can be taken into account in SWAT (Arnold et al., 2012), and monthly variable parameter values can be specified in HSPF, along with representation of variable management practices and land use changes through Scenario Builder in the HSPF-based Chesapeake Bay Watershed Model Phase 5.3.2 (USEPA, 2010).

Spatial and Temporal Resolutions of Weather Data

The magnitudes and variability of weather elements drive watershed response variables of interest (e.g., runoff, chemical loads). This section presents spatial and temporal considerations of weather data for watershed modeling. Because of the highly variable nature and importance of precipitation for watershed modeling, precipitation is given special emphasis.

Weather elements important to watershed hydrology modeling are those that affect the state of different hydrologic variables on the landscape during and between storms. Precipitation is the crucial input driver recharging soil and ground waters and causing runoff. Evapotranspiration (ET) between precipitation events is a major process affecting landscape soil-water depletion. Algorithms available to compute ET can require measurements of air temperature, solar radiation, dew point, wind speed, and relative humidity, often at a daily time resolution. Precipitation is often required with a daily resolution, but some models require subdaily values (hourly or less), and some models will disaggregate the daily total using a synthetic pattern of precipitation for different modeling needs (e.g., APEX; Steglich and Williams, 2013). Jeong et al. (2010) showed improved simulations of peak flows (but not low flows) by using a subhourly version of SWAT with Green-Ampt infiltration. These authors suggested that water quality modeling can be improved by incorporating subhourly data. The most spatially and temporally varying weather input is precipitation. In areas where orographic effects due to large relief dominate, precipitation generally increases with elevation (e.g., Hanson, 2001), with greater increases during winter. Over areas with less topographic relief, precipitation on leeward slopes has been shown to be larger than on windward slopes (Lentz et al., 1995). Ground-level precipitation also varies with wind direction and speed, wind obstacles, and aspect, even over a relatively small area. At the larger scale, three-dimensional representation of the temporal and spatial weather sequence may be necessary. For precipitation, this includes variation of precipitation amounts, intensities, and form with elevation in storms. Air temperature, wind, and other weather elements also vary with elevation in high-relief areas.

In arid regions, frequent convective storms are characterized by large spatial variability of rainfall. In Arizona, Faurès et al. (1995) showed that modeled runoff volume and peak flow results improved by incorporating four rain gauges over a 4.4 ha area as compared with using a single gauge. They concluded that a single rain gauge is not representative of the spatial variability of rainfall. Unless a model is designed to accept inputs at this level of spatial detail and data are available, spatial averaging is necessary for modeling regardless of associated modeling errors and uncertainty of the results.

In addition to spatial variability, precipitation measurements are fraught with errors due to wind, air temperature, and equipment. Measured precipitation can be inadequate for estimating the effects of management or land use through model simulation, i.e., scenario analysis, because of limited spatial availability, short durations of records, mixed sampling resolutions (i.e., time and depth resolutions may not be the same for all rain gauges during the same time period), changing climate, and horizontal and vertical variability. Even for small-scale applications, point data may not be representative of spatially variable precipitation (e.g., Faurès et al., 1995). These errors and biases have impacts on the representation of precipitation inputs, which are the driving force in all rainfall-runoff models, as discussed by Malone et al. (2014). Additional sources of error stem from potential spatial or temporal discontinuities and incongruity between different data sources. For example, aggregation of instantaneous data at a daily time step is not always based on the same reporting period; some agencies might use the 12:00 midnight to midnight period, while others use 7:00 a.m. to 7:00 a.m. (Saraswat et al., 2014). Awareness of these issues is important at any spatial and temporal scale but especially for large-scale models and long simulations because measurement errors may vary across the simulated area and/or during the simulation period (Malone et al., 2014). In most cases, precipitation must be averaged over an area (e.g., subbasin or subarea) to meet spatial and temporal precipitation input requirements of models. Averaging indirectly incorporates coherence of storms (natural spatial and temporal correlation). Common methods for averaging include depth-area curves, simple averaging, Thiessen polygons, and inverse-distance weighting. Depth-area curves reduce point rainfall amounts into areal intensities and introduce runoff volume errors. Simple averaging over a subbasin may not take full advantage of available data if the number of subbasins in a watershed is not increased (i.e., better spatial discretization of the watershed) concurrently with increasing rain gauge density. Simple averaging may result in reduced variability in hydrologic and water quality outputs, especially during seasons with large spatial variability due to thunderstorms (Cho et al., 2009). The Thiessen method was suggested as the best method for future use in SWAT (Cho et al., 2009).

Temporal averaging of precipitation over an area can also affect hydrographs compared with point precipitation (Berndtsson and Niemczynowicz, 1988). For example, if mass curves of precipitation are averaged over an area, intensities are shifted later, storm durations increase compared with point estimates, and storm coherence is not preserved. This affects the timing and magnitudes of all model output variables.

For models that do not require calibration, stochastically generated data may be advantageous because a synthesized data sequence can be generated for as many years as required and can incorporate seasonal and spatial variability. It may also be useful for scenario analysis with a previously calibrated/validated model. The statistics developed from measured precipitation data and used to generate synthesized data need to take into account potential non-stationary trends in measured data (e.g., climate change), atmospheric forcings (e.g., El Niño Southern Oscillation), or changes in recording methods (Groisman et al., 2013) in order to be statistically representative of long-term characteristics.

Watershed models assume temporal and spatial uniformity of precipitation inputs over the spatial elements of the model (e.g., HRU). Whether the data are measured or stochastically generated, these inputs originate from point weather data that are assumed to be spatially and temporally representative over the element. Consequently, coherence of weather inputs is not considered within an element. Natural coherence between elements is only approximated when there are a sufficient number of adequate weather stations to provide the underlying data for adjacent elements. Currently used stochastic precipitation generators do not incorporate coherence generally, leading to less coherent precipitation inputs than measured data. However, Wilks (1998) provides an example of incorporating stochastic spatial coherence in precipitation with a daily time step. Furthermore, spatial and temporal coherence are important when model inputs are derived from the outputs of global circulation models (GCM) for an entire large grid cell and must be spatially and temporally disaggregated.

NEXRAD radar data incorporate coherence characteristics and may provide valuable inputs for medium (100 km^2) and large-scale modeling applications. Moon et al. (2004) suggests that NEXRAD radar is a good alternative where there is a low-density rain gauge data network, such as in their 2608 km^2 study area. Sexton et al. (2010) suggested that NEXRAD data is a good alternative to a poorly distributed rain gauge network when simulating streamflows from a 50 km^2 area. However, problems with using NEXRAD data include calibration with non-representative rain gauge data and are summarized by Hunter (1996).

PRISM modeling (Daly et al., 1994; PRISM, 2013) offers monthly and/or daily precipitation data at grid sizes ranging from 800 m^2 to 4 km^2 over the U.S. and is another source of data useful for large-scale applications. An advantage of these data is that they are coherent, and some data sets are available on a daily basis. For data sets available on a monthly basis, a temporal disaggregation scheme is needed to develop a daily time series that can be used as precipitation inputs to models. A disadvantage of these data is that they are developed from raw precipitation measurements with underlying biases discussed above.

SYNTHESIS: CONSIDERING PROCESSES, DATA, AND MODEL OBJECTIVES

Considerations in the selection of appropriate spatial and temporal resolution of process-based hydrologic models include: (1) the processes simulated by the model, and (2) the objectives of the study. In addition, the temporal and spatial resolution of available input data may also limit the model selection. The selection of spatial and temporal resolution should be guided by the following principles:

Principle 1: The intended extent and resolution of the selected model should match the extent and resolution of the processes that need to be simulated.

Principle 2: The spatial discretization (resolution) of the simulated area and the temporal discretization (time step) of the simulated period should take into account the degree of variability necessary for the objectives of the study.

Principle 3: The spatial and temporal resolutions of input and calibration data should be compatible with the model spatial and temporal discretization levels, which is informed by study objectives.

Principle 4: Calibration and validation of models that involve multiple scales should be performed in successive steps considering the dominant processes, at scales that are appropriate for these processes.

As a corollary to the fourth principle, validation of a model for one extent does not imply validation for smaller or larger extents. In the absence of validation at the extent that is relevant for the analysis, results should not be extended beyond the scale for which the simulation was designed, parameterized, and calibrated. A general strategy to select the appropriate model and model resolution is summarized in table 3.

Table 3 also provides two suggestions when multiple spatial or temporal extents and resolutions are relevant:

1. When the modeling objectives must consider subwatershed or field scale processes, a complex watershed model may not be appropriate. Rather, the modeler should consider dividing the problem into smaller questions and using a field-scale model.

Table 3. Steps and principles for selecting the model and the spatial and temporal extents and resolutions best suited for a study.

Step 1	Step 2	Step 3	Principles
Identify modeling objectives	Identify processes that need to be simulated	Identify the spatial and temporal extent and resolution that are relevant for each process, taking into account the degree of variability necessary for the objectives of the study.	Single extent and resolution (e.g., field, day): • Select a model appropriate for the spatial and temporal extent and resolution of the critical processes (Principle 1) and for those of the objectives (Principle 2). • Use input and calibration data compatible with the model spatial resolution and temporal discretization (Principle 3). Multiple extents and resolutions (e.g., fields within a watershed, day and hours): • Select a model compatible with the required spatial and temporal resolutions. • Perform calibration and validation in successive steps considering the dominant processes, at resolutions appropriate for these processes (Principle 4). • Alternatively, use smaller single-extent/resolution models and develop linkages.

2. When the modeling objectives address interaction of spatial subunits or processes that operate over different extents, such as fields and watersheds, the modeler should consider using two models and, if feasible, develop a linkage to explicitly take into account the interactions that exist between the two extents. In this modeling approach, the outputs of small-scale models could override the equivalent output from the larger-scale model.

In the following section, we discuss the issues that can occur when there is a mismatch between the modeling objectives, the processes simulated in the model, and the extent and resolution of input and calibration data sets.

Issues Associated with Mismatching of Temporal Scales

The choice of an appropriate time step can be affected by: (1) the objectives of the study and the processes simulated and (2) numerical instabilities. To achieve meaningful results, model performance assessment must focus on the processes and model outputs that are relevant to the purpose of the modeling exercise using methods that reflect variation at appropriate temporal and spatial scales. Thus, the processes that need to be simulated and their associated temporal resolution need to be identified (Step 2, Principle 1). For example, if the issue of concern is the stability of a flood control structure during an extreme hydrologic event or the biological impact of high or low transient concentrations of toxic compounds, then dynamic hydrologic, geo-technical, or biological responses of the system are most critical. If the purpose is to design the needed size of a culvert or bridge opening, then validation should focus on peak runoff rates (Goodrich et al., 2012). If the purpose is to determine the size of a detention structure, then the objective function should focus on the runoff volume of extreme events. In contrast, if the objective of a study is to assess the long-term degradation of a soil resource, the long-term change in soil carbon, or the life expectancy of a large reservoir subject to sedimentation, then it is more critical to accurately predict the average rate of change than the short-term variability in that rate. In this case, calibration statistics reflecting the ability of a model to track short-term variation should not dominate over an assessment of long-term accuracy. The best model will match the dynamic response with minimum bias.

As resolution increases, variability increases. Consequently, temporal averaging causes variability to decrease and extremes to disappear from the range of values. For example, the variability of daily flows is larger than that of monthly flows, which is larger than that of annual flows. Regardless of model complexity, model performance measures should focus on the temporal variability that is critical to the purpose of the modeling exercise, whether it is short-term dynamic response or long-term impacts (Principle 2). If the modeling objective is to understand the long-term impact of management, climate, or land use changes, annual simulation results may be sufficient, or seasonal outputs could be analyzed from monthly simulation results. However, if the objective is to understand the variation at a finer time step, such as the impacts of a flood, a daily or subdaily time step is needed. Similarly, water quality processes evaluated on a daily time step may be very different from those evaluated on an hourly time step (Iudicello and Chin, 2013) because critical processes such as algae or bacteria growth and death occur on a subdaily time step (Vandenberghe et al., 2006). This can also affect the choice of the model.

If the model is not sensitive to or designed for the temporal resolution needed for the simulation, it may not be the best choice (Principle 1). For example, models that use daily precipitation amounts (mm) for hydrology simulation may not be suitable for analyzing the impacts of flood events because the modeling algorithm needs to be sensitive to the intensity of precipitation (millimeters per hour). Aggregating multi-day rainfall events into daily values starting at midnight can lead to pulsing hydrographs that may not resemble observed streamflows. Similarly, parameterization errors occur when we use constant values for a parameter that varies in time, such as a constant Manning coefficient along a stream segment.

Once the model and the temporal extent and resolution are defined, care should also be taken that the data used for parameterizing and calibrating the model match the intended use of the model (Principle 3). Appropriate resolution and representativeness of input parameters are critical for correct simulation of processes. Use of data at a resolution that is too coarse may result in poor performance, particularly with respect to extreme or infrequent events or biophysical settings. If data sets are not available, the study objectives may have to be revised or the study may have to be delayed until data can be collected. For example, it would be erroneous to use monthly data to calibrate a model ultimately intended to assess flow, concentrations, or transport at a daily or weekly level (Healy and Essaid, 2012). On the other hand, the opposite can be useful: obtaining good model performance at a time step smaller than required by modeling objectives suggests that the processes are correctly simulated. When data are available at multiple temporal resolutions, we suggest calibrating processes at progressively smaller time steps, ensuring vegetation biomass, water, and nutrient balance at annual time steps, followed by monthly flow and loadings, and finally at a daily time step to refine peak flows and recession curves.

Numerical instabilities may also affect the choice of temporal resolution. In some hydrologic and water quality models, a different time step may be selected for different processes and may further change with time. The choice of temporal resolution for different hydrologic processes is important to prevent numerical instability and reduce uncertainty of the results. Although in general the time steps of the processes within each subsystem (e.g., surface, vadose, saturated zones) are independent, they must converge to properly allow exchanges of water and solute fluxes. This leads to some restrictions on the specification of the maximum allowable time steps. As an example, in the MIKE SHE model, each of the main hydrologic components runs with independent time steps. If the river model in MIKE SHE (e.g., MIKE 11, a one-dimensional hydrodynamic flow model) is running with a constant time step, then the maximum overland flow time step must be a multiple of the MIKE 11 time step. On the other hand, if the modeler decides to run MIKE 11 with a variable time step, the actual overland time step will be truncated to match the nearest MIKE 11 time step. The overland flow time step is always less than or equal to the unsaturated zone time step, and the unsaturated zone time step is always less than or equal to the saturated zone time step.

Numerical instabilities can generally occur during periods of steep changes in state variables. For example, heavy rainfall after relatively dry conditions will cause a quick and large increase in soil water content in the vadose zone. Similarly, the application of agrochemicals will cause an abrupt increase in the concentration of the agrochemical in soil water. To reduce numerical instabilities, most integrated models have incorporated a time step control that successively reduces the time step until it satisfies the stability conditions of the numerical solver. For example, the nitrogen component of DRAINMOD (Youssef et al., 2005) simulates the reactive transport of different nitrogen species (nitrate, ammonium, and organic N) using an explicit finite difference solution to a multiphase form of the advection-dispersion reaction equation. The model automatically and successively decreases the time step by half until numerical stability is achieved. Time steps on the order of minutes could be necessary after the application of nitrogen fertilizer, which causes a sudden and large increase in the nitrate and/or ammonium concentration in the vadose zone.

In physically based models, simulation of the hydrologic and reactive solute transport processes is based on numerical solutions of differential equations under different spatial discretization schemes in which the time step plays an important role in the accuracy of the solution. In some cases, shortening of the time step leads to improved accuracy. However, although numerical instabilities are reduced, there may be no improvement in accuracy because data at the higher resolutions are often interpolated from those available at a coarser spatio-temporal resolution. In addition, available data are often averaged over time and space because of process heterogeneity.

Issues Associated with Mismatching of Spatial Scales

It is important that model performance evaluations consider whether all critical processes are reflected in the calibration (Principles 1 and 2), especially when measurements made at one spatial scale are extrapolated to larger scale. As discussed by Goodrich et al. (2012), at relatively small scales, carefully calibrated process-based models are superior to simpler models. However, at larger scales, inadequate knowledge of boundary conditions, critical inputs, representative properties, and the emergence of additional processes such as channel processes make up-scaling challenging. For example, if field-scale erosion and sediment transport are important processes to simulate, then a field or smaller scale model is necessary. If a watershed model is selected, it must consider the finer details of the physical processes occurring at field scale and route the edge-of-field losses through the stream network. A watershed model application will benefit from calibration and validation using field-scale measurements in addition to calibration at the watershed scale using stream gauge data (Principle 4). If the watershed model does not simulate the needed processes in the details prescribed by the modeling goal, a field-scale model would be a better choice.

As we have discussed previously, the scale at which a parameter value is determined can affect that value. Structural model errors inevitably occur when we use relationships derived from plot or edge-of-field data and apply them to larger watersheds without considering the scale at which parameters were derived. Process-based models can help extrapolate small-scale findings to larger watersheds, provided that processes becoming active for larger areas are appropriately represented (Principle 1). Similarly, scaling down from large extents, at which hydrologic monitoring is conducted and water resources management goals are defined, to smaller extents, at which agricultural management decisions are made, is a challenging task and can lead to misleading results if equifinality issues are not taken into account.

Scaling up Field or Farm Size Results

Scaling up is used to estimate the watershed or regional effects of a specific crop management or land use change on flow and water quality. Government agencies and water resource managers use such techniques to estimate flow, sediment, and nutrient loads discharged into a main regional or national water body under alternative land management based on results from experimental plots or small-scale models. Examples in the U.S. include the global effect of agriculture on the Ogallalla Aquifer, the Gulf of Mexico, or Chesapeake Bay in which the effects of modifications of the production systems and farming practices are being debated, including the effects of conservation and irrigation practices, reforestation, and land use change from agricultural to urban, from range to row crops, or from row crops to perennial bio-energy grasses. Several issues arise during this process.

Representation of small extent details. As computer resources improve, finer resolution becomes increasingly possible (Beven, 2001) with high-resolution maps and good soil characterizations. Since experimental soil characterization is impossible for medium and large watersheds, modelers have to rely on soil databases, with large assumptions of spatial uniformity embedded. Similar to temporal resolution issues, calibration of a model that involves multiple spatial resolutions should be done in successive steps (Principle 4). Aspects of the water balance should be calibrated at the landscape level, while stream processes should be calibrated at the subwatershed level to ensure that the variability in the dominant processes is captured (Arnold et al., 2012).

Lumped parameter values. As the spatial extent of a model increases, the number and size of hydrologic units generally increases. Ultimately, the user makes a compromise between resolution of the input data and the ability to manage these inputs, run the model, and analyze the outputs. The decision to represent spatial heterogeneity explicitly or to lump that heterogeneity into "effective" parameter values needs to be made on a case-by-case basis depending on the processes being simulated and the needed spatial resolution. For large watersheds and river basins, individual subunits almost always represent areas larger than a field, and the parameters that characterize these units lump more variability within their value. Current techniques of watershed discretization start with channel delineation, based on topography and minimum contributing area, and subbasin definition. Possible techniques for further subbasin characterization include using the dominant land use or soil type, splitting the subbasin between the most important soil, land use, and slope classes and assuming that non-represented classes are proportionally distributed between those retained, or trying to represent all possible combinations of soil, land use, and slope within the subbasin. When parameters are lumped, extreme values tend to disappear, resulting in a model that is representative of the average conditions in the watershed but cannot take into account extreme sources. When averaging, the modeler must pay attention to retaining what is important in the model (Principles 1 and 2). In particular, all combinations of soil, land use, and slope that play an important role in the watershed hydrology and stream water quality should be recognized and included. Pockets of urban areas are a good example of such combinations; they may be small, but they may produce more runoff than agricultural fields. Because of the nonlinearity of natural processes, Nowak et al. (2006) emphasized the concept of disproportionality and the importance of outliers, both in the physical setting and in terms of land management, to account for system environmental performance, i.e., small fractions of land contribute disproportionally to environmental problems. Depending on the objectives of a study, it may be important to retain these small fractions in a regional model.

Representation of processes that are active at subgrid or subtime-step scales. As the spatial and temporal extents increase, some of the processes active over small areas or during small time durations (e.g., field scale or subdaily time step) may be concealed by compensating processes. For example, sediment leaving the field may be deposited before it reaches the outlet of a watershed. A main assumption of most hydrologic models is that the representative element (e.g., HRU, representative elementary volume) can be considered homogenous for flow and transport in all dimensions. The representative element is in physical equilibrium, i.e., concentrations or fluxes at one corner of the element can be considered to be equal to those at the opposite corner. As extent increases, this assumption is increasingly violated, especially when the data do not have enough spatial and temporal resolution to properly represent the variability of a phenomenon within the representative element. For example, gully erosion is typically not taken into account in large watershed-scale models because the gullies are smaller than the channels simulated and the erosion equations implemented in the models typically do not include gully erosion. In contrast with this typical modeling approach, Momm et al. (2012) presented a watershed-scale approach to account for ephemeral gully erosion occurring at finer spatial scales than delineated channels.

A possible solution to this problem is to scale up only to a level at which the smallest hydrologic unit would be of a size comparable to that of the experimental data set, the field-scale model, or the area needed to represent all required processes. This constraint limits the spatial and temporal extents to which experimental, small-scale data sets can be extrapolated. For further scaling-up, we suggest using intermediate-extent models that satisfy this requirement and from which can be derived representative parameter values for an area or time step that are equivalent to either several subareas or several time steps. That representative value may be an arithmetic average, an area-weighted average, or a more complicated function. In cases where the spatial or temporal variability of the parameter is low, it may be that the value used for the smaller extent is suitable for the coarser resolution. Alternative techniques to scale up parameters of the vadose zone have been advanced (Vereecken et al., 2007), but this field of research is still in its infancy, lacks data sets to validate proposed upscaling techniques, and relies heavily on the numerical techniques suggested above.

While some parameters can be scaled up, and their calibration at the smaller scale can improve the performance of a larger-extent model, others cannot be scaled up (e.g., saturated hydraulic conductivity, K_{sat}). In the case of KINEROS2 applied to plots and to a hillslope, K_{sat} values were different for these two extents (Goodrich et al., 2012). In an example of the TOUGH model application, Finsterle et al. (2012) showed how the value of permeability (a property of a porous medium that is considered constant for an individual cell in the model) is dependent on application (i.e., its value depends on the size of the modeled area and incorporates unrepresented heterogeneity). It may also be biased to compensate for other misrepresentations of the system (e.g., if the simulated layers of the geological formation do not properly represent the actual system).

Alternatively, the effects of these subunit processes may be visible within a large area, but it may not be possible to represent them in the large-extent model because the elemental unit is too large to describe what happens at a subunit level. When representative elements are forced to represent homogeneous or equilibrium conditions (i.e., concentrations or fluxes are considered equal within the representative element, where the real world is not), the basic assumptions of the model are not valid anymore, and what cannot be spatially represented needs to be taken into account by other means. For example, surface and subsurface processes that take place in and at the upstream boundary of a grass filter strip adjacent to a row crop field may not be represented in a watershed model that does not simulate the spatial arrangement of individual hydrologic units. A solution to this problem consists of specifying that the hydrologic unit contains features that will cause certain processes to occur and to simulate them directly. For example, in the latest version of SWAT (2009 and later), if the user specifies that fields of a hydrologic unit contain a filter strip or a grass waterway, then processes specific to these features are simulated without formally identifying in the model where they are located. Guzman and Fox (2012) mixed the concept of equilibrium and non-equilibrium in a conceptual model based on RZWQM to represent the problem of rapid transport of bacteria in the presence of biopores. Jarvis (2007) discussed this issue based on the problem of macropore flow. Most of his concepts can be applied to the context of spatio-temporal extents, as in most cases the representative element is large enough to break the assumption of physical equilibrium (or homogeneity).

Representation and parameterization of processes not present at the small scale. This may include stream or lake processes, for example, or gully and stream erosion processes, as discussed earlier (fig. 2), as well as processes that take place in a hydrologic context that is different from that of the experimental site. For example, the region may include an aquiclude while the experimental conditions did not. Similarly, and most likely, it may include land uses and soils other than those featured in the field experiment or model. In these cases, the general parameters of the field model may not be valid for the larger area, and additional model calibration and validation are needed. In some cases, multiple models may have to be used and linked together.

Use of multiple models. Outputs from field-scale modeling can be combined to address watershed-scale questions. In some cases, field-scale models, focused on the processes occurring at the smaller area, can be loosely linked to watershed-scale models to evaluate their combined impacts on water yield or pollutant loads at the watershed outlet. Examples include linking SWAT and APEX to simulate processes related to farming practices (Saleh and Gallego, 2007; Wang et al., 2011; White et al., 2014), linking SWAT and REMM to simulate the effect of riparian buffers on assimilating edge-of-field nitrate nitrogen before this nitrogen enters the stream via groundwater flow (Liu et al., 2007), and linking SWAT and MODFLOW to fully simulate the interaction between the stream network and the aquifer (Kim et al., 2008). SWAT and other watershed models have also been used to simulate upland processes and routing to the outlet and have been linked to downstream models that simulate processes such as backwater effects (Betrie et al., 2011), lake processes (Ernst and Owens, 2009; Narashimhan et al., 2010; Park et al., 2013), and coastal water quality processes (Bougeard et al., 2011).

Scaling down the Results of a Model Parameterized for a Large Spatial or Temporal Context

Scaling down means that the model parameterized to simulate a large area is then used to infer or predict variables of interest for smaller extents. Examples of larger to smaller extents in the spatial context are watershed to field, or large area to soil pedon. An example in the temporal context is years to days. Reasons for doing this include understanding observed flow and constituent loads at the larger extent, attributing source to each subarea of the simulated space or each time increment of the temporal space, identifying the largest contributors or periods in the simulated space, and identifying the processes and the attributes that cause the greatest losses. For example, in the context of TMDL, once pollutant reduction goals have been defined for a stream, solutions need to be identified that will meet that goal. Process-based models are often used in this context because they link management and pollutant loss from the upstream landscape and from the point discharges in the watershed to stream loadings and concentrations. However, results may differ significantly depending on the resolution of the spatial inputs used in the model. Daggupati et al. (2011) showed that field soil losses estimated by downscaling the results of a SWAT model to existing fields could vary by as much as 75%, and the area targeted for treatment could double depending on the spatial resolution of the DEM, soil and land use maps, and detail of the management information used to parameterize the model. Thus, it is critical that input data have a resolution that is consistent with the scale at which the results will be analyzed.

While several sets of parameters can lead to good model performance at the watershed outlet or on an annual basis because of equifinality, they may not produce equally good results for fields within that watershed or at a daily time step. Consequently, simulated processes need to be verified at the time step or spatial unit relevant for the model objectives by obtaining input and calibration data and validating the model at these scales. This can be challenging, as these data may be only partially available, for example from one set of experimental plots within a watershed but not for every land use and soil type found in that watershed. Sometimes, small-scale data (field data or daily data) are not available at all, which may be the reason the modeling study was undertaken. In previously published studies, the validation of processes at smaller scales used various sources of data. In the spatial context, county-level annual crop yields in the U.S. (USDA-NASS, 2013) can be used as an indication that water and nutrient plant uptakes are correctly simulated on agricultural fields. Similarly, forage yields can be used to verify that pastures support the known grazing densities across the simulated area. More recently, long-term (1971-2000) county ET maps (Sanford and Selnick, 2013) can be used to verify the evapotranspiration term of the water balance equation. Alternatively, or in addition to model validation for small spatial or temporal units, parameter optimization and uncertainty analysis can provide sets of input parameters that all produce good results for the larger area and provide ranges of predicted values for the smaller spatio-temporal units. These corresponding ranges are likely to be wider for the smaller spatio-temporal units because of the averaging that occurs when integrating in time or in space.

CONCLUSIONS

Hydrologic and water quality models cover a range of spatial and temporal scales: they simulate processes that occur over durations ranging from seconds to centuries and over spatial units ranging from soil cores to river basins, their parameterization and calibration require data that have matching spatial and temporal resolution, and the results may be analyzed for different extents depending on the objectives of the study. The selection of spatial and temporal extent and resolution is inherently linked to the simulated hydrologic processes and to the modeling objectives. For a modeling study to be successful, we recommend: (1) that the intended extent and resolution of the selected model match the extent and resolution of the processes that need to be simulated, (2) that the extent and resolution of the model application match the extent and resolution necessary to achieve the objectives, (3) that representative input and calibration data are available at a spatial and temporal extent and resolution that match those of the model and the objectives of the study, and (4) that the model is calibrated in successive steps at the spatial and temporal resolutions that match those of the critical processes and of the modeling objectives. While the selection of a model, extent, and resolution is frequently based on modeler expertise or available data, consideration of these recommendations should prevent mismatch between the temporal and spatial extent and resolution of a modeling application and its objectives.

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