Hydrologic and Water Quality Models: Documentation and Reporting Procedures for Calibration, Validation, and Use

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Abstract. *The increasing use of hydrologic and water quality (H/WQ) models for technical, policy, and legal decision making calls for greater transparency in communicating the methods used and decisions made when using H/WQ models. The objectives of this article are to: (1) provide guidelines to properly document H/WQ model calibration, validation, and use, and (2) raise issues about how to improve model documentation and reproducibility, and encourage open discussion of these topics in the H/WQ modeling community. First, eight recommended elements of model documentation and reporting are identified and described, and good examples are provided for each. Next, steps to move the H/WQ modeling community toward a culture of full model reproducibility are discussed. The use by model practitioners of the consistent and comprehensive elements described herein for documentation and reporting of H/WQ model calibration, validation, and use will allow better interpretation of published modeling studies, improve the utility of modeling studies, and allow more systematic advancement of H/WQ models.*

Keywords. *Documentation, Model calibration, Model validation, Performance criteria, Performance measures, Reporting.*

Proper documentation of model calibration, validation, and use is a critical element of good hydrologic and water quality (H/WQ) modeling practice. Thorough documentation provides information needed by reviewers and editors to assess the scientific merit and allows others to ensure that the calibrated model is appropriate for the intended use, especially as models are increasingly used to support technical, policy, and legal decision-making. Proper documentation enables the scientific findings of a particular modeling study to be used by others to draw more generalizable lessons to advance the science. Inadequate documentation may result in duplication of efforts and even lack of confidence in the results; therefore, improving documentation of the procedures used can increase modeling's scientific credibility.

A basic principle of scientific documentation is that a report should provide enough details for others to reproduce the findings (Nature, 2013). Sharing source code, data, metadata, and software may also be necessary for computational research to be truly reproducible (Peng, 2011). In recent years, robust discussion of the concept of "reproducible research" in computational science has taken place in many disciplines (NRC, 2003; Donoho, 2010; Eddy et al., 2012). However, a similar rigor in H/WQ model documentation has not yet been widely discussed or agreed on. H/WQ modeling results are difficult to reproduce, in part due to variability of input data, large numbers of parameters, availability of alternative calibration approaches, and the role of modeler experience.

A major reason for the lack of detailed documentation is that the allowable length and publication costs of scientific articles may limit the detail provided. With complex models, even thorough documentation often does not provide enough detail for the research to be reproduced. Therefore, many journals provide electronic supplements where the documentation can be provided, while other repositories provide secure locations for source code, data, and other elements of model use. Although the practice of depositing data and code in such a repository has not yet become widely used in H/WQ modeling, this article suggests the

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means by which it could increase.

The overall objectives of this article are to: (1) provide guidelines to properly document H/WQ model calibration, validation, and use, and (2) raise the issue of documentation and publication practices, in the hope that reproducibility is more openly discussed and applied in the H/WQ modeling community. While other articles in this special collection describe other important issues related to model calibration and validation, the objective of this article is to discuss how to document these elements clearly and concisely to facilitate better communication of model calibration/validation procedures and results. Specifically, this article discusses proper reporting of model calibration and validation procedures and provides a list of elements that should be reported in H/WQ modeling applications. This article also discusses methods to overcome the barriers to reproducibility in H/WQ model calibration, validation, and use.

There are two major sections in this article. The first section lists eight broad documentation topics and identifies key elements to be documented, with good examples of appropriate documentation from the literature. The topics are: (I) intended model use, (II) model description, (III) study area, (IV) observed data used for model calibration and validation, (V) input data, (VI) calibration parameters, (VII) calibration and validation strategy, and (VIII) performance assessment methods. The second section discusses how the H/WQ modeling community can move toward more rigorous documentation of model calibration, validation, and use procedures, and eventually toward a "culture of reproducibility" (Peng, 2011) in which calibration data and code are shared to advance the understanding and management of water resources.

ELEMENTS TO BE DOCUMENTED

I. INTENDED MODEL USE

The model's intended purpose and end-user expectation should be clearly defined and documented. Each purpose carries an implied expectation of accuracy and resolution that often is not clarified but is essential in setting model calibration and validation targets and interpreting model results. Harmel et al. (2014) established three general categories of intended model use (i.e., exploratory, planning, and regulatory/legal) and emphasized that each category warrants differing model performance expectations. Different end users also may have different expectations of model performance. At a minimum, the purpose of the modeling study should be stated; ideally, the implications on model performance expectations should be specified.

Many modeling studies clearly state the modeling purpose, for example: quantifying performance improvements gained by specific model enhancements (Youssef et al., 2005; Parajuli et al., 2009a; Bosch et al., 2010; Moriasi et al., 2013; Negm et al., 2014) or model input enhancements (Daggupati et al., 2011; Gali et al., 2012); targeting or prioritizing sub-areas within a watershed for specific water quality interventions (Tuppad et al., 2010b; Pai et al., 2011); comparing performance of different models (Parajuli et al., 2009b; Thorp et al., 2009; Ale et al., 2013); forecasting the H/WQ impacts of climate change (Thompson et al., 2009; Sheshukov et al., 2011), land use change (Srinivasan et al., 2010; Powers et al., 2011), and land use management (e.g., drainage; Thorp et al., 2009); defining site-specific nutrient source loads and reductions among agricultural management practices and their distribution within a watershed to support development of a water quality trading system (Lee and Douglas-Mankin, 2011); or setting cost-share payments for conservation practice implementation according to modeled sediment-yield reductions (Douglas-Mankin et al., 2013).

Although these studies state their purpose, no studies have been found that describe how these purposes relate to developing a project-specific calibration and validation strategy. Harmel et al. (2014), however, discussed recommendations for model performance interpretation for exploratory, planning, and regulatory/legal modeling applications. Similarly, Moriasi et al. (2007) indicated the need for performance ratings that vary according to the intended model but did not provide guidance on how to incorporate such differences in their performance expectations. Further research and discussion, as suggested by Bennett et al. (2013) and Harmel et al. (2014), needs to occur in the modeling community to explore the tradeoffs between model utility and accuracy and the importance of setting and documenting performance expectations.

II. MODEL DESCRIPTION

Providing an adequate model description enables readers to assess the model's suitability for the intended use and increases their understanding of the modeling study. The level of model description may vary depending on the type of the model and the purpose of the study; however, an adequate model description will generally summarize the following points:

- Model name, version, and release date (to facilitate reproducibility).
- Model type (e.g., mechanistic, quasi-mechanistic, or empirical), spatial and temporal scales (e.g., point to watershed; sub-hourly to yearly), and model structure and components (e.g., hydrology, nutrients, sediment, chemicals, carbon, vegetation).

Model Name, Version, and Release Date

For example, the SWAT model has both a release version (e.g., SWAT 2009, SWAT 2012) and a version number identifying the executable file (e.g., rev. 627 released on 24 June 2014). If no system is used to identify different model versions, then the date of model download should be listed, as a minimum. We recommend that model developers number each release or version and provide a brief list of improvements made in each version through appropriate citations.

Model Type, Spatial and Temporal Scales, Structure, and Components

While almost all modeling studies provide some aspects of this information, care should be taken to document all key information. Many H/WQ models consist of various submodels that may individually be categorized simply as process-based or empirical, but they become more difficult to categorize when combined with other submodels in an H/WQ model. Many process-based models use empirical representation of key processes that are difficult to represent mechanistically. For instance, SWAT and other watershed-scale models use the empirical curve number method (USDA-SCS, 1972) for runoff estimation and use a modified version of the Universal Soil Loss Equation (Wischmeier and Smith, 1978) to estimate soil erosion. Some models simulate H/WQ at different spatial scales. For example, DRAINMOD and APEX can simulate individual fields or small watersheds. Models may also use different time steps to simulate different processes. For example, DRAINMOD uses hourly and daily time increments for simulating hydrologic processes (Skaggs et al., 2012) and uses sub-hourly time increments for simulating nitrogen transport (Youssef et al., 2005).

As model complexity increases, providing a detailed description of the model becomes a challenge, especially for watershed-scale, multi-component, and mechanistic models. Adequate documentation can be achieved by providing a brief description of the model structure and different model components followed by more detailed description of specific model aspects relevant to the study. Modeling studies focusing on further development and testing should provide detailed description of newly added or modified aspects. For instance, Moriasi et al. (2013) provided a detailed description of DRAINMOD-based routines incorporated into SWAT to enhance modeling of watersheds dominated by tile-drained cropland. If development involves linking existing models, a brief description of the model components should be followed by a description of the linkage and the level of integration. For example, Negm et al. (2014) and Tian et al. (2012) developed whole-system models for agricultural and forest ecosystems on high water table soils by linking the hydrologic model DRAINMOD, the soil carbon and nitrogen model DRAINMOD-NII, and vegetation growth models (DSSAT for crops, 3-PG for tree growth). After providing brief descriptions of the component models, they provided detailed description of the linkage and how the newly developed models represent the interaction and feedback occurring among individual hydrological, biogeochemical, and plant growth processes. If the purpose is to compare the performance of two or more models, the descriptions should highlight the main differences among the models. For instance, Thorp et al. (2009) and Ale et al. (2013) compared DRAINMOD-NII to RZWQM-DSSAT and ADAPT, respectively. In both studies, differences between the models were clearly highlighted. Additionally, modeling studies that involve calibration and validation should provide adequate description of key processes included in calibration and validation (discussed in subsequent sections).

III. Study Area

A general description of the study area is important to clarify the setting in which the model is used. Study area descriptions should include the following information:

- Location, including size of study area, latitude and longitude, and a map showing the study area. The coordinates and map allow readers to access much of the remaining site information even if it is not included. The point of interest for which the latitude and longitude should be provided is intuitive for point-scale studies, but for field-scale and watershed-scale studies it could be the edge-of-field or the watershed outlet. Often it is appropriate (and recommended) to include the Hydrologic Unit Code (HUC) for watersheds in the U.S. or other identifying watershed code internationally.
- Topography, which should include a general description (e.g., floodplain, rolling hills, mountainous), range of elevation, and slopes (average, maximum, and minimum).
- Soil and geology characteristics, especially those that affect hydrology and biogeochemistry, extent and distribution of major soil groups or types (depending on scale, with soil taxonomic name, textural class, and/or hydrologic soil group information), and relevant geological formations and materials.
- Land use and land cover, which should include summary information about the types, extent, and distribution of land use (e.g., crop type, percent of watershed area, regions having the greatest density), any changes during the study period, and typical management practices (e.g., tillage, agrochemical application, irrigation, drainage, and/or fire management descriptions and timing).
- Water resource structures (e.g., ditches or other constructed waterways, drainage structures, terraces, water detention ponds, or reservoirs) and other constructed or natural watershed features (e.g., canals, wetlands, vegetative filter strips or riparian buffers, connected floodplains).
- Climate, which should include long-term average temperatures, precipitation, and comparison of the weather during the modeling period to the longer-term climate record.
- Locations, volumes, and constituent concentrations from point sources, such as wastewater treatment plants (WWTP) that discharge into stream reaches (for watershed models).
- Specific features of interest, highlighting unique features that help readers understand key aspects of the watershed or location.

The level of necessary detail varies by model, study area, and modeling purpose; therefore, no single example from the literature can demonstrate an ideal level of documentation. Baker and Miller (2013) provided maps with latitude and longitude and included extensive climate and vegetation information for a SWAT application in Kenya. Daggupati et al. (2011) and Pai et al. (2011) provided good examples of the use of detailed maps, text, and tables to summarize stream network, slope, soil, and land use characteristics. Tuppad et al. (2010a) provided detailed descriptions of both ground-based and radar precipitation data to support an analysis of SWAT streamflow response to type and scale of precipitation data. Forester et al. (2013) included information about changes to the natural hydrology, in this case important stream channelization that occurred over a several-year period in their watershed, which otherwise would likely have been unavailable to the reader. Pai et al. (2011) provided a detailed account of point sources in the Illinois River watershed in Arkansas, along with assumptions made to make WWTP data compatible with SWAT. To document gauge location, Sheshukov et al. (2011) used a single, minimally acceptable sentence: "The outlet of the watershed was selected to coincide with U.S. Geological Survey (USGS) gauge station 06889500 at coordinates 39° 6′ 0″ N and 95° 43′ 29″ W (USGS, 2009)." On the other hand, Pai et al. (2011) provided a map (see fig. 2 in Pai et al., 2011) showing the exact location of the seven gauges within the watershed that were used for calibration and validation, along with subwatersheds that drain into each gauge. Subsequently, they documented their rationale for the order in which sites were calibrated.

IV. Observed Data Used for Model Calibration and Validation

Observed data are the benchmark for calibration and validation. Documenting methods used to collect these data is critical for understanding the relative uncertainty of calibration and validation results. Information provided should be adequate to allow the estimation of the uncertainty of the measured data (e.g., using the method of Harmel et al., 2009). Similarly, Harmel et al. (2006) provided typical uncertainty ranges that can be used in the absence of project-specific uncertainty estimates. The following information is considered essential to describing observed data:

- Location and description of monitoring stations, including physical location shown on a study site map.
- For measurement of streamflow:
  - From a publicly available source, such as USGS, report the gauge location, station number, frequency and/or timing of measurements, and quality information provided by the source, or:
  - From another entity, report equipment model, type (e.g., bubbler, pressure transducer, float sensor, sonic sensor), and description; methods; location and orientation of sensor in water column; equipment maintenance and calibration; method used to convert stage to streamflow (including dimensions of weir or flume, or methods used to characterize channel cross-section, profile, and bed characteristics); uncertainty or data quality information from the source (if available); and citation of standard methods. Examples of important information to report for streamflow measurement and water quality constituents are presented by Harmel et al. (2006, 2009).
- For measurement of other constituents (e.g., sediment, nutrients, and chemicals), report or cite references for the following details:
  - Direct measurement (instrument, accuracy, frequency, and location of *in situ* measurement in water column, equipment maintenance and calibration, and citation of standard methods), or:
  - Sample collection (method, frequency, location of sample collection in water column, equipment maintenance and calibration), preservation and storage (method, environmental conditions, and duration), and analysis (method, accuracy, and citation of standard methods), as well as any other factors that may have influenced data accuracy.
- Method used to derive constituent mass loads from streamflow and concentrations. Examples of methods used to measure flow and flow-weighted nutrient concentrations (total N and P) using a V-notch weir and an autosampler, respectively, at individual terrace outlets in a crop field and standard analytical methods are provided by Douglas-Mankin et al. (2010).
- Citation of any quality assurance and quality control (QA/QC) protocols for streamflow measurement, field instrument use, or sample collection, preservation/storage, and analysis. Ideally, all monitoring data would meet strict QA/QC protocols, such as those reported for USGS continuously collected constituents by Wagner et al. (2006).
- For multi-site calibration studies using watershed models, it is useful to document in what order the sites were selected for model calibration.
- Temporal or spatial discontinuity between data sources needs to be reported. For example, many 24-hour precipitation values are recorded for a 7:00 a.m. to 7:00 a.m. period (or some other standard time), whereas the 24-hour USGS streamflow values are reported for a 12:00 midnight to 12:00 midnight period.

Translating data collection and analysis methods to a quantitative estimate of data uncertainty is a critical, yet often neglected, aspect of documenting the calibration and validation process. For example, Harmel et al. (2006) quantified error estimates associated with various methods of streamflow measurement and sample collection, preservation/storage, and analysis that may be useful for documenting the uncertainty of data used in calibration and validation. Their analysis found that the worst-case cumulative uncertainty values associated with measured data may exceed 40% for streamflow, 100% for TSS, and 150% to 400% for nutrients. Documenting the degree of uncertainty in measured data used for calibration and validation allows appropriate interpretation of any limitations in the calibration and validation results brought about by their use. Procedures to use uncertainty estimates for measured data in evaluation of model performance were developed by Harmel and Smith (2007) and Harmel et al. (2010).

V. Input Data

Required model input data such as study area boundaries, soil, land use, topography, and site-specific management data must be clearly documented. Weather data, particularly precipitation data, are among the most important elements in model calibration, validation, and use, and often require processing before use. The following information on input data, along with any modifications made, should be clearly documented:

- Citation of a source that includes the metadata, if published data are used. Published datasets often specify a preferred citation, which should be used. When input data are not from a published source, basic information should be included, and the full dataset should be uploaded to an electronic repository if possible.
- Dates for which each source is used if more than one data source is combined (e.g., to fill incomplete weather records).
- Modifications, simplifications, or "data cleaning" procedures used in preparing the input data, including any assumptions made to acquire or process site-specific management data to make it compatible with the model.
- For geospatial input data, the resolution of the vector/raster dataset should be noted. For derived geospatial data, such as a thematic map (e.g., land use raster), the acquisition date for the original imagery is essential for proper temporal representation of study area features.

Several examples in the literature provide good examples for documenting model input data. For instance, Wang et al. (2006) described three sources of weather data that were combined in their study. Published data sets often provide a preferred citation (i.e., Fry et al., 2011, for the National Land Cover Data), which should be used rather than simply a link to the data or citation of a secondary data source (i.e., data clearinghouse). Price et al. (2012) and Daggupati et al. (2011) provided good examples of citing nationally available databases, such as land use and land cover data (NLCD, NASS), soil data (SSURGO, STATSGO), and topographic data using the preferred citation format. To document grazing and urban lawn management practices, Pai et al. (2011) provided details of how data were acquired and processed to derive specific SWAT-compatible management data (see tables 2 and 3 in Pai et al., 2011) and documented how various categories were merged to make them consistent with each other and compatible with SWAT (see table 1 in Pai et al., 2011). Tuppad et al. (2010a) and Gali et al. (2012) both reported precipitation gauge timing details, which were important in ensuring consistency with aggregation of hourly NEXRAD data (including daylight saving time adjustments), but did not discuss the inconsistency with USGS streamflow timing.

VI. Calibration Parameters

Documentation of calibration parameters is a critical, yet often overlooked, part of modeling studies. Selection of calibration parameters from the many possibilities usually takes place by model default, prior knowledge, field data, empirical calibration, or some combination of these. The following information on parameter selection and testing during calibration is considered essential to report:

- The approach used to select calibration parameters (e.g., sensitivity analysis, experience with model, literature review, expert opinion, etc.).
- A table and associated text should provide the following information for each important model parameter:
    - For default parameters (determined by model developers without user modification), cite references.
    - For baseline parameters (determined by model user based on *a priori* knowledge), provide justification and/or citation to support each value.
    - For calibration parameters (modified after comparison to some response variable), provide the range of each parameter tested during calibration, citing references to justify reasonable ranges, and the resolution of each final parameter (±0.1 unit, ±5%, etc.). This information should be provided even if the parameter retains its default value after calibration.

The literature provides several good examples of parameter selection documentation. For instance, Spruill et al. (2000) conducted a sensitivity analysis of 15 SWAT parameters, described the physical processes related to each parameter, and then discussed how selected parameters related to their study watershed. Knisel and Douglas-Mankin (2012) listed and discussed sensitive parameters related to erosion, pesticide, and plant nutrient cycling in CREAMS/GLEAMS. Similarly, Arnold et al. (2012) discussed the parameterization process and provided a typical list of parameters for SWAT calibration. The process of hydrologic, sediment, and nonpoint-source calibration was discussed in detail by Duda et al. (2012) for HSPF; however, readers were referred to the BASINS website to obtain details concerning the parameterization process.

VII. Calibration and Validation Strategy

Details related to model calibration and validation are described by Daggupati et al. (2015); however, this section outlines recommended documentation of calibration and validation. The results of the calibration and validation process can only be interpreted by knowing which data were used, how they were used, and in what sequence. The following are recommended calibration and validation strategy elements that need to be documented:

- Sites and processes for which the model is calibrated (these should be consistent with the calibration and validation data sources, described earlier).
- Process and sequence of adjusting parameters and assessing output. Several fundamental approaches are described in detail by Daggupati et al. (2015) under the classifications of the following approaches: single-stage, stepwise single-pass, stepwise iterative with limited parameter space, and stepwise iterative with extensive parameter space.
- Allocation of the spatio-temporally distributed data (i.e., data splitting) for either calibration or validation. Several fundamental approaches are described

in detail by Daggupati et al. (2015) under the classifications of temporal split-sample, proxy basin, differential split-sample, and proxy-basin differential split-sample.

- Description of automated calibration processes or algorithms used, including:
  - Algorithm or software name and revision or version number
  - Objective function
  - Parameters optimized
  - Sampling method
  - Number of simulations
  - Any assumptions related to statistical distribution of the parameters
  - Likelihood function, prior, and posterior distributions for Bayesian-type approaches.
- Additional diagnostics used to document model performance, why they were used, and other information appropriate to the specific approach used. Assessment and documentation of non-target model outputs also provide greater insight and confidence into model performance. For example, for hydrology calibration, in addition to reporting streamflow simulation performance, it is recommended that other components of the water budget (e.g., rainfall, ET, groundwater, runoff) be evaluated for reasonableness and documented for confidence building. Similarly, if the model has been evaluated for crop yield prediction, graphical or tabular comparison of observed and predicted crop yield should be included. The use of diagnostics is discussed in detail by Daggupati et al. (2015).

There are numerous examples in the literature in which authors provided an adequate description of their calibration and validation strategy. For instance, while performing manual calibration for SWAT, Santhi et al. (2001) used a flowchart to document the sequence of outputs that were calibrated. Thorp et al. (2009) documented almost all of the elements outlined above in a detailed description of the calibration and validation process for DRAINMOD-NII. In two multi-site calibration studies, White and Chaubey (2005) and Pai et al. (2011) documented the sequence in which various sites were calibrated. Following completion of satisfactory calibration and validation using site-specific observed data, Pai et al. (2011) performed additional diagnostics wherein they compared the relative sediment and nutrient loadings from subwatersheds with respective land use distribution to evaluate if the relative spatial distribution of loadings were reasonable.

VIII. Performance Assessment Methods

Information on model evaluation is provided in a separate article in this special collection (Moriasi et al., 2015). In this section, we focus on the important documentation points when presenting the model performance assessment, which should include:

- Discussion of the methods used to assess model performance for each parameter (statistics, graphical methods, etc.).
- Description of criteria used to determine when the calibration and validation process is deemed successful, as recommended by ASCE (1993).
- Documentation of model calibration results for each parameter, including comparison of observed and modeled values, model performance statistics, and using an appropriate combination of text, tables, and graphics.
- The precise objective function used for assessing the model performance should be given in the form of equations and/or citations to standard references. If multiple objective functions are used, the sequence or combination of their use should be described. If more than one site is calibrated, the method of combining them should be included.

A great deal of information has been published on this subject. Publications such as Willmott (1981), Loague and Green (1991), ASCE (1993), Legates and McCabe (1999), Moriasi et al. (2007), Jain and Sudheer (2008), Harmel et al. (2010), and Bennett et al. (2013) are highly cited and provide valuable information on model performance assessment. These publications stress the importance of using multiple techniques to produce more comprehensive assessments.

There are several good examples of how authors have provided documentation of model performance assessment methods. As shown by Skaggs et al. (2012), including cumulative curves for variables such as drain flow on daily/monthly time series plots is highly recommended, as this additional representation not only shows the differences in daily/monthly values but also illustrates if the model over- or under-predicted a variable during the entire calibration/validation period. Similarly, when observed data are available from replicated treatments of an experiment, reporting standard deviations of observed data (Ale et al., 2009, 2012) and including of upper and lower bounds on observed data series are desirable to better understand the variation in observed data and to verify if the predicted values are within the range of observed values. White and Chaubey (2005) used a multi-objective function that combined relative error, Nash-Sutcliffe efficiency, and R^2 over three sites. Jain and Sudheer (2008) also discussed the use of statistical measures for assessing model performance. Another good example of presenting model calibration and validation results is Wang et al. (2012), who included the 5% and 95% confidence intervals of simulated corn yield while comparing the best simulated and observed yields over the calibration period.

Providing Needed Documentation

The documentation suggested in this article is extensive, and including all elements will likely raise concerns regarding the length added to journal articles, especially because of page limits and/or publication cost. However, in the age of digital communication, article length should not be a barrier to proper documentation, as many journals provide e-repositories where supplemental materials can be deposited. Similarly, repositories for data and code are becoming more and more widespread.

A first step in advancing the science of H/WQ modeling through improved documentation would be to expect researchers to routinely provide all eight documentation elements described herein either in the main body of the article or in an electronic supplement. As an accompaniment to the manuscript, most journals now include the facility to provide supplementary material. A table with policies for supplemental information adopted by key hydrologic journals is provided as an appendix to this article. The authors encourage all journals, including ASABE journals, to provide permanent digital repositories for supplemental information. In addition, we encourage colleagues to provide all details of their model calibration, validation, and use described above by supplementing the essential details with important details made available through a digital repository.

Additional supplementary information includes non-target model outputs (e.g., soil water, evapotranspiration, and crop yield) that are simulated by the model as well as the targeted outputs (e.g., streamflow, sediment, and chemical transport). While it is understood that the confidence in non-target outputs is low, this information could be useful for future modelers and could provide a valuable source of information for model advancement.

Valuable as they are, electronic supplements usually consist of text, tables, and figures designed to be read, not to be used directly in additional modeling studies. For research to be reproduced and built upon, the code along with all input files needs to be shared, as large and complex models may have thousands of parameters that are intricately connected. A journal supplement may not be the best way to do this. Most journals (e.g., *Science*) place broad size limits on supplementary material so that authors can ensure that the file sizes are reasonable and that the material is genuinely needed. Non-journal avenues to publish reproducible models include RunMyCode (www.runmycode.org), Research Compendia (www.researchcompendia.org), and SWAT Share (http://water-hub.org/swat-tool). A simple method of assembling all data and files is often provided by the model itself. For instance, in SWAT (Arnold et al., 2012), the output.std text file contains average annual values of major outputs for the entire basin. In the HSPF model (Duda et al., 2012), the hyd_man.WaterBalance.txt file produces annual-scale water balance simulations.

Discussion

Toward Reproducible Research in Model Calibration, Validation, and Use

Reproducibility of published research is not only recommended but may become mandatory in the future. In fact, the White House Office of Science and Technology Policy has instructed major federal funding agencies to develop plans to make both the datasets and research articles resulting from their grants publicly available (OSTP, 2013). Obviously, this mandate would trickle down to H/WQ modeling projects, many of which are federally funded.

Journal requirements are also moving computational research toward the goal of reproducibility. Numerous journals have developed policies requiring researchers to provide data and code. These policies were synthesized for 50 top journals by Alsheikh-Ali et al. (2011), although they have not always resulted in freely shared data and code (Stodden et al., 2013). Recent research has compared publications for which data are shared and not shared, and found that "willingness to share research data is related to the strength of the evidence and the quality of reporting of statistical results" (Wicherts et al., 2011) and "sharing detailed research data is associated with increased citation rate" (Piwowar et al., 2007). The most rewarding part of this exercise is that modelers can publicly claim that their work is reproducible and invite further improvement.

Whereas submission of code along with a manuscript is practiced widely in several other scientific disciplines, we understand that the concept of reproducibility is novel to the H/WQ community. In addition, because of the nature of H/WQ modeling, complexities due to parameter uncertainty/equifinality, and modeler bias, some of the concepts of reproducibility that have worked well for other fields, e.g., biostatistics (Peng, 2011) and signal processing (Vandewalle et al., 2009), may not directly apply to the H/WQ community. Through this article, we hope to start a discussion on how the H/WQ modeling community might start preparing itself to meet the challenges faced by regulatory open data sharing. Several legitimate concerns exist, which would need deliberation by the larger community, such as:

- Assembling: additional efforts that would be required to clean up a model to prepare its release and reuse.
- Free-riding: use of material (model and its inputs) available in the repository without proper acknowledgement or reference. A related issue is intellectual rights to an open model, particularly when used in commercial settings.
- Inspection: additional burden on traditional journals and reviewers to test a model before publication.
- Unintended consequences: use of a calibrated and validated model in a manner for which it was not originally intended.

We invite our peers to discuss these (and other) concerns, pose questions, and provide suggestions on how these concerns could be addressed so that we can start moving toward greater transparency in documenting H/WQ calibration and validation. We also recommend that the H/WQ community refer to the extensive literature available from Stanford University (Victoria Stodden, retrieved from http://web.stanford.edu/~vcs/Papers.html).

Moving toward reproducible model calibration, validation, and use will not be a one-time change but is rather a continuum (fig. 1). The current norm is to discuss calibration, validation, and use of H/WQ models through publication only. However, we suggest that authors take an additional step by providing details of calibration and additional ancillary items as supplemental material. In the long-term, the science of H/WQ modeling, as well as the decisions that are supported by such modeling, will advance most effectively when scientists and engineers share files and code for full reproducibility.

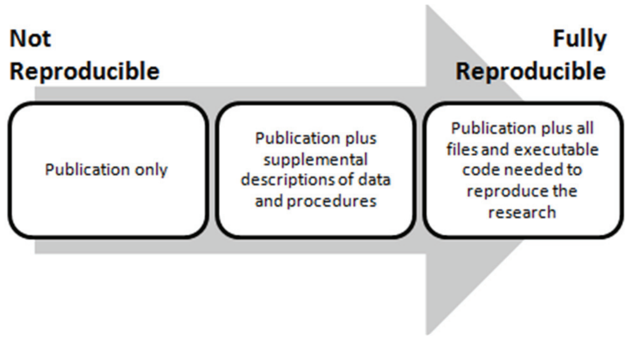

Figure 1. Moving toward reproducibility in hydrologic and water quality modeling (after Peng, 2011).

from Stanford University (Victoria Stodden, retrieved from http://web.stanford.edu/~vcs/Papers.html).

Moving toward reproducible model calibration, validation, and use will not be a one-time change but is rather a continuum (fig. 1). The current norm is to discuss calibration, validation, and use of H/WQ models through publication only. However, we suggest that authors take an additional step by providing details of calibration and additional ancillary items as supplemental material. In the long-term, the science of H/WQ modeling, as well as the decisions that are supported by such modeling, will advance most effectively when scientists and engineers share files and code for full reproducibility.

Summary and Conclusions

This article describes documentation procedures for hydrologic and water quality models for eight key reporting elements: (I) intended model use, (II) model description, (III) study area, (IV) observed data used for model calibration and validation, (V) input data, (VI) calibration parameters, (VII) calibration and validation strategy, and (VIII) performance assessment methods. The discussion was interspersed with appropriate good examples of elements from published literature. This article is one of a collection of nine articles that provides a comprehensive description of H/WQ model calibration and validation concepts and process.

This article recognizes and supports the increased requirements by federal funding agencies in the U.S. and the insistence by journals publishing computationally intensive research to provide additional data, metadata, and model code to improve research reproducibility. The concept of reproducibility is not novel, but the requirements for reproducible H/WQ model results with robust performance across widely variable biogeophysical conditions may require special consideration in the H/WQ modeling community. This article initiates a discussion to prepare the H/WQ modeling community for meeting the challenges faced by open data sharing.

Proper and adequate documentation is key to reproducing complex H/WQ modeling studies carried out from point to watershed scales. Comprehensive documentation of a study may require authors to rely on providing ancillary information as supplemental material to be accessed from some form of digital or online repository. Therefore, a discussion of the challenges, concerns, and opportunities for providing greater transparency in documenting H/WQ model calibration, validation, and use is needed for gaining public confidence in modeled outputs.

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APPENDIX

The following table lists the supplementary material policies for journals that typically publish hydrologic and water quality modeling work. No policies were found for *Journal of Water Resources and Engineering* (published by World Academic Publishing) nor for *Transactions of the ASABE* and *Applied Engineering in Agriculture* (published by ASABE).

Journal Title	Publisher	Supplementary Material Policy
Hydrological Processes	Wiley	Supporting information can be a useful way for an author to include important but ancillary information with the online version of an article. Examples of supporting information include additional tables, data sets, figures, movie files, audio clips, 3D structures, and other related nonessential multimedia files. Supporting Information should be cited within the article text, and a descriptive legend should be included. (More details are available at: http://onlinelibrary.wiley.com/journal/10.1002/(ISSN)1099-1085/homepage/ForAuthors.html).
Hydrology	MDPI	Authors are strongly encouraged to make their experimental and research data openly available either by depositing into data repositories or by publishing the data and files as supplementary information in this journal. Supplementary data and files can be uploaded as “supplementary files” during the manuscript submission process. The supplementary files will be offered to the referees as part of the peer-review process, although referees are not specifically asked to review supplementary files. Large data sets and files should be deposited to specialized service providers (such as Figshare) or institutional/subject repositories, preferably those that use the DataCite mechanism. For a list of specialized repositories for the deposit of scientific and experimental data, please consult databib.org or re3data.org. (Available at: www.mdpi.com/journal/hydrology/instructions#supplements).
Hydrology and Earth System Sciences	European Geosciences	Other possible review files are supplementary material (if available) as *.zip archive or single *.pdf file. Authors of larger supplements are kindly asked to submit their files to a reliable data

	Union	repository and to insert a link in the manuscript. Ideally, this linkage is realized through DOIs (digital object identifier). (Available at: www.hydrology-and-earth-system-sciences.net/submission/manuscript_submission.html).
Journal of Hydrologic Engineering	ASCE	Supplemental Data is considered to be data too large to be submitted comfortably for print publication (e.g., movie files, audio files, animated .gifs, 3D rendering files), as well as color figures, data tables, and text (e.g., Appendixes) that serve to enhance the article but are not considered vital to support the science presented in the article. A complete understanding of the article does not depend upon viewing or hearing the supplemental data. Supplemental data must be submitted for inclusion in the online version of any ASCE journal via Editorial Manager at the time of submission. (Available at: www.asce.org/Audience/Authors,--Editors/Journals/General-Journal-Information/Supplemental-Data/).
Journal of Hydrology *Journal of Hydrology: Regional Studies* *Water Research* *Advances in Water Resources* *Agricultural Water Management* *Environmental Modelling and Software* *Computers and Geosciences*	Elsevier	Elsevier accepts electronic supplementary material to support and enhance your scientific research. Supplementary files offer the author additional possibilities to publish supporting applications, high-resolution images, background datasets, sound clips, and more. Supplementary files supplied will be published online alongside the electronic version of your article in Elsevier Web products, including ScienceDirect (www.sciencedirect.com). Authors should submit the material in electronic format together with the article and supply a concise and descriptive caption for each file. (Available at: www.elsevier.com/journals/journal-of-hydrology/0022-1694/guide-for-authors#87000).
Journal of the American Water Resources Association	Wiley-Blackwell	If there is supplemental material that will be available online but not with the print version of the paper, include a Supporting Information section directly before the Acknowledgments and Literature Cited and after any Appendices. (More details are available at: www.awra.org/jawra/JAWRA%20Instructions%20for%20Authors.pdf).
Nature	Nature Publishing Group	An inherent principle of publication is that others should be able to replicate and build upon the authors' published claims. Therefore, a condition of publication in a Nature journal is that authors are required to make materials, data, and associated protocols promptly available to readers without undue qualifications. Any restrictions on the availability of materials or information must be disclosed to the editors at the time of submission. Any restrictions must also be disclosed in the submitted manuscript, including details of how readers can obtain materials and information. If materials are to be distributed by a for-profit company, this must be stated in the paper. Supporting data must be made available to editors and peer-reviewers at the time of submission for the purposes of evaluating the manuscript. Peer-reviewers may be asked to comment on the terms of access to materials, methods, and/or data sets; Nature journals reserve the right to refuse publication in cases where authors do not provide adequate assurances that they can comply with the journal's requirements for sharing materials. (Available at: www.nature.com/authors/policies/availability.html).
Vadose Zone Journal *Journal of Environmental Quality*	ASA, CSSA, and SSSA	Supplemental material may be included with articles at the discretion of the journal editor and production editor. Authors are encouraged to submit material that contributes to the content and quality of the article. The material must be submitted along with the original manuscript for peer review. The production editor may limit the quantity of supplemental material posted per issue. Extra images, video, or large tables are examples of appropriate supplemental material. When using supplemental material to shorten the text of a manuscript, keep in mind that the Materials and Methods section should provide enough detail to allow the reader to determine whether the interpretations are supported by the data. Supplemental material must undergo peer review and should be submitted along with the original manuscript. (Author instructions are available at: https://dl.sciencesocieties.org/publications/authors).
Water Resources Research	American Geophysical Union	The purpose of the auxiliary material, known as supporting materials or supplementary information, is to enable authors to provide and archive auxiliary non-print information such as data tables, figures, video, or computer software in digital formats so that other scientists can use them. (Available at: http://publications.agu.org/author-resource-center/author-guide/auxiliary-materials-guidelines/).