Water Resour Manage
DOI 10.1007/s11269-013-0260-0

Application of Hierarchy Theory to Cross-Scale Hydrologic Modeling of Nutrient Loads

Liem T. Tran · Robert V. O'Neill · Elizabeth R. Smith · Randall J. F. Bruins · Carol Harden

Received: 27 August 2011 / Accepted: 1 January 2013

Abstract We describe a framework called **R**egional **Hy**drologic **M**odeling for **E**nvironmental **E**valuation (RHyME^2) for hydrologic modeling across scales. Rooted from hierarchy theory, RHyME^2 acknowledges the rate-based hierarchical structure of hydrological systems. Operationally, hierarchical constraints are accounted for and explicitly described in models put together into RHyME^2. We illustrate RHyME^{2}with a two-module model to quantify annual nutrient loads in stream networks and watersheds at regional and subregional levels. High values of R^2 (>0.95) and the Nash–Sutcliffe model efficiency coefficient (>0.85) and a systematic connection between the two modules show that the hierarchy theory-based RHyME^2 framework can be used effectively for developing and connecting hydrologic models to analyze the dynamics of hydrologic systems.

Keywords Hierarchy theory · Dynamic regional hydrologic modeling · Annual nitrogen load · Water quality · Cross-scale analysis

1 Introduction

Scale arguably has been one of the major challenges to hydrology (Beven 1987, 2001; Yevjevic 1991; Blöschl 2001; Gentine et al. 2012). Due to various scale-related issues (e.g.,

L. T. Tran (✉) · C. Harden
Department of Geography, University of Tennessee, 1000 Phillip Fulmer Way, Knoxville, TN 37996-0925, USA
e-mail: ltran1@utk.edu

R. V. O'Neill
Oneida Total Integrated Enterprises (OTIE), Oak Ridge, TN 37830, USA

E. R. Smith
U.S. Environmental Protection Agency, Office of Research and Development, National Exposure Research Laboratory, Research Triangle Park, NC 27711, USA

R. J. F. Bruins
U.S. Environmental Protection Agency, Ecological Exposure Research Division, National Exposure Research Laboratory, Cincinnati, OH 45268, USA

Published online: 10 January 2013

insufficiencies of knowledge on hydrological processes and their interactions across scales), it is not uncommon that a model works well on a particular spatiotemporal scale but not on others (Beven 2002; Gentine et al. 2012). This is true for both mechanistic (i.e., process-based) and empirical (i.e., statistical) models (Xu and Singh 2004; Perveen and James 2010; Thampi et al. 2010). While mechanistic models often have higher complexity in terms of mass balance structure and hydrologic processes at finer spatiotemporal resolution (e.g., SWAT—Soil Water Assessment Tool, (Arnold et al. 1990); HSPF—Hydrologic Simulation Program-Fortran, (Bicknell et al. 2001); and Gaddis and Voinov's model (Gaddis and Voinov 2010)), they often require intensive data and calibration effort plus priori assumptions on many parameters which are not calibrated or tested in most applications. In contrast, statistical models (e.g., Howarth et al. 1996; Goolsby and Battaglin 2001; Caraco et al. 2003) tend to be simpler in model structure or processes being described and at coarser spatiotemporal resolutions. However they are often able to provide quantified uncertainty information on model parameters and outputs. Regardless of the pros and cons of each approach, both mechanistic and empirical models debatably are scale-dependent, making the use of a single model for cross-scale hydrologic modeling questionable. This is also true for hybrid mechanistic-empirical models. An example is the Spatially Referenced Regression on Watershed attributes (SPARROW) model (Smith et al. 1997). SPARROW has been applied to assess the effect of sources and attenuation factors on stream nutrient loading at the national scale (Smith et al. 1997; Alexander et al. 2000; Schwarz et al. 2006) and for various regions and river basins (e.g., Preston and Brakebill 1999; McMahon et al. 2003; Moore et al. 2004; Alexander et al. 2008; Hoos and McMahon 2009; and García et al. 2011). However, those national and regional SPARROW models are very much stand-alone applications with very little cross-scale connection. In brief, given the scale-dependent nature of existing hydrologic models, they are not suitable for cross-scale hydrologic studies.

The purpose of this paper is to present a framework, which is rooted from hierarchy theory (Simon 1962, 1969, 1973; Allen and Starr 1982; O'Neill et al. 1986), for hydrologic modeling across scales. Central to hierarchy theory is the concept that differences in process rates can hierarchically structure a system. The structure imposed by differences in rates is sufficient to decompose a complex system into organization levels and into discrete components within each level (Overton 1974). System behaviors corresponding to higher levels occur at slower rates and lower levels conversely show rapid rates. From the hierarchy theory perspective, hydrological systems can be hierarchically grouped into similar classes with similar rates even though hydrological dynamics occur over a wide spectrum of interrelated spatiotemporal scales. For example, soil at micro scales responds rapidly to momentary changes in nitrogen through various processes of nitrogen fixation, mineralization, nitrification, and denitrification. The behavior of a small catchment regarding nitrogen export responds at a slower rate and integrates those micro-scale changes. Changes in nitrogen flux of the whole region at the size of the Mississippi River Basin (MRB) occurs even more slower, requiring months, years, decades, or even longer. To illustrate, while intensive fertilizer applications in MRB have been observed since 1950's, nitrate concentration data in the Mississippi–Atchafalaya River Basin indicate stable concentrations after 1975 after increasing trends in the previous 25 years (1950–1975) (Aulenbach et al. 2007). Apparently the system has shifted its nutrient export behavior from supply-limited before 1950's to transport-limited since mid-1970's after a lag time of several decades to accumulate legacy nutrient sources (Basu et al. 2010).

We refer to the modeling framework described here as **R**egional **Hy**drologic **M**odeling for **E**nvironmental **E**valuation ($RHyME^2$). In $RHyME^2$, the dynamics of fast variables at a lower level are described by equations in which slower variables at a higher level appear as parameters which in turn can be characterized by equation with still slower variables as parameters. The current RHyME^2 framework consists of two modules at two different organization levels corresponding to distinct spatiotemporal scales: regional-decadal versus subregional-annual.

2 Materials and Study Area

2.1 Study Area

The RHyME^2 regional module in this study was developed for the Upper Mississippi River Basin (UMRB). Encompassing an area of roughly 492,000 km^2 (190,000 mi^2) in the upper mid-western United States, the UMBR covers the headwaters of the Mississippi River in upper Minnesota, extends southward through Minnesota, Wisconsin, Iowa, Illinois, and Missouri, and ends at the confluence with the Ohio River near Cairo, Illinois (Fig. 1). The subregion module was developed for an area of five cascading subbasins (i.e., 8-digit hydrologic unit code [HUC-8] 0730001, 0730002, 0730003, 0730004, and 0730005) that include four US Geological Survey (USGS) monitoring sites 30001, 30002, 30003, and 30004 (Fig. 1). Observed flow and nutrient load at the USGS sites were used to develop the subregional module. As a proof of concept, we use a relatively small number of input variables of nutrient sources and physical and landscape properties in this study. They are discussed below.

2.2 Stream Network and Watershed Infrastructure

The NHDPlus digital network (version 1) developed by the US Environmental Protection Agency and the USEPA (2006) is used as the model framework of streams, reservoirs, and drainage topology. NHDPlus consists of various components, e.g., the improved 1:100 K National Hydrography Dataset (NHD); a set of value-added attributes for stream network navigation, analysis, and display; and catchment characteristics (USEPA and USGS 2006). We used the NHDPlus mean annual flow at bottom of flowline as computed by the unit runoff method in NHDPlus to represent the long-term balanced flow term described in the methodology section.

2.3 Land Use

The National Land Cover Dataset (NLCD) of 1992 from the Multi-Resolution Land Characteristics (MRLC) initiative (Vogelmann et al. 2001) was used to quantify certain diffuse sources of nitrogen (e.g., wetland) and to refine the spatial distribution of nitrogen sources (e.g., refining data reported at county level to catchment/flowline level).

2.4 Nitrogen Sources

Nitrogen sources from commercial fertilizers for farm and non-farm uses, livestock manure of confined and unconfined animals, and atmospheric deposition are from data described in Ruddy et al. (2006). To refine data from county to catchment/flowline level, nitrogen inputs from fertilizer and manure were allocated to various NLCD92 land-cover classes within each catchment as described in Table 3 in Ruddy et al. (2006). Nitrogen input from atmospheric deposition was allocated to all land-cover classes. As data in Ruddy et al. (2006) are not

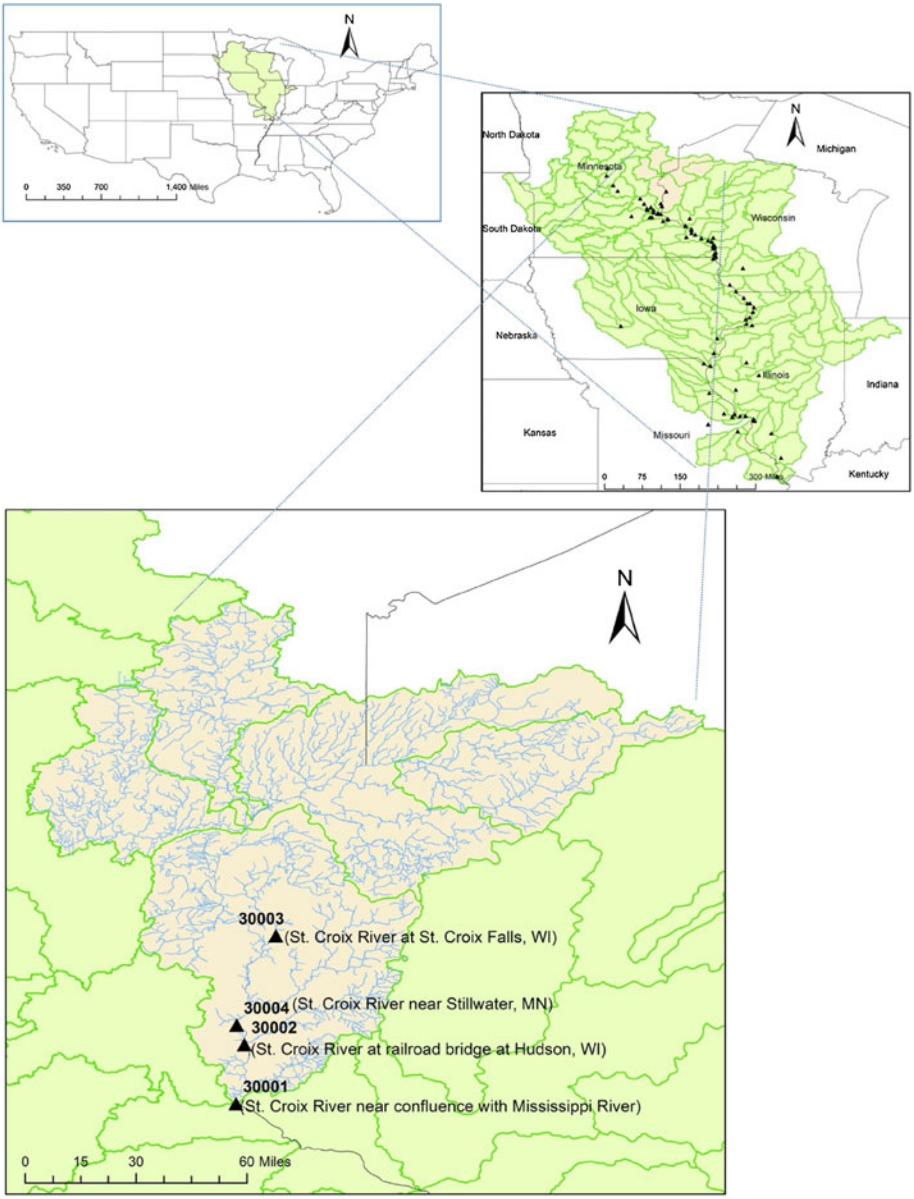


Fig. 1 Upper Mississippi River Basin and the subregion study area

available for the same years for all nitrogen sources (e.g., commercial fertilizers for farm/non-farm uses are available from 1987 to 2001, atmospheric deposition from 1985 to 2001, confined/unconfined livestock manure for four single years of 1982, 1987, 1992, and 1997), we selected years when data of different nitrogen sources have the most overlap to develop RHyME^2. Table 1 shows how nitrogen source data in Ruddy et al. (2006) are used in the development of the RHyME^2 regional and subregional modules.

Table 1 Nitrogen source data used in $RHyME^2$ regional and subregional modules

Nitrogen sources	$RHyME^2$ regional module	$RHyME^2$ subregional module					
		1987	1988	1990	1991	1992	1993
On-farm fertilizer [a]	1987–1997 average	1987	1988	1990	1991	1992	1993
Off-farm fertilizer [a]	1987–1997 average	1987	1988	1990	1991	1992	1993
Confined livestock manure [a]	Average of 1987, 1992, and 1997	1987	1987	1992	1992	1992	1992
Unconfined livestock manure [a]	Average of 1987, 1992, and 1997	1987	1987	1992	1992	1992	1992
Atmospheric deposition [a]	1987–1997 average	1987	1988	1990	1991	1992	1993
Point source [b]	1977–1981 average	1977–1981 average	1977–1981 average	1977–1981 average	1977–1981 average	1977–1981 average	1977–1981 average

[a] Ruddy el al. (2006)'s dataset

[b] USGS' "County-Level Point-Source Data for the United States" dataset

Nitrogen input from domestic and industrial point-sources are from the USGS' "County-Level Point-Source Data for the United States" dataset (available at http://water.usgs.gov/nawqa/sparrow/wrr97/point/point.html) which are, in turn, derived from a Resources for the Future (RFF) national inventory of wastewater discharges from 32,000 facilities, including industries, municipal wastewater treatment plants, and small sanitary waste facilities for the years 1977–1981. As the dataset is not available at the yearly level, the average for the whole period of 1977–1981 is used in both the regional and subregional modules as displayed in Table 1.

2.5 Soil Characteristics

Soil permeability is from the USGS "Soils Data for the Conterminous United States" dataset (available at http://water.usgs.gov/GIS/metadata/usgswrd/XML/ussoils.xml) which are derived from the NRCS State Soil Geographic (STATSGO) data base. The data contain multi-layered physical soil characteristics in vector format which are rasterized at 30-m resolution to refine data to catchment/flowline level.

2.6 Climate

Precipitation and temperature data are from the NHDPlus dataset which are in turn derived from the PRISM, 2.5-min (approximately 4 km) resolution data by Daly and Taylor (1998).

2.7 Annual Instream Nitrogen Load

Data of annual instream nitrogen load are from the Upper Mississippi Basin Loading Database (available at http://www.umesc.usgs.gov/data_library/sediment_nutrients/sediment_nutrient_page.html) which was generated by the USGS Upper Midwest Environmental Sciences Center (UMESC). Eighty-one out of 93 monitoring sites in the database were used to develop RHyME[2]; the remainder was eliminated due to data deficiency or being outside of the study area. Data from the Upper Mississippi Basin Loading Database are available at both monthly and yearly time steps. To create more annual nitrogen load data, monthly nitrogen load data were used in a 12-month window moving average fashion (i.e., five and a half months before and after a particular month), producing 12 observed data points for a single year. For example, there are 12 1987 data points, with the first being the average of the period from (half of) July, 1986, to (half of) July, 1987. Therefore, there are 72 (=12 points/year x 6 years) observed nitrogen load data points for each of the four monitoring sites for the six years used to develop the subregional module. On the other hand, there is only one simulated value for a single year at each monitoring site from the subregional module. As a result, one simulated output from the subregional module is compared with 12 observed annual nitrogen load data points for a particular year.

3 Method

First we model annual nitrogen load $Load_i$ as a non-linear function of flow:

$$Load_i = Load_{i,ltbf} * \left(Q_i / Q_{ltbf}\right)^{\alpha_i} \tag{1}$$

where Q_{ltbf} is the long-term balanced flow at reach i, $Load_{i,ltbf}$ is the nutrient load at reach i corresponding with Q_{ltbf}, and α is the load-versus-flow coefficient. $Load_{i,ltbf}$ in turn is modeled as a non-linear function of nitrogen sources, landscape and stream characteristics, and anthropogenic factors which control on-land and in-stream nitrogen attenuation processes:

$$Load_{i,ltbf} = \left(\sum_{k \in K(i)} Load_{k,ltbf}\right)^{*} A_i + \left(\sum_{n=1}^{N} S_{n,i} D_n\right)^{*} A_i^{'} \tag{2}$$

where $Load_{k,ltbf}(k \in K(i))$ is the nutrient load from upstream reach(es) k, A_i is in-stream attenuation function applied to upstream nitrogen load as it enters and travels along the stream channel of reach i. A_i is modeled as first-order decay exponential function of the mean water time of travel t_i along reach i for different stream-size classes such that:

$$A_i = \exp\left(-\theta_{Q_{ltbf}} t_i\right) \tag{3}$$

where $\theta_{Q_{ltbf}}$ are first-order stream loss coefficients calibrated for various stream-size classes defined by different ranges of long-term balanced stream flow Q_{ltbf}.

$S_{n,i}$ $(n \in N(i))$ are nitrogen sources in the catchment which contributes water to reach i (e.g., nitrogen from commercial fertilizers, manure, and point-source wastewater, and atmospheric deposition). D_n is the land-to-water delivery function for source n in catchment i. D_n is modeled as a series of exponential functions of physical and landscape characteristics (e.g., soil permeability, stream density, temperature and precipitation) that control the on-land nitrogen attenuation process and determine the amount of nitrogen delivered to streams. Each physical and landscape characteristic in the land-to-water delivery function D_n is associated with a delivery coefficient β_n.

$A_i^{'}$ is an in-stream attenuation function applied to the nitrogen load from catchment i as it enters and travels along the stream channel of reach i. $A_i^{'}$ is similar in form to the stream delivery function A_i defined above (3). In RHyME^2, $A_i^{'}$ of reach i is assumed equal to the square root of A_i.

Steps of model development include:

(a) Separating the direct influence of flow on annual nitrogen load: we calibrated the load-versus-flow coefficients α in (1) at each stream monitoring site by using nonlinear least-squares optimization to simultaneously minimize the correlation between $Load_{i,ltbf}$ and Q_i and maximize the correlation between $Load_i$ and $\left(Q_i/Q_{ltbf}\right)^{\alpha_i}$. As the correlation coefficient between $Load_{i,ltbf}$ and Q_i is minimal, nitrogen load corresponding with long-term balanced flow level $Load_{i,ltbf}$ arguably is not directly influenced by annual flow Q_i.

(b) Transforming annual nitrogen load $Load_i$ to long-term-balanced-flow nitrogen load $Load_{i,ltbf}$: we derived $Load_{i,ltbf}$ at stream monitoring sites such that:

$$Load_{i,ltbf} = Load_i \Big/ \left(Q_i/Q_{ltbf}\right)^{\alpha_i} \tag{4}$$

(c) Developing the regional module (4): we calibrated the regional module with average of $Load_{i,ltbf}$ ($\overline{Load_{i,ltbf}}$) at 81 monitoring sites and average nitrogen sources (see Table 1) such that:

$$\overline{Load_{i,ltbf}} = \left(\sum_{k \in K(i)} \overline{Load_{k,ltbf}}\right)^{*} A_i + \left(\sum_{n=1}^{N} \overline{S_{n,i}} D_n(\beta_n)\right)^{*} A_i^{'} \tag{5}$$

First we used all 81 data points to calibrate the initial model. Then we used the same 81-point dataset in a bootstrap[1] setting to develop the final model.

(d) Creating a "background" annual nitrogen load dataset in the subregion of interest: we used the regional module calibrated in step (c) along with temporal nitrogen source ($S_{n,i}$) data (see Table 1) to simulate "background" annual nitrogen load ($Load_{i,ltbf}{}^{*}$) for monitoring sites in the subregion of interest. The term "background" means, with the regional variables to be applied as parameters at subregional level, a subregion would produce an "average" annual nitrogen load similar to the simulated "background" nitrogen load dataset.

(e) Developing the subregional module: we calibrated the subregional module with both temporal nitrogen load data $Load_{i,ltbf}$ derived in step (b) and the background nitrogen load $Load_{i,ltbf}{}^{*}$ such that:

$$Load_{i,ltbf} = \left(\sum_{k \in K(i)} Load_{k,ltbf} \right) {}^{*}A_i + \left(\sum_{n=1}^{N} S_{n,i} D_n(\beta_n) \right) {}^{*}A_i' \tag{6}$$

First we used all data of $Load_{i,ltbf}$ and $Load_{i,ltbf}{}^{*}$ $\left(\left[\left(12 Load_{i,ltbf}\, \text{data/site/year} \times 6\ \text{years}\right) + \left(12 Load_{i,ltbf}{}^{*}\text{data/site/year} \times 6\ \text{years}\right)\right] \times 4\ \text{sites} = 576\ \text{data points}\right)$ to calibrate the initial model. Then we used the same 576-point dataset in a bootstrap fashion to develop the final model.

(f) Generating annual nitrogen load $Load_i$: first we applied the subregional module calibrated in step (e) to derive $Load_{i,ltbf}$. We then used (4) to calculate annual nitrogen load $Load_i$.

Operationally, we used the *lsqnonlin* function in MATLAB's (version 7.8) optimization toolbox (MathWorks 2011) for non-linear least-squares regression problems in steps (a), (c), and (e), including the bootstrap analyses in (c) and (e). Results of the regional and subregional modules are presented and discussed in the following section.

4 Results and Discussion

Values of the load-versus-flow coefficient α derived in step (a) at 81 monitoring sites range from 0.63 to 1.62 and display a normal distribution with a mean of 1.08 (Fig. 2). The correlation coefficient between the load-versus-flow coefficient α and Q_{ltbf} across 81 stations equals 0.368 (p-value<0.001), showing a light trend that nitrogen load tends to level out in small streams ($\alpha<1$) and boost up in large streams ($\alpha>1$) when flow increases relatively to its long-term balanced flow.

At each monitoring station, the correlation coefficient between $Load_i$ and $\left(Q_i/Q_{ltbf}\right)^{\alpha_i}$ is close to 1 (p-value<0.0001) while those between $Load_{i,ltbf}$ and Q_i is near zero and statistically insignificant. Namely, the nitrogen load associated with long-term balanced flow ($Load_{i,ltbf}$) is not influenced directly by the annual stream flow Q_i.

[1] Bootstrap analysis involves resampling with replacement from among the original size-n dataset (e.g., the 81-point and 576-point datasets in steps (c) and (e)) to create samples with the same size n in all iterations (Davison and Hinkley 1997).

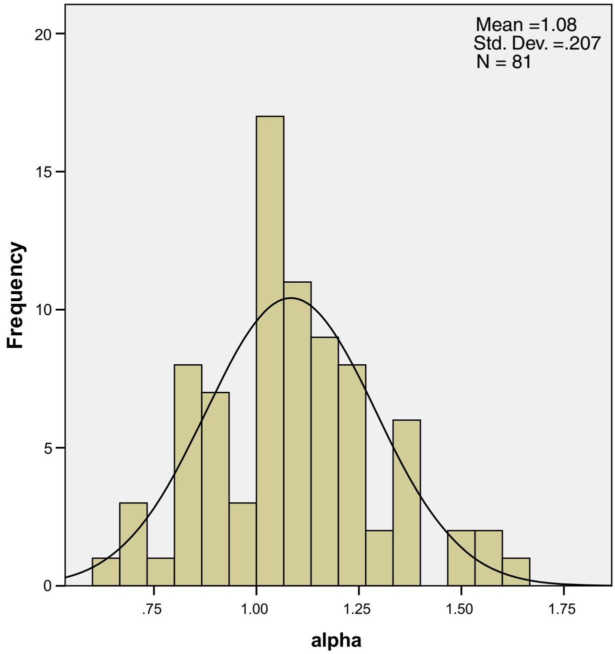


Fig. 2 Histogram of the load-versus-flow coefficient α

The model R^2 (Table 2) shows that the regional module explains about 92 % of the spatial variability of the log-transformed values of the average annual nitrogen load associated with the long-term balanced flow. However, the regional module tends to slightly overpredict loads from a couple small areas and underpredict loads from several large areas (Fig. 3).

The model-estimated coefficients β_n for six nitrogen source variables (Table 2) represent the land-delivery ratio for that source. For example, β_n for commercial fertilizers applied to farm land, 0.244 kg/kg, means that for each kilogram of nitrogen from commercial fertilizers applied to farm land in a catchment, RHyME[2] estimates that 0.244 kg is delivered to the stream network in that catchment. The balance of 0.755 kg is removed by a combination of crop harvest and on-land attenuation.

The land-to-water delivery coefficients for soil permeability, stream density, temperature, precipitation, and wetland (Table 2) show the effect of each physical and landscape characteristic to the land-to-stream delivery function in a spatially-relative term. For example, if soil permeability changes by 10 % relative to the averaged soil permeability of the whole study area, the land-to-stream delivery function will change by a factor of 0.975 (i.e., $e^{-0.252*0.6}/e^{-0.252*0.5} = e^{-0.252*0.1} = 0.975$) provided other physical and landscape variables remain unchanged. The positive values of the coefficients for stream density, temperature, and precipitation indicate that the land-to-stream delivery function increases when those variables increase. In contrast, soil permeability and wetland have negative values for their coefficients, implying that these variables tone down the land-to-stream delivery.

Values of the first-order stream loss coefficients for four stream-size classes (Table 2) are all statistically significant. While these values are not completely consistent with the concept that attenuation decreases with the increase of stream size for all four classes, the overall pattern is reasonable (e.g., the coefficients for the two large stream-size classes are smaller than those of the two smaller stream-size classes). Furthermore, values of the first-order

Table 2 Calibration results for the RHyME^2 regional module

Parameters	Coefficient units	Initial model	Final model (bootstrap)		
			Mean coefficient	Standard error	p-value
Nitrogen sources (β_n)					
Nitrogen in commercial fertilizers applied to farm land	kg/kg	0.234	0.244	0.006	<0.001
Nitrogen in commercial fertilizers applied to non-farm land	kg/kg	0.208	0.184	0.004	<0.001
Manure from confined livestock	kg/kg	0.043	0.043	0.002	<0.001
Manure from unconfined livestock	kg/kg	0.034	0.037	0.002	<0.001
Atmospheric deposition	kg/kg	0.505	0.474	0.004	<0.001
Domestic and industrial point sources	kg/kg	0.879	0.837	0.012	<0.001
Land-to-water delivery					
Soil permeability	dimensionless	−0.244	0.252	0.007	<0.001
Stream density	dimensionless	0.233	0.200	0.003	<0.001
Temperature	dimensionless	0.227	0.191	0.002	<0.001
Precipitation	dimensionless	0.092	0.086	0.003	<0.001
Wetland	dimensionless	−0.252	0.263	0.007	<0.001
In-stream removal $\left(\theta_{Q_{ltbf}}\right)$					
Time of travel in reach where Q_{ltbf}<2.8 m^3/s	day	0.221	0.197	0.004	<0.001
Time of travel in reach where Q_{ltbf}>2.8 and <28 m^3/s	day	0.247	0.265	0.008	<0.001
Time of travel in reach where Q_{ltbf}>28 and <280 m^3/s;	day	0.010	0.015	0.005	0.001
Time of travel in reach where Q_{ltbf}>280 m^3/s	day	0.138	0.137	0.002	<0.001
Model R^2 (on log-transformed values of the average annual nitrogen load associated with Q_{ltbf})	0.923				
Mean square error	0.251				

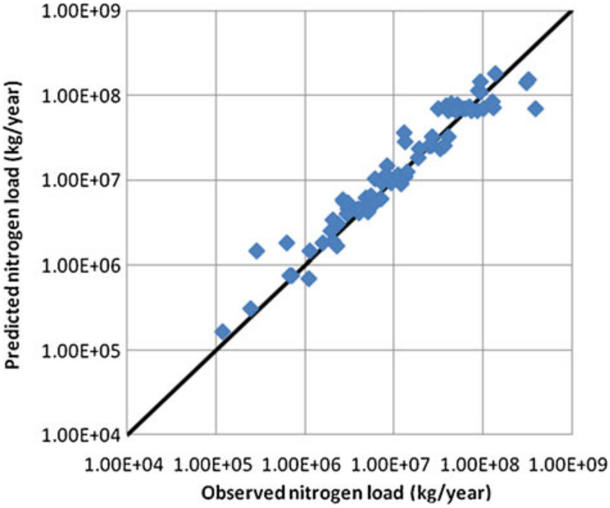
stream loss coefficients for the subregional module are not too different from results of experimental studies (Howarth et al. 1996; Gibson and Meyer 2007; Mulholland et al. 2008, 2009).

Except for atmospheric deposition, the values of β_n in the subregional module (Table 3) are greater than those in the regional module. Furthermore, the values of β_n for each nitrogen source are statistically different between the two modules (p-value<0.001, two independent-sample t tests; two samples are parameter estimates in two bootstrap analyses).

Comparing the land-to-water delivery coefficients of the two modules, there is no statistical difference for stream density (p-value=0.12) but a difference at 5 % level for precipitation (p-value=0.04) and at 1 % for the other four coefficients (p-value<0.001). The first-order stream loss coefficients for four stream-size classes are also statistically different (p-value<0.001) from one module to the other. Furthermore, different from those in the regional module, the first-order stream loss coefficients in the subregional model are consistent with the concept that attenuation decreases with the increase of stream size.

Figure 4 displays observed and RHyME^2 simulated (12-month moving average) annual total nitrogen load $Load_i$ at four USGS monitoring sites. The model performed quite well at

Fig. 3 Scatterplot of predicted versus nitrogen load, RHyME^2 regional module



two sites, 30002 and 30003, and somewhat underestimated at the other two stations. Model R^2 and the Nash–Sutcliffe model efficiency coefficients (Nash and Sutcliffe 1970) at the four

Table 3 Calibration results for the RHyME^2 subregional module

Parameters	Coefficient units	Initial model	Final model (bootstrap)		
			Mean coefficient	Standard error	p-value
Nitrogen sources (β_n)					
Nitrogen in commercial fertilizers applied to farm land	kg/kg	0.281	0.269	0.002	<0.001
Nitrogen in commercial fertilizers applied to non-farm land	kg/kg	0.264	0.214	0.001	<0.001
Manure from confined livestock	kg/kg	0.098	0.070	0.002	<0.001
Manure from unconfined livestock	kg/kg	0.079	0.056	0.017	<0.001
Atmospheric deposition	kg/kg	0.479	0.515	0.001	<0.001
Domestic and industrial point sources	kg/kg	0.954	0.954	0.001	<0.001
Land-to-water delivery					
Soil permeability	dimensionless	−0.207	0.219	0.001	<0.001
Stream density	dimensionless	0.190	0.205	0.001	<0.001
Temperature	dimensionless	0.185	0.200	0.001	<0.001
Precipitation	dimensionless	0.075	0.093	0.001	<0.001
Wetland	dimensionless	−0.217	0.228	0.001	<0.001
In-stream removal $\left(\theta_{Q_{ltbf}}\right)$					
Time of travel in reach where Q_{ltbf}<2.8 m^3/s	day	0.228	0.263	0.001	<0.001
Time of travel in reach where Q_{ltbf}>2.8 and <28 m^3/s	day	0.198	0.213	0.001	<0.001
Time of travel in reach where Q_{ltbf}>28 and <280 m^3/s;	day	0.197	0.206	0.001	<0.001
Time of travel in reach where Q_{ltbf}>280 m^3/s	day	0.097	0.101	0.001	<0.001

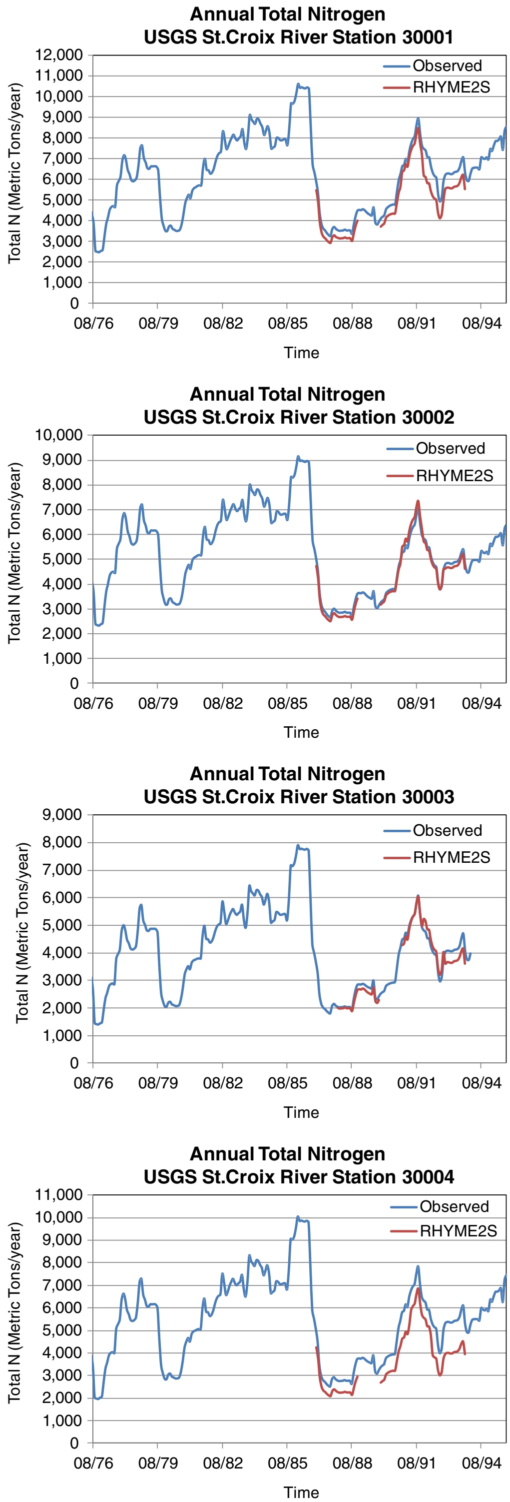


Fig. 4 Observed and RHyME^2 simulated (12-month moving average) annual total nitrogen load at four USGS St. Croix River monitoring sites

monitoring sites (Table 4) are relatively high and the root mean square errors are reasonable (e.g., ranging between 3 % and 17 %). Overall, RHyME^2 sufficiently captured the magnitude and pattern of the annual nitrogen load at all four stations.

The use of $Load_{i,ltbf}$— the nitrogen load corresponding with long-term balanced flow—allows the separation of annual flow's direct impact on nitrogen load from those caused by physical and landscape factors operating at longer temporal scales, e.g., from decades to centuries or longer. Moreover the temporal pattern of $Load_{i,ltbf}$ as a function of long-term physical and landscape factors is revealed (Fig. 5). Note that the approach of separating the direct impact of flow on nitrogen load is different from averaging out nitrogen load ($\overline{Load_i}$) in several aspects:

- Value: $\overline{Load_{i,ltbf}}$ are very different from $\overline{Load_i}$ (e.g., $\overline{Load_{i,ltbf}}/\overline{Load_i}$ in metric tons/year: 5,753/6,274; 5,150/5,590; 4,035/4,120; and 5,079/5,478 at sites 30001, 30002, 3003, and 30004, respectively). Arguably, $\overline{Load_{i,ltbf}}$ reflects the non-linear relationship between nitrogen load and long-term balanced flow as well as their often non-normal distribution better than $\overline{Load_i}$ (e.g., the non-linear relationship is taken care of via the load-versus-flow coefficient before $Load_{i,ltbf}$ is derived).
- Temporal pattern: the temporal dimension is completely removed in $\overline{Load_i}$. In contrast, while $\overline{Load_{i,ltbf}}$ is used in the regional module, the time series $Load_{i,ltbf}$ is used in developing the subregional module.
- Relationship between nitrogen load and flow: Eq. (1) explicitly portrays the non-linear relationship between nitrogen load and flow. The equation is consistent with field observations and is proven statistically in this study. It facilitates the simulation of $Load_i$ through the use of $\overline{Load_{i,ltbf}}$ and $Load_{i,ltbf}$ at regional and subregional levels, respectively. In contrast, it is not possible to do that with $\overline{Load_i}$.

We use $\overline{Load_{i,ltbf}}$ but $Load_{i,ltbf}$ for the regional module to reflect the fact that the regional and subregional modules operate at two different organization levels (i.e., different spatio-temporal scales). The use of $\overline{Load_{i,ltbf}}$ also preserves the mass balance across the whole region at a longer temporal scale (e.g., decadal). Meanwhile, operating at a lower organization level with faster changes in various factors (e.g., nitrogen sources, precipitation, and temperature), $Load_{i,ltbf}$ might have different temporal patterns in different subregions. For example, $Load_{i,ltbf}$ at USGS monitoring site 30001 displays an increasing trend while the opposite is observed at site 190001 (Fig. 5). As the time frame for change of $Load_{i,ltbf}$ from one subregion to take effect on other downstream subregions is not accounted for, the use of $Load_{i,ltbf}$ to develop the regional module might violate the mass balance principle. On the other hand, the trend of $Load_{i,ltbf}$ is often consistent within a subregion (e.g., an increasing

Table 4 Model performance of RHyME^2 on annual total nitrogen at four USGS St. Croix River monitoring sites

Model performance indicators	USGS St. Croix River monitoring sites			
	30001	30002	30003	30004
R^2	0.97	0.99	0.96	0.96
Root mean square error (mean) of annual nitrogen load in Metric Tons/year	630 (6,274)	175 (5,590)	249 (4,120)	945 (5,478)
Nash–Sutcliffe model efficiency coefficient	0.87	0.99	0.96	0.87

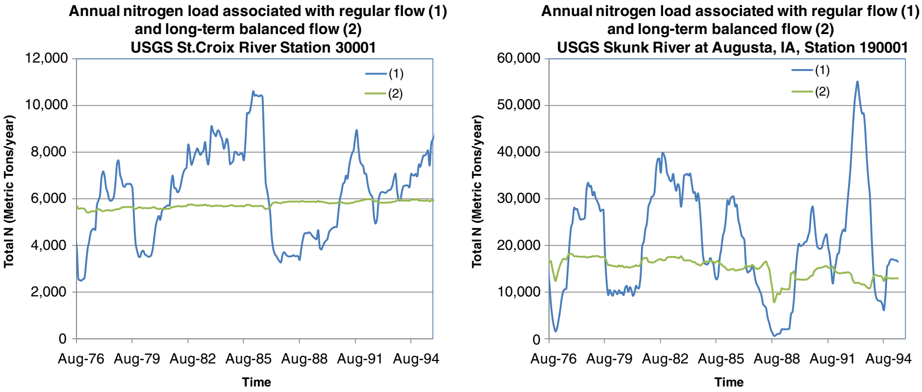


Fig. 5 Annual nitrogen load associated with regular flow $Load_i$ and long-term balanced flow $Load_{i,ltbf}$ at two USGS monitoring sites 30001 and 190001

trend is observed at all four monitoring sites 30001, 30002, 30003, and 3004 in the studied subregion). Hence the use of $Load_{i,ltbf}$ in the subregional module exposes the impact due to changes through time of nitrogen sources and/or physical and landscape factors on nitrogen load in a subregion.

Methodologically, the regional and subregional modules in RHyME^2 are quasi-mechanistic given their mass-balance structure in simulating hydrologic and contaminant transport processes. On the other hand, all parameters in the two modules are estimated statistically, providing robust measures of uncertainty in both model coefficients and outputs. Namely, the complexity of RHyME^2 is fully supported by the data.

Our goal in this paper is not to introduce "another" hydrologic model but to present RHyME^2 as a framework for hydrologic modeling across spatiotemporal scales. As mentioned above, hydrologic dynamics at a specific level is constrained by the higher-level system of which it is a part. When one studies a hydrologic system with a particular scientific question in mind, that person focuses on a specific spatiotemporal scale of observation, e.g., a hillslope, a catchment, or a basin. The problem arises in extrapolating observation at a specific scale to observation at other scales. For example, when a model originally developed at catchment scale is applied for a large basin over a long period of time (i.e., linear up-scaling), it might not sufficiently account for constraints at higher levels (e.g., groundwater movement at basin scale). Furthermore, such linear up-scaling model emphasizes what system is allowed to do under mainly the very low-level constraints. As a result, the model cannot simulate what the system is capable of doing if higher-level constraints are changed. The common sensitivity analysis and calibration practices to improve the performance of a mechanistic model often focus on only a subset of parameters to which the model is the most sensitive. Because the tendency is to deal with fast-rate behavior of the lowest entities, those parameters often correspond to low-level constraints. Consequently parameters associated with higher-level constraints are often left as uncalibrated constant in the model, making the model insensitive or falsely behave to (changes in) higher-level constraints.

Different from mechanistic models, statistical models are rarely used in cross-scale applications. Often a statistical model is developed at a specific spatial-temporal scale to answer a specific research question at that scale (e.g., long-term nitrogen flux at regional scale). If one has a similar research question but focuses on a different spatial-temporal scale (e.g., annual nitrogen flux at subregional scale), the previous model is likely not appropriate.

A common practice in empirical modeling is to develop another model with observation at that specific spatial-temporal scale which is independent from the model with observation at another scale. While comparison of model structure or results can be made, there is often no clear systematic and/or theoretical connection between the two models. In that context, RHyME^2 is to facilitate such systematic connection among models at different scales in the light of hierarchy theory.

The regional module in this study was derived from observation at regional scale (i.e., long-term average of nutrient load $\overline{Load_{i,ltbf}}$ and climatic and landscape factors). In the subregional module which is at a lower organization level, the faster variables (e.g., annual nutrient load, annual climatic variables) were described by equations in which slower variables from the regional module appear as parameters. Such hierarchical connection between the two modules provides a theoretically and operationally framework to understand the nitrogen flux pattern at two different scales. While the equations in the two modules might look similar, the focused entities, level of observation, and parameters in each module are very different (i.e., mathematic equation is not a sole factor in defining the structure of a model). In the same context, models with different structures (e.g., mechanistic versus empirical) at different spatiotemporal scales can be put together under RHyME^2 if hierarchical constraints can be defined and dealt with properly in each model (e.g., by describing faster variables in equations/models in which slower variables appear as parameters, and so on).

In this paper we have proposed RHyME^2 as a framework for hydrologic modeling across scales based on the hierarchy theory. The principle of RHyME^2 is to acknowledge the rate-based hierarchical structure of hydrological systems. Operationally, hierarchical constraints should be accounted for and explicitly described in models put together into the framework. With that, RHyME^2 can be used for integrating hydrologic models developed at different spatiotemporal scales to understand the cross-scale dynamics of hydrologic systems.

References

Alexander RB, Smith RA, Schwarz CA (2000) Effect of stream channel size on the delivery of nitrogen to the Gulf of Mexico. Nature 403:758–761

Alexander RB, Smith RA, Schwarz GE, Boyer EW, Nolan JV, Brakebill JW (2008) Differences in phosphorus and nitrogen delivery to the Gulf of Mexico from the Mississippi River Basin. Environ Sci Technol 42 (3):822–830

Allen TFH, Starr TB (1982) Hierarchy: perspectives for ecological complexity. University of Chicago Press, Chicago

Arnold JG, Williams JR, Nicks AD, Sammons NB (1990) SWRRB—A basin scale simulation model for soil and water resources management. Texas A&M University Press, College Station

Aulenbach, BT, Buxton HT, Battaglin WA, Coupe RH (2007) Streamflow and nutrient fluxes of the Mississippi–Atchafalaya River Basin and sub–basins for the period of record through 2005, U.S. Geol. Surv. Open File Rep., 2007–1080

Basu NB et al (2010) Nutrient loads exported from managed catchments reveal emergent biogeochemical stationarity. Geophys Res Lett 37(L23404):1–5

Beven K (1987) Towards a new paradigm in hydrology, Water for the Future: Hydrology in perspective (Proceedings of the Rome Symposium, April 1987). IAHS Publ. no.164

Beven K (2001) How far can we go in distributed hydrological modelling? Hydrol Earth Syst Sci 5(1):1–12

Beven K (2002) Towards an alternative blueprint for a physically based digitally simulated hydrologic response modeling system. Hydrol Process 16:189–206

Bicknell BR, Imhoff JC, Kittle JL Jr, Jobes TH, Donigian AS Jr (2001) Hydrological simulation program-Fortran, HSPF version 12 user's manual. AQUA TERRA Consultants, Mountain View, 873p

Blöschl G (2001) Scaling in hydrology. Hydrol Process 15:709–711
Caraco NF, Cole JJ, Likens GE, Lovett GM, Weathers KC (2003) Variation in NO_3 export from flowing waters of vastly different sizes—Does one model fit all? Ecosystems 6:344–352
Daly C, Taylor G (1998) United States average monthly or annual precipitation, 1961–90. Spatial Climate Analysis Service at Oregon State University, Corvallis
Davison AC, Hinkley D (1997) Bootstrap methods and their application. Cambridge Series in Statistical and Probabilistic Mathematics, Cambridge
Gaddis EJB, Voinov A (2010) Spatially explicit modeling of land use specific Phosphorus transport pathways to improve TMDL load estimates and implementation planning. Water Resour Manag 24:1621–1644
García AM, Hoos AB, Terziotti S (2011) A regional modeling framework of phosphorus sources and transport in streams of the Southeastern United States. JAWRA J Am Water Resour Assoc. doi:10.1111/j.1752-1688.2010.00517.x
Gentine P, Troy TJ, Lintner BR, Findell KL (2012) Scaling in surface hydrology: progress and challenges. J Contemporary Water Res Education 147:28–40
Gibson CA, Meyer JL (2007) Nutrient uptake in a large urban river. J Am Water Resour Assoc 43(3):576–587
Goolsby DA, Battaglin WA (2001) Long-term changes in concentrations and flux of nitrogen in the Mississippi River basin, USA. Hydrol Process 15(7):1209–1226
Hoos AB, McMahon G (2009) Spatial analysis of instream nitrogen loads and factors controlling nitrogen delivery to streams in the southeastern United States using spatially referenced regression on watershed attributes (SPARROW) and regional classification frameworks. Hydrologic Processes. doi:10.1002/hyp.7323
Howarth et al (1996) Regional nitrogen budgets and riverine N and P fluxes for the drainages to the North Atlantic Ocean—natural and human influences. Biogeochemistry 35:75–139
MathWorks (2011), MatLab User Guide, Available at http://www.mathworks.com/help/techdoc/matlab_product_page.html
McMahon G, Alexander RB, Qian S (2003) Support of TMDL programs using spatially referenced regression models. ASCE J Water Resour Plann Manag 129:315–329
Moore RB, Johnston CM, Robinson KW, Deacon JR (2004) Estimation of total nitrogen and phosphorus in New England streams using spatially referenced regression models, U.S. Geological Survey Scientific Investigations Report 2004–5012, 50p
Mulholland PJ et al (2008) Stream denitrification across biomes and its response to anthropogenic nitrate loading. Nature 452:202–205
Mulholland PJ et al (2009) Nitrate removal in stream ecosystems measured by 15 N addition experiments: denitrification. Limnol Oceanogr 54(3):666–680
Nash JE, Sutcliffe JV (1970) River flow forecasting through conceptual models part I — A discussion of principles. J Hydrol 10(3):282–290
O'Neill RV, DeAngelis DL, Waide JB, Allen TFH (1986) A hierarchical concept of ecosystems. Princeton University Press, Princeton
Overton WS (1974) Decomposability: a unifying concept? In: Levin SA (ed) Ecosystem analysis and prediction. SIAM, Philadelphia, pp 297–298
Perveen S, James LA (2010) Multiscale effects on spatial variability metrics in global water resources data. Water Resour Manag 24:1903–1924
Preston SD, Brakebill JW (1999) Application of spatially referenced regression modeling for the evaluation of total nitrogen loading in the Chesapeake Bay watershed. U.S. Geological Survey Water-Resources Investigations Report 99–4054, 12p
Ruddy BC, Lorenz DL, Mueller DK (2006) County-Level Estimates of Nutrient Inputs to the Land Surface of the Conterminous United States, 1982–2001. U.S. Geological Survey Scientific Investigations Report 2006–5012, 17 p
Schwarz GE, Hoos AB, Alexander RB, Smith RA (2006) The SPARROW surface water-quality model: Theory, application and user documentation, U.S. Geological Survey Techniques and Methods Report, Book 6, Chapter B3, 2006
Simon HA (1962) The architecture of complexity. Proc Am Philos Soc 106:467–482
Simon HA (1969) The sciences of the artificial. MIT Press, Cambridge
Simon HA (1973) The organization of complex systems. In: Pattee HH (ed) Hierarchy theory. Braziller, New York, pp 3–27
Smith RA, Schwarz GE, Alexander RB (1997) Regional interpretation of water-quality monitoring data. Water Resour Res 33(12):2781–2798
Thampi SG, Raneesh KY, Surya TV (2010) Influence of scale on SWAT model calibration for streamflow in a river basin in the humid tropics. Water Resour Manag 24:4567–4578

USEPA and USGS (2006) National Hydrography Dataset Plus (NHDPlus). Available at http://www.horizon-systems.com/nhdplus/

Vogelmann JE et al (2001) Completion of the 1990's national land cover data set for the conterminous United States. Photogramm Eng Remote Sens 67:650–662

Xu CY, Singh VP (2004) Review on regional water resources assessment models under stationary and changing climate. Water Resour Manag 18:591–612

Yevjevic V (1991) Tendencies in hydrology research and its applications for 21st century. Water Resour Manag 5:1–23