HYDROLOGIC AND WATER QUALITY MODELS: USE, CALIBRATION, AND VALIDATION

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ABSTRACT. *To provide a common background and platform for consensual development of calibration and validation guidelines, model developers and/or expert users of the commonly used hydrologic and water quality models globally were invited to write technical articles recommending calibration and validation procedures specific to their model. This article introduces a special collection of 22 research articles that present and discuss calibration and validation concepts in detail for 25 hydrologic and water quality models. The main objective of this introductory article is to introduce and summarize key aspects of the hydrologic and water quality models presented in this collection. The models range from field to watershed scales for simulating hydrology, sediment, nutrients, bacteria, and pesticides at temporal scales varying from hourly to annually. Individually, the articles provide model practitioners with detailed, model-specific guidance on model calibration, validation, and use. Collectively, the articles in this collection present a consistent framework of information that will facilitate development of a proposed set of ASABE model calibration and validation guidelines.*

Keywords. *ASABE, Calibration, Guidelines, Hydrologic models, Hydrology, Validation, Water quality, Watershed.*

Hydrologic and water quality (H/WQ) models are increasingly used to evaluate the impacts of climate, land use, and land and crop management practices on the quantity and quality of land and water resources. Calibration and validation of these models are necessary before using them in research and/or real-world applications. No universally accepted procedures or guidelines for calibration and validation currently exist in the literature. However, there are numerous viewpoints among model developers and model practitioners as to how calibration and validation should be implemented and reported to assist the peer-review process and to withstand legal scrutiny (Refsgaard and Storm, 1995; Refsgaard and Storm, 1996; Refsgaard, 1997; Santhi et al., 2001; Jakeman et al., 2006; Moriasi et al., 2007; Engel et al., 2007; Bennett et al., 2010).

Numerous issues related to calibration and validation of H/WQ models have been discussed by researchers. Topics include philosophical frameworks for calibration and validation (Beven and Binley, 1992; Beven, 1993), statistical and graphical model performance evaluation methods (Loague and Green, 1991; ASCE, 1993; Legates and McCabe, 1999), general procedures for calibration and validation (Donigian et al. 1983; Santhi et al., 2001; Donigian, 2002; White and Chaubey, 2005; Engel et al., 2007; Moriasi et al., 2007), autocalibration (Beven, 1993; Gupta et al., 1998, 1999; van Griensven and Bauwens, 2003; Abbaspour et al., 2007), incorporation of uncertainty analyses in model simulations (Beven and Binley, 1992; Beven, 1993; Shirmohammadi et al., 2006; Harmel and Smith, 2007; Harmel et al., 2010), and guidance on model performance criteria (Refsgaard and Henriksen, 2004; Engel et al., 2007; Moriasi et al., 2007; Harmel et al., 2010). Even with this large body of literature on model calibration and validation, it is difficult to compare modeling results from different studies because there are no universally accepted guidelines, and users utilize different calibration and validation methods.

The acceptance of guidelines for model calibration and validation provides many specific advantages to the modeling community, which include:

- Consistent assertions of model applicability, which results in increased credibility of modeling studies (Refsgaard and Henriksen, 2004).
- Better documentation and transparency in modeling studies, which allows others to audit, reconstruct, repeat, and reproduce the modeling process and its results (Refsgaard and Henriksen, 2004).
- A more standard and uniform peer-review process in the publication of modeling results (Douglas-Mankin et al., 2010).
- Improved assessment and comparison of different models applied in the same study area, or the same model(s) applied in different areas.

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- A consistent basis for assigning typical parameters and ranges for use in manual or automatic calibration and uncertainty analyses for a given model (Douglas-Mankin et al., 2010; Tuppad et al., 2011).
- Providing a platform to capture the knowledge and recommendations from experienced model developers or users.
- Providing a platform for future model developers and users to improve or expand knowledge on H/WQ model calibration and validation to increase credibility of model outputs.

In 2010, two subcommittees (in essence, Process and Communication) were established by ASABE with the goal of developing modeling guidelines. In order to provide a common background and platform for consensus building, model developers and/or expert users of the commonly used H/WQ models were invited to write technical articles on recommended calibration and validation procedures for their specific models. These recommended procedures are captured in this special collection. These articles not only set the stage for developing appropriate model calibration and validation guidelines but are also invaluable in the proper application and reporting of results for chosen models. The objective of this introductory article is to introduce and summarize key aspects of the quality H/WQ models presented in this special collection.

SUMMARY OF HYDROLOGIC AND WATER QUALITY MODELS

There are 22 research articles in this special collection, comprising 25 models (table 1). Each model is introduced with a description of the purpose for which the model was developed and its recommended spatial and temporal scales. For each model, the authors also provide information on the developmental history of their model(s), research and/or real-world applications, availability of source code, and technical user support. Recommended calibration and validation methods include discussion of recommended data screening and of ideal or minimum acceptable calibration and validation results. A case study is provided to demonstrate the application of calibration and validation recommendations. Finally, the strengths and weaknesses of the model as well as directions for future developments are discussed.

Tables 1 through 3 summarize important information for each of the models. Specifically, table 1 presents the processes (variables) simulated and the spatial and temporal scales for the models included, which vary in spatial context from field to watershed scale and in the watershed components represented (e.g., hydrology, sediment, nutrients, and pesticides components). Of the 25 models represented, 20 models simulate both hydrology and water quality (sediment, nutrients, pesticides, etc.); two models simulate hydrology, heat transfer, and solute transport (HYDRUS, Šimůnek et al., 2012; VS2DI, Healy and Essaid, 2012); and one each simulates only hydrology (DRAINMOD, Skaggs et al., 2012), solute transport in soils and groundwater (STANMOD, van Genuchten et al., 2012), and hydrology and heat transfer (SHAW, Flerchinger et al., 2012). MT3DMS (Zheng et al., 2012) is the only model focusing solely on groundwater. There are six field-scale models and six watershed-scale models; the rest simulate either at the point scale or cover ranges of scales, from point to field, plot to field, or plot to watershed. The temporal scales range from minutes to decades.

Table 2 presents information regarding whether or not the model currently has open source code, contains a GIS interface, and has available user support. Sixteen of the 25 models are open source code. For the HYDRUS (Šimůnek et al., 2012) models, the HYDRUS-1D code is publicly available, whereas the code for HYDRUS (2D/3D) is distributed commercially for a nominal fee. Eighteen models, ranging from soil-column to watershed scale, have a GIS interface to help with input preparation and data manipulation during the calibration and validation process. Most of the models currently provide some form of user support. The support types include theoretical documentation, user's manuals, GIS and Windows interface manuals, developer's manual, e-mail newsletters, website user groups, applications guides, tutorial manuals, and workshop training.

Finally, table 3 presents information regarding calibration and validation strategies and the model performance evaluation methods demonstrated in the case studies presented in each article. All the models discussed in this collection require calibration in one form or another, as demonstrated by the case studies. Calibration procedures vary with models, with some supporting manual calibration alone and others allowing both manual and auto calibration. Most of these models also support and recommend model validation, with a split-sample strategy as the most common method. MT3DMS (Zheng et al., 2012) is the only model that does not include model validation because the authors state that "others have argued that, at least philosophically, a groundwater model, like any scientific hypothesis, cannot be validated in the absolute sense and thus the term 'model validation' should be avoided (Konikow and Bredehoeft, 1992)." Most models in this collection utilize both graphical and statistical methods to evaluate model performance. The graphical methods used include time series plots, scatter plots, cumulative frequency distribution, and contour maps. Some of the statistics used include root mean square error, Nash-Sutcliffe efficiency (Nash and Sutcliffe, 1970), index of agreement, percent error, mean absolute error, correlation coefficient, mean error, absolute mean error, relative error, relative bias, standard error of estimate, coefficient of model-fit efficiency, Kolmogorov-Smirnov test, coefficient of determination, mean absolute error, model efficiency, normalized root mean square error, root mean square difference, minimum value of the nonlinear weighted objective function, percent bias, root mean square error to standard deviation ratio, mean error, 95% confidence interval to account for uncertainty, means, and standard deviation. Detailed definitions of these statistics can be obtained from the model-specific articles and elsewhere (e.g., Legates and McCabe, 1999; Moriasi et al., 2007). A few models provide performance ratings, includ-

Table 1. Summary of simulated processes (variables) and spatial and temporal scales for H/WQ models in this collection.

Model	Simulated Processes (Variables)	Spatial Scale	Temporal Scale	Reference
ADAPT	Hydrology, erosion, nutrients, pesticides, subsurface tile drainage.	Field	Daily	Gowda et al., 2012
BASINS/ HSPF	Hydrology, snowmelt, pollutant loadings, erosion, fate and transport.	Watershed	Daily	Duda et al., 2012
CREAMS/ GLEAMS	Hydrology, erosion, pesticides, sediments, nutrients, plant growth.	Field	Daily	Knisel and Douglas-Mankin, 2012
CoupModel	Hydrology, nitrogen, carbon, plant growth, heat, tracer, chloride.	User defined	Minutes to years	Jansson, 2012
Daisy	Water, snowmelt, carbon cycle, energy balance, nitrogen cycle, crop production, pesticides.	One to several fields	Minutes to daily	Hansen et al., 2012
DRAINMOD	Hydrology: water table depth, tile flow, surface runoff, depth of irrigation water applied, wetland hydrology. Plant growth: crop yield.	Point to watershed	Hourly and daily	Skaggs et al., 2012
EPIC and APEX	Hydrology: surface runoff, streamflow, tile flow. Plant growth: erosion, sediments, nutrients, pesticides.	EPIC: field; APEX: field to watershed	Daily to annual	Wang et al., 2012
HYDRUS	Water flow, solute transport, heat transfer, carbon dioxide.	Column to field	Minutes to years	Šimůnek et al., 2012
MACRO	Macropore flow, pesticides.	One-dimensional flow; field	Minutes to decades of simulations	Jarvis and Larsbo, 2012
KINEROS/ AGWA	Runoff, erosion, sediments.	Plot to watershed	Event	Goodrich et al., 2012
MIKE-SHE	Surface and subsurface water dynamics, interception, evapotranspiration, overland flow, channel flow, unsaturated flow, saturated zone flow, water levels; surface and groundwater quality.	Watershed	Seconds to daily	Jaber and Shukla, 2012
MT3DMS	Multispecies solute transport, groundwater.	Plot to watershed	Hourly to daily	Zheng et al., 2012
RZWQM	Hydrology, plant growth, nutrients, pesticides.	Plot to field	Hourly to daily	Ma et al., 2012
SHAW	Hydrology, heat transfer.	Point scale	Hourly to daily	Flerchinger et al., 2012
STANMOD	Solute transport in soils and groundwater.	One- and multi-dimensional transport; laboratory and field	Events	van Genuchten et al., 2012
SWAT	Hydrology, plant growth, sediments, nutrients, pesticides.	Basin	Daily	Arnold et al., 2012
SWIM	Water and solute movement.	Field section to field	Days to annual	Huth et al., 2012
TOUGH2	Multiphase, multicomponent fluids in porous and fractured geologic media.	No inherent limitation: pore-scale to reservoir	Generally short time steps used to solve differential equations	Finsterle et al., 2012
VS2DI	Water, solute, heat transport.	No inherent limitation; point to watershed	Seconds to decades	Healy and Essaid, 2012
WAM	Hydrology, sediments, nutrients.	Watershed	Daily, monthly	Bottcher et al., 2012
WARMF	Hydrology, sediments, nutrients, acid mine, carbon, bacteria.	Watershed	Daily	Herr and Chen, 2012
WEPP	Hydrology, soil erosion.	Hillslope and small watershed	Single storm to hundreds of years	Flanagan et al., 2012

ing BASINS/HSPF (Duda et al., 2012), DRAINMOD (Skaggs et al., 2012), EPIC and APEX (Wang et al., 2012), HYDRUS (Šimůnek et al., 2012), and SWAT (Arnold et al., 2012).

FUTURE WORK

The next steps in development of the model calibration and validation guidelines will be determined by the Process and Communication subcommittee members. These steps may include, but are not limited to:

- Identification of calibration and validation issues and topics to be included in the ASABE guidelines.
- Synthesis of relevant information from this special collection and the existing literature.
- Formation of groups to write, review, and revise the guidelines.
- Approval and publication of the guidelines by the ASABE Soil and Water Division Standards Committee.

Table 2. Access to code, presence of GIS interface, and availability of user support for H/WQ models in this collection.

Model	Open Source Code	GIS Interface	User Support Provided	Reference
ADAPT	Yes	No	Little support available	Gowda et al., 2012
BASINS/ HSPF	No	BASINS: yes; HSPF: no	Yes, HSPF user's manual and application guide.	Duda et al., 2012
CREAMS/ GLEAMS	Yes, available at: www.tifton.uga.edu/sewrl/Gleams/gleams_y2k_update.htm	Yes	Yes, available at: www.tifton.uga.edu/sewrl/gleams/gleams_y2k_update.htm	Knisel and Douglas-Mankin, 2012
CoupModel	No	Yes, available at: www2.lwr.kth.se/CoupModel/NetHelp/default.htm	Yes, user group from KTH has interactive forum for users; informal courses and tutorials are available from KTH.	Jansson, 2012
Daisy	Yes, available at: http://code.google.com/p/daisy-model/	No	Yes, website with supporting information and potential assistance available at: http://code.google.com/p/daisy-model/	Hansen et al., 2012
DRAINMOD	No, but provided to researchers by contacting developers at: www.bae.ncsu.edu/soil_water/drainmod/index.html	Yes, available at: www.bae.ncsu.edu/soil_water/drainmod/index.html	Yes, user's guide published by USDA-NRCS; incorporated in model software.	Skaggs et al., 2012
EPIC and APEX	Yes	Yes	Yes	Wang et al., 2012
HYDRUS	HYDRUS-1D available at: www.pc-progress.com/en/Default.aspx?hydrus-2d; HYDRUS (2D/3D): distributed commercially for nominal fee.	Yes, available at: www.pc-progress.com/en/Default.aspx?hydrus-2d	Yes, available at: www.pc-progress.com/en/Default.aspx?hydrus-2d	Šimůnek et al., 2012
KINEROS/ AGWA	Yes, available at: www.tucson.ars.ag.gov/kineros/	Yes, available at: www.tucson.ars.ag.gov/agwa/	Yes, available at: www.tucson.ars.ag.gov/kineros	Goodrich et al., 2012
MACRO	No	No	Yes, as allowed by time and resources constraints.	Jarvis and Larsbo, 2012
MIKE-SHE	No	Yes, available at: www.mikebydhi.com	Yes, documentation at the Danish Hydraulic Institute; support available at: www.mikebydhi.com	Jaber and Shukla, 2012
MT3DMS	Yes	Yes	Yes	Zheng et al., 2012
RZWQM	Yes, upon request: rzwqmsupport@ars.usda.gov	No	Yes, upon request from: rzwqmsupport@ars.usda.gov	Ma et al., 2012
SHAW	Yes, available at: ftp.nwrc.ars.usda.gov/public/ShawModel/	Yes	Yes, upon request from: gerald.flerchinger@ars.usda.gov	Flerchinger et al., 2012
STANMOD	Yes	No	Web-based with manuals.	van Genuchten et al., 2012
SWAT	Yes, available at: http://swatmodel.tamu.edu/	Yes, available at: http://swatmodel.tamu.edu/	Yes, theoretical documentation, user's manual, ArcSWAT and Map Window interface manuals, developer's manual, and email newsletter available at: http://swatmodel.tamu.edu/. There are other user groups worldwide.	Arnold et al., 2012
SWIM	Yes, available at: www.apsim.info	Yes (APSIM user interface)	Yes, available at: www.apsim.info	Huth et al., 2012
TOUGH2	No, source code copyrighted by University of California	No	Website with supporting documents available at: http://esd.lbl.gov/files/research/projects/tough/documentation/TOUGH2_V2_Users_Guide.pdf	Finsterle et al., 2012
VS2DT	Yes, available at: http://water.usgs.gov/software/ground_water.html	Yes, available at: http://water.usgs.gov/software/ground_water.html./	Yes, available at: http://water.usgs.gov/software/ground_water.html	Healy and Essaid, 2012
WAM	No, but can provide source code to model reviewers, university students and faculty, and other collaborators.	Yes	Yes, available at: www.swet.com/WAM.htm	Bottcher et al., 2012
WARMF	No, maintained by Systech Water Resources, Inc.	Yes	Yes, available at: www.epa.gov/Athens/wwqtsc	Herr and Chen, 2012
WEPP	Yes	Yes	Yes	Flanagan et al., 2012

Table 3. Summary of calibration and validation approaches and performance evaluation methods and criteria as suggested by the developers and/or expert users of the H/WQ models in this collection (continued).

Model	Calibration Approach	Validation Approach	Suggested Performance Evaluation Methods and Criteria	Reference
ADAPT	Partition flows, compare annual water and nutrient budget to measured or literature-reported values. Sensitivity coefficient to identify most important parameters.	Divide record into two equal periods or use alternative years covering extremes in both calibration and validation.	Statistical: Root mean square error, Nash-Sutcliffe efficiency, index of agreement, percent error, mean absolute error, correlation coefficient. Graphical: 1:1, time series.	Gowda et al., 2012
BASINS/ HSPF	Iterative procedure of parameter evaluation and refinement.	Split-sample	Statistical: Mean error, absolute mean error, relative error, relative bias, standard error of estimate, linear correlation coefficient, coefficient of model-fit efficiency, Kolmogorov-Smirnov test. Graphical: Time series, scatter, cumulative frequency distribution. Performance criteria: Provided in article.	Duda et al., 2012
CREAMS/ GLEAMS	Manual fine-tuning to achieve best comparison between simulated and observed data. Stepwise procedure: hydrology, sediment, nutrients/pesticides.	Split sample, adjacent watershed	Statistical: Index of agreement, coefficient of determination, Nash-Sutcliffe efficiency, relative error. Graphical: Time series.	Knisel and Douglas-Mankin, 2012
CoupModel	Simple stepwise systematic procedure, use of double mass plot technique. Manual and automated (GLUE).	Split sample	Statistical: Coefficient of determination, Nash-Sutcliff efficiency. Graphical: time series.	Jansson, 2012
Daisy	Defines objective functions. Stepwise procedure: bioclimate parameters, vegetation and field management parameters, soil parameters.	Split sample	Statistical: Comparison between observed and predicted means and standard deviations, model efficiency, root mean square error, index of agreement.	Hansen et al., 2012
DRAINMOD	Possible to determine inputs without calibration; calibration recommended for some inputs.	Split sample	Statistical: Mean absolute error, coefficient of determination, Nash-Sutcliffe efficiency. Graphical: Time series. Performance criteria: Provided in article.	Skaggs et al., 2012
EPIC and APEX	Determine calibration parameters, manual and automated, multi-site (if data available).	Split sample	Statistical: Coefficient of determination, Nash-Sutcliffe efficiency, root mean square error, percent bias, objective functions, autocorrelation, cross-correlation, nonparametric tests, t-test. Graphical: 1:1, time series, bar. Performance criteria: Provided in article.	Wang et al., 2012
HYDRUS	Simple gradient-based local optimization approach (based on Marquardt-Levenberg method) or automated.	Split sample	Statistical: Coefficient of determination, objective functions. Graphical: Time series.	Šimůnek et al., 2012
KINEROS/ AGWA	Simple manual to complex automated calibration (GLUE). Recommend stepwise, multi-scale calibrations.	Split sample, adjacent watershed	Statistical: Nash-Sutcliffe efficiency. Graphical: Time series.	Goodrich et al., 2012
MACRO	Forward, sequential and iterative procedure most common; also Monte Carlo methods.	Focus on individual processes	Statistical: Root mean square error, Nash-Sutcliffe coefficient.	Jarvis and Larsbo, 2012
MIKE-SHE	Warm-up period, manual and automated (AUTOCAL, GLUE).	Split sample	Statistical: RMSE, index of agreement. Graphical: Time series.	Jaber and Shukla, 2012
MT3DMS	Manual and automated. Variance-covariance matrix, and resulting uncertainty in predictions can be quantified using prediction linear and nonlinear confidence intervals and Bayesian credible intervals.	No	Statistical: Mean of weighted residuals, variance of weighted residuals errors, linear correlation coefficient. Graphical: Contour maps of heads and concentrations, time series plots. Performance criteria: Depends on application.	Zheng et al., 2012
RZWQM	Manual	Split sample	Statistical: Normalized root mean square error. Graphical: Time series.	Ma et al., 2012
SHAW	With/without calibration, sensitivity analysis, manual calibration, or automated (PEST). Stepwise, trial and error, optimization algorithm.	Split sample	Statistical: Root mean square difference. Graphical: Time series.	Flerchinger et al., 2012
STANMOD	Weighted nonlinear least square method.	No	Statistical: Minimum value of nonlinear, weighted objective function. Graphical: Time series.	van Genuchten et al., 2012

Table 3 (continued). Summary of calibration and validation approaches and performance evaluation methods and criteria as suggested by the developers and/or expert users of the H/WQ models in this collection.

Model	Calibration Approach	Validation Approach	Suggested Performance Evaluation Methods and Criteria	Reference
SWAT	Systematic process: hydrology, sediments, nutrients, pesticides (including budgets). Manual and automated.	Split sample, adjacent watershed	Statistical: Coefficient of determination, Nash-Sutcliffe efficiency, root mean square error, percent bias, objective functions, autocorrelation, cross-correlation, nonparametric tests, t-test. Graphical: Time series.	Arnold et al., 2012
SWIM	Manual, water balance.	Split sample, adjacent watershed	Statistical: Nash-Sutcliffe efficiency, root mean square error to standard deviation ratio mean error, mean absolute error, 95% confidence interval. Graphical: Time series.	Huth et al., 2012
TOUGH2	Weighted least squares objective function with several minimization algorithms.	Use uncertainty analysis based on linear or first-order second-moment error.	Statistical: Minimum value of objective function.	Finsterle et al., 2012
VS2DI	Manual, parameter-estimation programs (e.g., PEST).	Split sample	Statistical: Weighted correlation coefficient. Graphical: Time series.	Healy and Essaid, 2012
WAM	Process-based: source cell nutrient load and flow generation, cell to stream routing, and in-stream routing.	Split sample	Statistical: Nash-Sutcliffe, coefficient, root mean square error. Graphical: Hydrographs.	Bottcher et al., 2012
WARMF	Systematically adjust model input parameters within normal ranges to match simulated results to observed data, beginning with flow. Manual and automated.	Split sample	Statistical: Relative error, absolute error Graphical: Time series.	Herr and Chen, 2012
WEPP	Stepwise procedure: hydrology, erosion.	Split sample, adjacent watershed	Statistical: Means, standard deviation, root mean square error, percent bias, Nash-Sutcliffe coefficient, relative root mean square error.	Flanagan et al., 2012

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