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Modeling the hydrochemistry of the Choptank River Basin using GWLF and Arc/Info: 1. Model calibration and validation

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Abstract. We modeled nutrient export in the Choptank River Basin on the coastal plain of the Chesapeake drainage, using a modified version of a lumped-parameter, hydrochemical model (GWLF). Calibration was performed using long-term (WY1980–WY1990) hydrochemistry data from a gauged site. The calibrated model reproduced water yields, TN, and TP export with cumulative errors of $<1\%$ over the 11-year calibration period and with annual RMS errors of 10–50%. Model validation was done with independent measurements at the same gauged site (WY1991 to WY1996) and at another nearby independently gauged site (WY1991 to WY1995). Local adjustment of the groundwater recession coefficient and the dissolved N concentration in agricultural stormflow was essential for successful application at the second site. GWLF appears to be a useful model for estimation of fluxes of water, N and P from ungauged areas with accuracies of 10–50% at annual time scales.

Introduction

The eutrophication of North American estuaries has been caused by nutrient enrichment from their surrounding watersheds. Enhanced supplies of N and P have resulted from the past 300 years of anthropogenic watershed disturbance, beginning in the 17th century and continuing to the present as the primary land use changed from forested to intensively managed agriculture and urban. As the human population increased, greater amounts of N and P entered aquatic systems via atmospheric inputs of N (Fisher & Oppenheimer 1991), agricultural activities (Beaulac & Reckhow 1982), and sewage discharges (Peierls et al. 1990). Characteristics of eutrophied estuaries include enhanced nutrient concentrations, phytoplankton blooms, seasonal anoxia in bottom waters, accumulation of nuisance macroalgae and decreased importance of benthic microalgae and submerged vascular plants (Orth & Moore 1983; Office et al. 1984; Seliger et al. 1985; Malone et al. 1988; Valiela et al. 1990; Cooper & Brush 1991).

The Chesapeake Bay is an anthropogenically enriched estuary (Nixon 1987). Over several centuries, primary production has shifted from benthic diatoms and sea grasses to plankton, in a sequence typical of eutrophying aquatic systems (Cooper & Brush 1993). More recently, increases in inputs of nitrogen (N) and phosphorus (P) over several decades have increased N and P concentrations in saline waters of the Bay (Harding 1994). Due to the volume, length, and relative clarity of the Chesapeake, inputs of N and P are largely removed by the growth of phytoplankton (Malone et al. 1988; Fisher et al. 1988), which provides a large supply of sinking organic matter to create seasonal anoxia (Seliger et al. 1985; Malone 1992).

The historical rate of nutrient export that caused the eutrophication of Chesapeake Bay is poorly known. Even in gauged areas, systematic chemistry measurements began only in 1984, and the accuracy of the nutrient flux or load depends on the number of water chemistry samples relative to the volume of flow represented. Nutrient export from ungauged areas of the land is not well known and is difficult to appraise (Gardner et al. 1997). The estimated flux from a nearby gauged area is often normalized per unit area and extrapolated over ungauged areas to compute fluxes from similar, adjacent watersheds or portion of a watershed in which land use, soils, or other watershed characteristics may vary. This problem is particularly acute in coastal plain watersheds with low relief, in which gauged areas often represent $<25\%$ of the basin area.

In the coastal plain region of the Chesapeake watershed, agriculture is the primary land use. Agriculture results in large and variable losses of nutrients from coastal plain watersheds (Beaulac & Reckhow 1982). Mayers and Fisher (in press) reported that the N yield (kg N ha^{-1} y^{-1}) increased by about a factor of 10 as agriculture increased from ca. 40% to 90% of land use within subbasins. Similar results have been observed in variety of coastal plain watersheds (Jordan et al. 1997). Therefore, spatial variations in land use within a basin hinder extrapolation of nutrient yields from a small gauged portion of a basin.

The goal of our research was to develop a method to extrapolate over the ungauged areas of a coastal plain basin where direct measurements of nutrient losses were difficult or impractical. In this manuscript, we describe the calibration and validation of the hydrochemical model GWLF using existing detailed data sets of hydrochemistry at two gauged sites. A subsequent manuscript will use spatial variations in landscape features such as topography, soil, and land use to apply the calibrated model to ungauged areas using local terrestrial attributes. The hydrochemical model GWLF was developed for estimating streamflow and nutrient loads from ungauged watersheds (Haith & Shoemaker 1987) and has been applied successfully to the West Branch of the Delaware River watershed in NY (Haith & Shoemaker 1987), in the Hudson River watershed, NY (Howarth et al. 1991), and for modeling water quality in NY City's water supply system (http://www.cinyc.nyu.us/html/dep/html/tmdl/html).

Study area

The Choptank River Basin is a coastal plain catchment in the Chesapeake Bay watershed and is located on the Delmarva Peninsula (Figure 1). Agriculture represents 52% of the land use within this basin, and 26% is covered by forest (Mayers & Fisher, in press). Table 1 shows selected landscape attributes of the entire Choptank Basin and the two gauged subbasins. The subbasin at Greensboro gauged by USGS (293 km^2) contains a greater percent of forest and poorly drained soils (D drainage class) than the entire basin, whereas German branch (51 km^2), studied by Jordan et al. (1997), contains a greater percentage of agriculture and poorly drained soils (Table 1).

The entire Choptank Basin is underlain by the surficial Columbia aquifer. This formation has a relatively continuous aquiclude, and local groundwater flow paths are <2 km through soils with relatively high hydraulic conductivity and flat topography (Carpenter 1983; Bachman & Phillips 1996). The area contains two hydrogeomorphic regions, well-drained uplands with a small proportion of forested wetlands and poorly drained lowlands with a large proportion of forested wetlands (Phillips et al. 1993).

Water quality parameters vary seasonally and spatially within this basin (Fisher et al. 1998; Mayers & Fisher, in press). In a one-year spatial survey of 34 ungauged subbasins, the mean TN concentrations varied exponentially with agricultural land use over the range of 1–8 mg N L^{-1} (70–600 μM), of which an average of 69% was nitrite + nitrate-N. Mean TP concentrations varied from 0.03–0.13 mg P L^{-1} (1–4 μM), of which an average of 28% was phosphate-P. Particulate and dissolved organic N (PON and DON, respectively) were relatively small fractions of the TN, but PP and DOP were much more important fractions of the TP. In an intensive, long-term study from WY1980 to WY1990 at the gauged basin at Greensboro, Fisher et al. (1998) found that total phosphorus (TP) demonstrated no significant trends; however, PO_4^{3-} decreased exponentially over the decade. NO_3^- increased linearly at $\sim$0.03 mg NO_3^--N L^{-1} y^{-1} ($\sim$2 μM y^{-1}), although there was no significant trend for [TN].

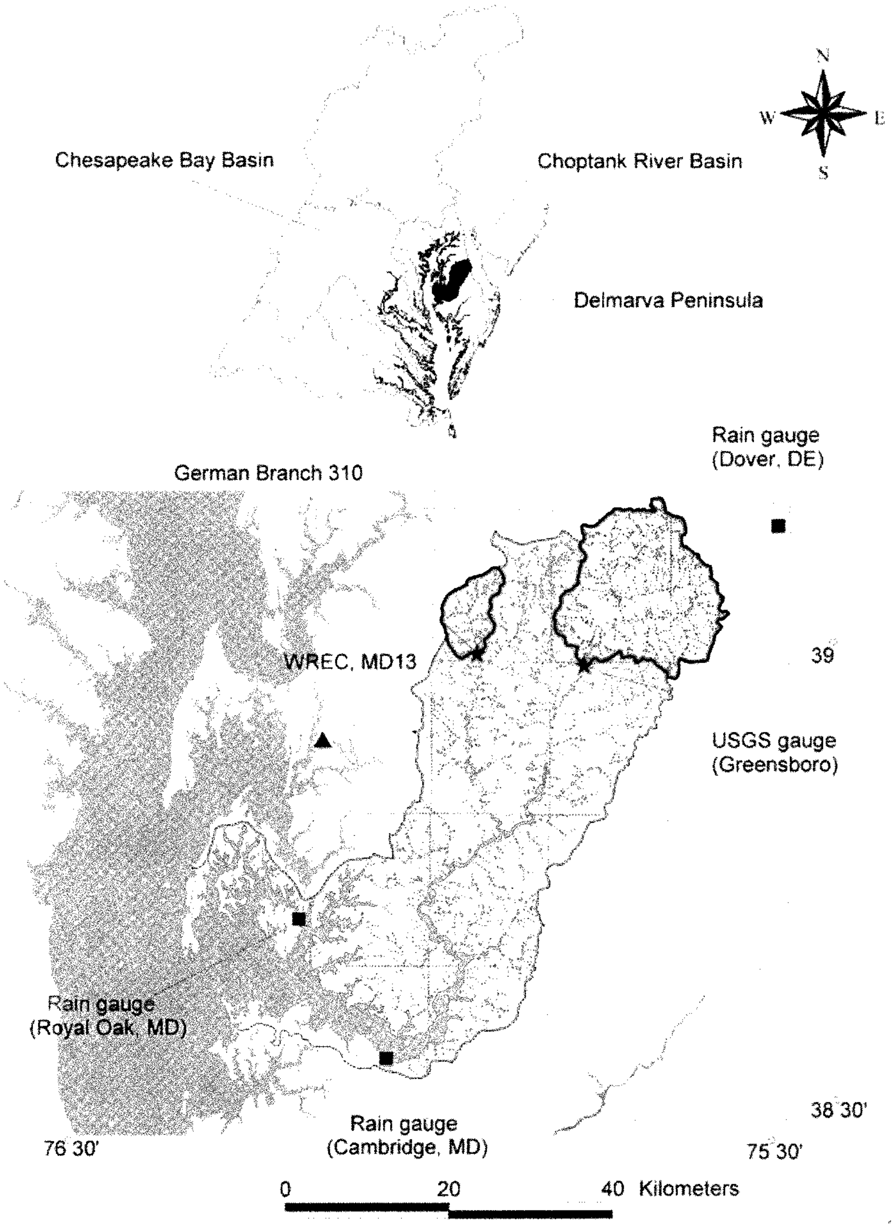

Figure 1. Upper: Position of the Choptank River Basin within the Chesapeake Bay watershed. Lower: the Greensboro subbasin gauged by USGS and German Branch subbasin (310) are represented by polygons within the basin. The locations of rain gauge stations are represented by squares, a local NADP station is a triangle, and the gauging stations are shown as stars.

Table 1. Landuse, soil drainage, human populations, and wastewater treatment plants (WWTP) of the entire Choptank Basin and the two gauged watersheds. The gauged site at Greensboro is a Chesapeake Bay program monitoring station with a 45-year history of hydrologic measurements by USGS. German Branch (basin 310) is a recently gauged watershed on which applications of best management practices have been studied (Jordan et al. 1997; Primrose et al. 1997). Basin areas include land and water (estuarine area + stream + lakes + surface depressions). Soil drainage represents hydrologic classes, from well-drained (A) to poorly drained (D). Human population data were obtained from the US Census Bureau. Wastewater treatment plants are licensed point sources with maximum discharges of millions of gallons per day (MGD). The data were compiled from Mayers (1998), Mayers and Fisher (in press), and Walters (1990).

Attribute	Unit	Choptank	Greensboro	German Branch
Landuse (1990)	km^2	2057.0	293.0	51.0
Forest	%	26.4	45.7	26.3
Agriculture	%	52.0	48.9	72.5
Developed	%	4.6	4.6	0.2
Feedlot	%	0.5	0.4	0.9
Wetland	%	1.9	0.2	0.0
Water	%	15.0	0.2	0.0
Soil drainage				
A	%	25.1	15.4	0.7
B	%	33.2	12.4	36.3
C	%	15.0	13.0	11.6
D	%	26.7	59.2	51.4
Human population (1990)				
Density	# km^{-2}	35	36	13
Total	#	72177	10536	631
WWTP				
	#	10	0	0
	MGD	4.7	0	0

Notes: Water + Wetland = 0.0% shown here at German Branch watershed is slightly different from values of 0.3% reported in Jordan et al. (1997).

Methods

A QuickBasic version of GWLF (General Watershed Loading Function v2.0) was obtained from Dr. D. Haith at Cornell University and translated into object-oriented Visual Basic Code (Microsoft Visual Basic-5.0 1997) to utilize the Active X component of VB5 to integrate with NT Arc/Info. With an Arc Macro Language (AML) program, this integration can activate Arc/Info within the VB5 version of GWLF and shorten the processing time needed to obtain land use and soils from Arc/Info. The original output module of GWLF was modified to produce output with a monthly sequence in plain text format, with the following columns: rain (cm month^{-1}), ET (cm month^{-1}), deep seepage (cm month^{-1}), baseflow (cm month^{-1}), stormflow (cm month^{-1}), streamflow (cm month^{-1}), sediment (Gg month^{-1} = 10^9 g month^{-1}), TN (Mg month^{-1} = 10^6 g month^{-1}), and TP (Mg month^{-1}). Copies of the modified program are available upon request.

GWLF computes the concentrations of dissolved and solid-phase N and P in streamflow as the sum of baseflow (groundwater), stormflow (overland flow), and point sources. Groundwater contributes only dissolved N and P (adjusted for local conditions), and largely reflects land use. Stormflow contributes both dissolved and particulate N and P from each land use; particulate losses are computed via the universal soil loss equation. Urban nutrient losses are assumed to be entirely solid-phase (Haith et al. 1992), as described in Amy et al. (1974). Point sources are assumed to be entirely dissolved; however, we used values of total N and P, which include particulate and dissolved forms. A detailed description of GWLF can be found in Haith and Shoemaker (1987) and Haith et al. (1992).

Input data

Water discharge at Greensboro MD (USGS gauge #01491000) was obtained from USGS. Discharge was separated into daily base and storm flow components using the USGS software RORA (Rutledge 1993). Water chemistry (NH_4, NO_3, TN, Fe, PO_4, and TP) at the USGS gauge has been monitored independently of USGS at a frequency of 50–150 samples per year since Oct. 1979 (Fisher et al. 1998). Calibration of GWLF was accomplished using these data from water year 1980 to 1990 (October 1979 to September 1990). Areas of land use for 1990 were extracted from an Arc/Info coverage of Mayers (1998) to compute curve number; the land use coverage was compiled using digital files from MD Dept. of Planning and a manually digitized version of a land use map from DE Dept. of Agriculture. We used six simplified land use categories: agriculture, forest, developed, feedlots, water, and wetland. Other data layers employed here include stream networks, soils, topography, and basin or subbasin boundaries.

A census block boundary from the 1990 Census was provided in Arc/Info I/O format by the Consortium for International Earth Science Information Network (CIESIN; http://plue.sedac.ciesin.org/plue/ddcarto/). Linking these block boundaries with point attribute data (STF1B) of the census developed the population-density data layers for the entire basin and each gauged subbasin. Digital watershed boundaries (Greensboro, German Branch 310, and Choptank River Basin) were used to confine those point attribute data within each basin to estimate the population size in 1990 with spatial coordinates.

GWLF requires daily average temperature and precipitation to compute a daily water balance. Meteorological data from National Weather Service Stations were obtained on CD-ROM from EarthInfo Corp. We selected three rain gauge stations with long-term records within or close to the Choptank River Basin in order to estimate average conditions in the basin. The three local stations with long-term (∼45 y) records are Dover DE, Cambridge MD, and Royal Oak MD (see Figure 1). Daily minimum and maximum temperature records at the stations were averaged prior to input to GWLF.

Parameters of GWLF

Table 2 lists the hydrology and nutrient parameters used by GWLF. For example, curve number was employed to compute stormflow, and KLSCP represents the components of the Universal Soil Loss Equation. Local calibration of all model parameters for the Greensboro watershed was accomplished in four steps:

(1) We defined reasonable ranges for each parameter through a literature survey to provide initial values for model calibration (see literature ranges in Table 2).

(2) We estimated the local hydrologic parameters (e.g., the recession coefficient and the seepage coefficient). The baseflow recession coefficient (r) describes the rate at which baseflow declines following a storm event and is parameterized as

$$r = \ln[F_{(t1)}/F_{(t2)}]/(t_2 - t_1), \tag{1}$$

where F_t = daily streamflow (cm) at different times. This was initially determined as 0.052±0.004 d^{-1} for the USGS gauging station as a result of analysis of six hydrographs using the straight-line method and fixed-base methods of Linsley et al. (1975), Dunne and Leopold (1978) and Chow et al. (1988). The seepage coefficient was initially set to a default value of zero since no standard techniques are available to compute this coefficient (Haith et al. 1992).

(3) We chose values for each parameter in an optimization procedure which minimized errors at the decadal time scale. We manually varied each parameter and plotted the cumulative errors (CE, sum of predicted – observed over 11 water years) as a function of parameter value. We then chose the parameter value which minimized the cumulative error (CE) over the 11 water year calibration period (1980–1990), sometimes at less than minimal values of the root-mean-square errors (RMS) for monthly predictions. The cumulative error at the decadal time scale was

Table 2. Hydrology and nutrient parameters in GWLF. The initial values were obtained from a literature survey, and the calibrated values were chosen by optimization (*: USGS Water Resources Data: Maryland and Delaware Water Year 1992–1995).

Parameter	Description	Unit	Variable	Initial value	Calibrated value	Literature range /comments	Group	Reference
Curve number (II)	For computing surface runoff	None	• Agriculture • Feedlots • Forest • Wetland • Water	83 88 68 99 99	83 88 68 99 99	Site-dependent	1	Haith et al. (1992); Dunne & Leopold (1978)
KLSCP	Components of Universal Soil Loss Equation	None	• Agriculture • Feedlots • Forest • Wetland • Water	0.214 0.016 0 0 0	0.0125 0.0125 0 0 0	Site-dependent	2	Mills et al. (1985); Haith et al. (1992)
Sediment/ delivery ratio	Annual sediment yield/annual erosion	None		0.08	0.08	Site-dependent	1	Haith & Shoemaker (1987); Haith et al. (1992); Novotny & Olem (1994)
KU	Cover coefficient for estimating evapotranspiration	None	Jan, Feb, Mar Apr, May, June July, Aug, Sep Oct, Nov, Dec	0.90, 0.89, 0.84 0.77, 0.80, 0.75 0.82, 0.99, 0.79 0.85, 0.86, 0.88	0.90, 0.89, 0.84 0.77, 0.80, 0.75 0.82, 0.99, 0.79 0.85, 0.86, 0.88	Site-dependent	2	Haith et al. (1992); Novotny & Olem (1994); Zipparro & Hasen (1993)
Baseflow recession	Groundwater recession coefficient	day^{-1}	r	0.052	0.0461	0.01–0.2	1	Haith et al. (1992)
Seepage	Deep seepage coefficient (loss)	day^{-1}	s	0.000	0.0191	Calibration	1	Haith et al. (1992)
IUS	Initial unsaturated storage	cm	IUS	10	10	Only affects first few months	3	Haith et al. (1992)
UAWC	Unsaturated available water capacity	cm	UAWC	10	11	Calibration	1	Haith et al. (1992)
ISS	Initial saturated storage	cm	ISS	0	0	Only affects first few months	3	Haith et al. (1992)

Table 2. Continued.

Parameter	Description	Unit	Variable	Initial value	Calibrated value	Literature range /comments	Group	Reference
IS	Initial snow	cm	IS	0	0	Only affects first few months	3	Haith et al. (1992)
Agricultural runoff	Agricultural land	mg L^{-1}	Dissolved N Dissolved P	2.9 0.26	2.18 0.05	0–29 0.1–5.1	1	Dornbush et al. (1974)
Forest runoff	Forested land	mg L^{-1}	Dissolved N Dissolved P	0.19 0.006	0.11 0.001	0.19–5 0.006–0.067	1	Dornbush et al. (1974)
Feedlot	Intensive animal opeations	mg L^{-1}	Dissolved N Dissolved P	29 5.1	9 0.7		1	Haith et al. (1992)
Urban-buildup	Nutrient accumulation and wash off on urban surfaces	kg ha^{-1} day^{-1}	Solid N Solid P	0.1 0.01	0.1 0.005	0.012–0.1 0.002–0.01	1	Kuo et al. (1988)
Groundwater	Nutrient concentration in groundwater	mg L^{-1}	Dissolved N Dissolved P	8 0.0001	1.17 0.031	1.7–4.3 (NO_3^-) 0.1–19 (TN) 0.2–0.4 (NO_3^-)	1	Phillips & Bachman (1996); USGS*; Lichtenberg & Shapiro (1997)
Tank effluent	Nutrient loads in septic tank effluent	g day^{-1}	Dissolved N Dissolved P	12 2.5	10 2.5	10–12 1.5–2.5	2	Haith et al. (1992)
Uptake per capita	Nutrient uptake by plants growing over the septic system	g day^{-1}	Dissolved N Dissolved P	1.6 0.4	1.6 0.4	0–1.6 0–0.4	2	Haith et al. (1992)
Sediment	Solid-phase nutrient from rural sources	mg kg^{-1}	Solid N Solid P	550 300	400 176	500–900 220–393	1	Mills et al. (1985)
1990 population	Total human population within watersheds	Choptank Greensboro German Branch	72,177 10,536 631	72,177 10,536 631			1	1990 Census STF1B

considered to be more important than the monthly RMS error because there are more scientific and management applications at the larger time scales. Model output was optimized by adjusting parameters individually in the following order: the recession coefficient, the seepage coefficient, unsaturated available water capacity, dissolved nutrient concentrations in groundwater, and export losses from each land use.

(4) Finally we compared the optimized parameters with values obtained in the literature survey to be certain that the optimized value was within that range.

Statistics

Linear regressions, correlations, and *t*-tests were used for examining the significance of relationships or differences. The significance of these tests were indicated as "not significant" (NS, $p > 0.05$), "significant" (*, $0.01 < p < 0.05$), or "highly significant" (**, $p < 0.01$).

Results

Model calibration

We calibrated GWLF by varying each model parameter individually and comparing model output with observations at Greensboro (Fisher et al. 1998). Model parameters describing initial stored water influenced only the output of the first few months of data (IUS, IS, and ISS, see Table 2). Haith et al. (1992) recommended running the model for a year prior to the time period of interest to avoid the effects of these parameters. We accepted the default values of these parameters and started the model one-year prior to our time period of interest.

Other model parameters strongly influenced the output during the entire period. For example, the seepage coefficient (s, d^{-1}) is a sensitive parameter which controls the loss of near-surface groundwater through the aquaclude to deeper layers. This parameter creates large cumulative errors in baseflow as it varies from 0 to 0.025, although storm flow is relatively unaffected (Figure 2(A, B)). In the case of s, we chose the optimized value of $s = 0.0191$, which produced a cumulative error of zero for baseflow and stormflow (Figure 2(A)), and RMS errors of 0.9 cm month^{-1} for baseflow, 1.1 cm month^{-1} for stormflow and 1.4 cm month^{-1} for streamflow (Figure 2(B)). The value of this parameter implies that ∼2% of the water in the saturated zone is lost daily to deeper aquifers underlying the gauged basin. A cumulative error of zero with an RMS error of ∼1 cm month^{-1} for the seepage coefficient indicates that monthly predictions are expected to be within ± 1 cm month^{-1} of the observed values, and that these errors cancel to zero over larger time intervals.

We chose to minimize cumulative errors in the model output (summed values of predicted – observed) over the 11 year calibration period, sometimes at the expense of monthly RMS errors (square root of the average of squared values of predicted – observed), as in the example above, to produce more accurate predictions of output at annual to decadal time scales (i.e., lower cumulative errors). We also used % cumulative error and % RMS error to examine the model deviations from observations relative to the cumulative or mean values. In this case, % cumulative error was defined as the cumulative errors (sum of predicted – observed) over the entire 11 water year period expressed as a percent of the observed cumulative measurements, and % RMS error was defined as the RMS error expressed as a % of the average value (either monthly or annually).

Another example of optimization of a hydrologic parameter is the adjustment of the baseflow recession coefficient, r (d^{-1}). This parameter controls how quickly baseflow returns to pre-storm levels (Equation 1) and is highly site dependent. Based on our initial estimate of $r = 0.052$, we varied the recession coefficient from 0.01 to 0.1 (Figure 2(C, D)). We selected $r = 0.0461$, which sets the cumulative error of baseflow and stormflow to zero (Figure 2(C)). The resulting RMS errors were 1.15 cm month^{-1} for stormflow and 0.97 cm month^{-1} for baseflow (Figure 2(D)).

Following the calibration of hydrologic parameters, we continued to calibrate the nutrient parameters. For example, dissolved N and P concentrations assumed by the model for agricultural stormflow were calibrated by a similar procedure (Figure 2(E, F)). As described above, we minimized cumulative errors of exported N and P (to zero) to improve predictive ability at larger time scales. In this case, RMS errors were relatively unaffected by the choice of dissolved N and P concentrations. Procedures similar to those described above were employed for other parameters, and a summary of initial and optimized values is given in Table 2.

Model output

Following calibration, we compared monthly GWLF predictions with observed monthly streamflow, baseflow, stormflow, and export of N and P (Figure 3). Generally, GWLF was able to capture the seasonal and interannual variations of streamflow at Greensboro (Figure 3(A)). However, the model under- and over-predicted wet and dry periods <1 y due to our choice of minimizing cumulative errors at the expense of RMS errors. For example, the model over-predicted stormflow during a hurricane event in October 1986

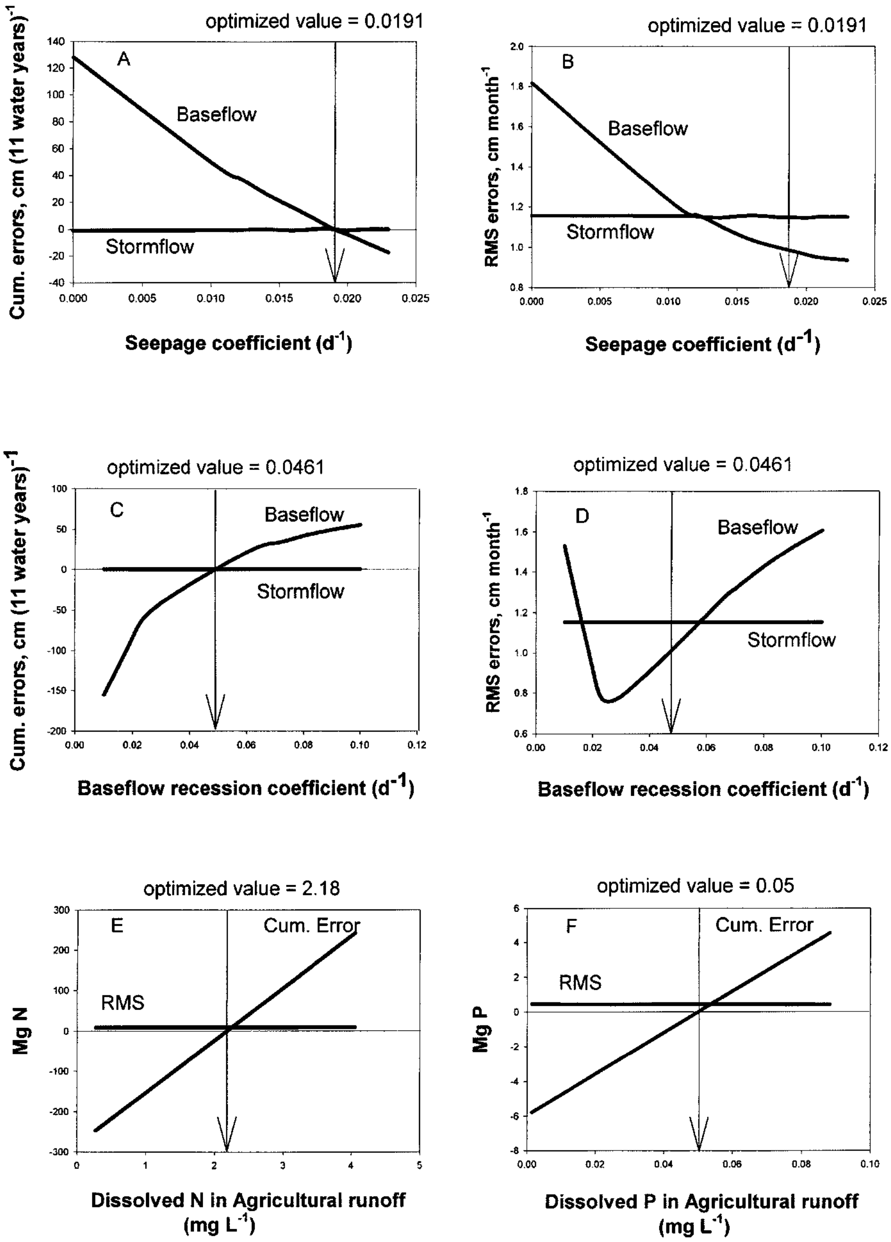

Figure 2. The optimization procedure employed to minimize cumulative and RMS errors for the seepage coefficient (A, B) and baseflow recession coefficient (C, D). Both coefficients primarily influence baseflow, with only minimal effects on stormflow. Arrows represent the optimized values for each parameter, chosen to minimize cumulative errors (A, C); the resulting RMS errors are shown in the B, D. Panels E, F indicate the selection of optimized values for dissolved N and P in agricultural stormflow. The units used for cumulative errors and RMS errors in the bottom panels are Mg (11 water years) $^{-1}$ and Mg month^{-1}, respectively (Mg = 10^6 g).

(Figure 3(A, B)), and under-predicted baseflow during August–October in most years (Figure 3(C)). Under-prediction of baseflow during late summer and early fall is the model's weakest performance. In Figure 3(D, E), the model captured the basic seasonal pattern of N and P export (high in spring, low in summer/fall), primarily because export is flow-driven. Errors for some months could be quite large ($>$100% of observed), and P export was consistently overestimated in late summer and fall during low flow. Nonetheless, in spite of these errors for individual events or seasons, the model clearly reproduced the general pattern of hydrochemistry in the gauged basin.

To quantify the model's performance statistically, we compared the predicted and observed values of export of water, N, and P at decadal, annual, and monthly time scales (Table 3). Over the 11 water years (WY1980–WY1990), the model predicted the watershed output very well, with cumulative errors of $\pm$0.01 cm for water, and $\pm$0.1 kg for N and P. This corresponds to very small% cumulative errors ($\pm$0.001%) for water, N, and P at the decadal time scale (Table 3) and indicates excellent predictive capability at the decadal time scale.

At the annual time scale, the model's performance degraded somewhat. Observed baseflow was predicted well, with no model bias (Figure 4(C), slope = 1, $r^2 = 0.91^{**}$); RMS errors were 10% (Table 3). Stormflow predictions were less precise (Figure 4(B), $r^2 = 0.44^{*}$), and there was model bias (slope $<$1, and intercept significantly $>$0, Table 3). Average RMS errors for stormflow were 5 cm y^{-1} (46%). For total streamflow (baseflow + stormflow), the results were intermediate with significant model bias (Figure 4(A)), and average RMS errors were 4 cm y^{-1} or 12% (Table 3). At this time scale, TN and TP were predicted well by the model (Figure 4D, E, $r^2 = 0.98^{**}$, 0.82^{**}), although the slopes were not 1:1. Average annual RMS errors were 17%–38% (Table 3).

At the monthly time scale, model performance degraded again somewhat. Observed streamflow was predicted well by the model ($r^2 = 0.78^{**}$), and the data points scattered about the 1:1 line (Figure 5(A)), consistent with our attempts to minimize cumulative errors. Monthly RMS errors were 1.4 cm month^{-1} or 45% (Table 3). However, at this time scale, baseflow and stormflow were predicted less well than total streamflow (Figure 5(B, C)), with some model bias (Table 3). Observed monthly export of TN and TP were predicted well by GWLF ($r^2 = 0.77^{**}$ and 0.62^{**}) with 48%–77% RMS errors, although the model tended to over predict TN and TP at low flows and underpredict at high flows (Figure 5(D, E); Table 3).

The above data show both the strength and the limitations of the calibrated model. At the decadal time scale, the model performs as well as can be expected, with cumulative errors $\ll$1% and well within the experimental

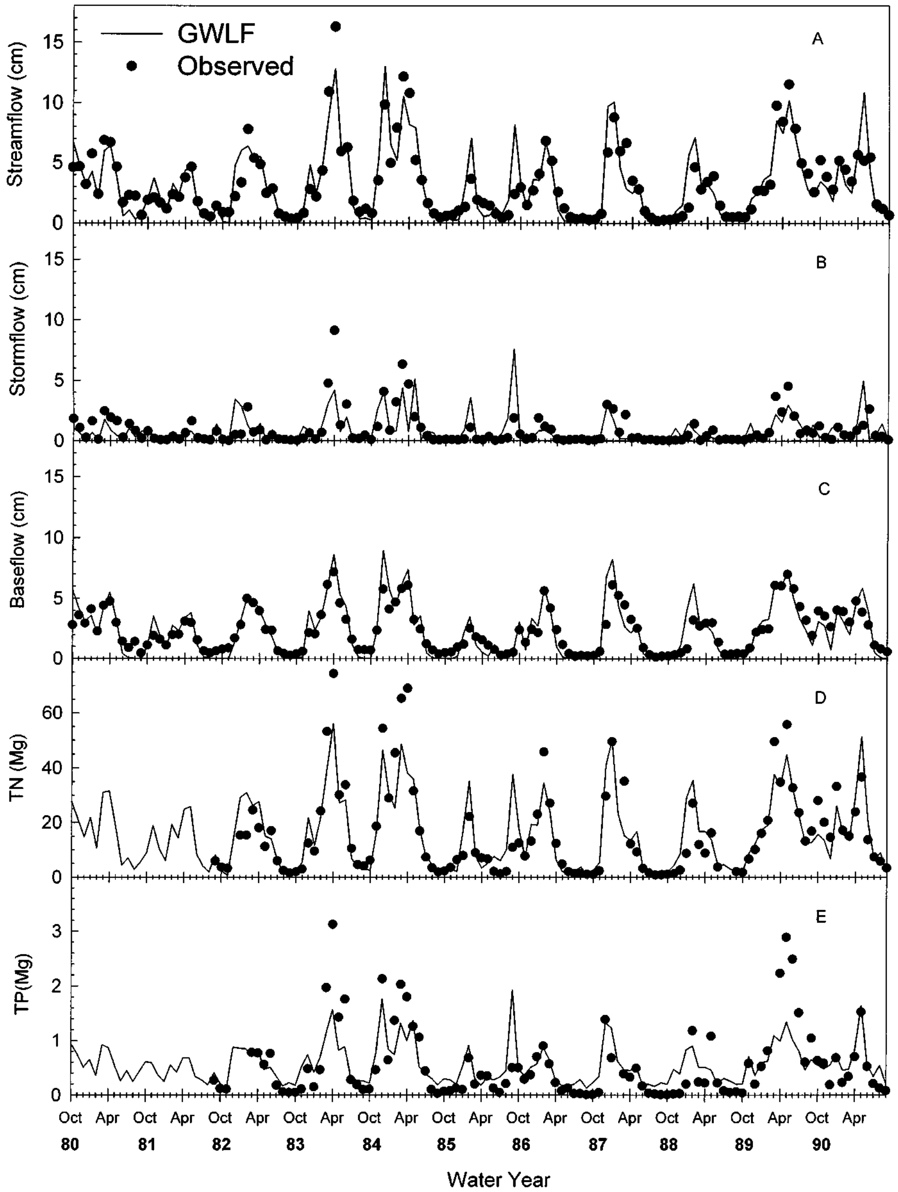

Figure 3. Time-series of observed monthly means at the gauged Greensboro subbasin compared with discharge and export of N and P modeled with GWLF. Export modeled with GWLF is shown as lines; observed data (Fisher et al. 1998) are points.

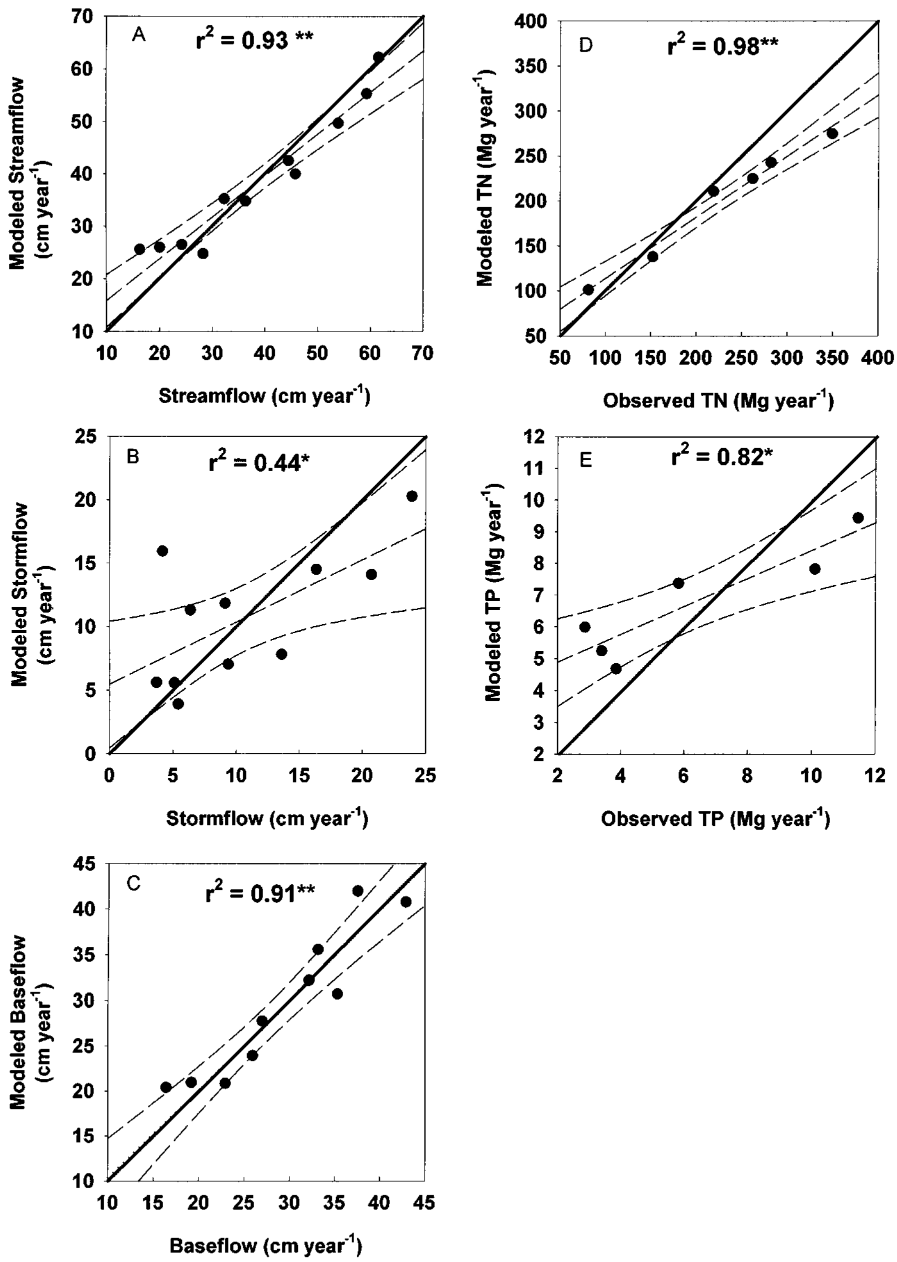

Figure 4. Correlations between modeled and observed annual measurements during the calibration period from WY1980–WY1990 at the Greensboro watershed. Solid line is the 1:1 line; dashed lines represent the line of best fit with 95% confidence limits.

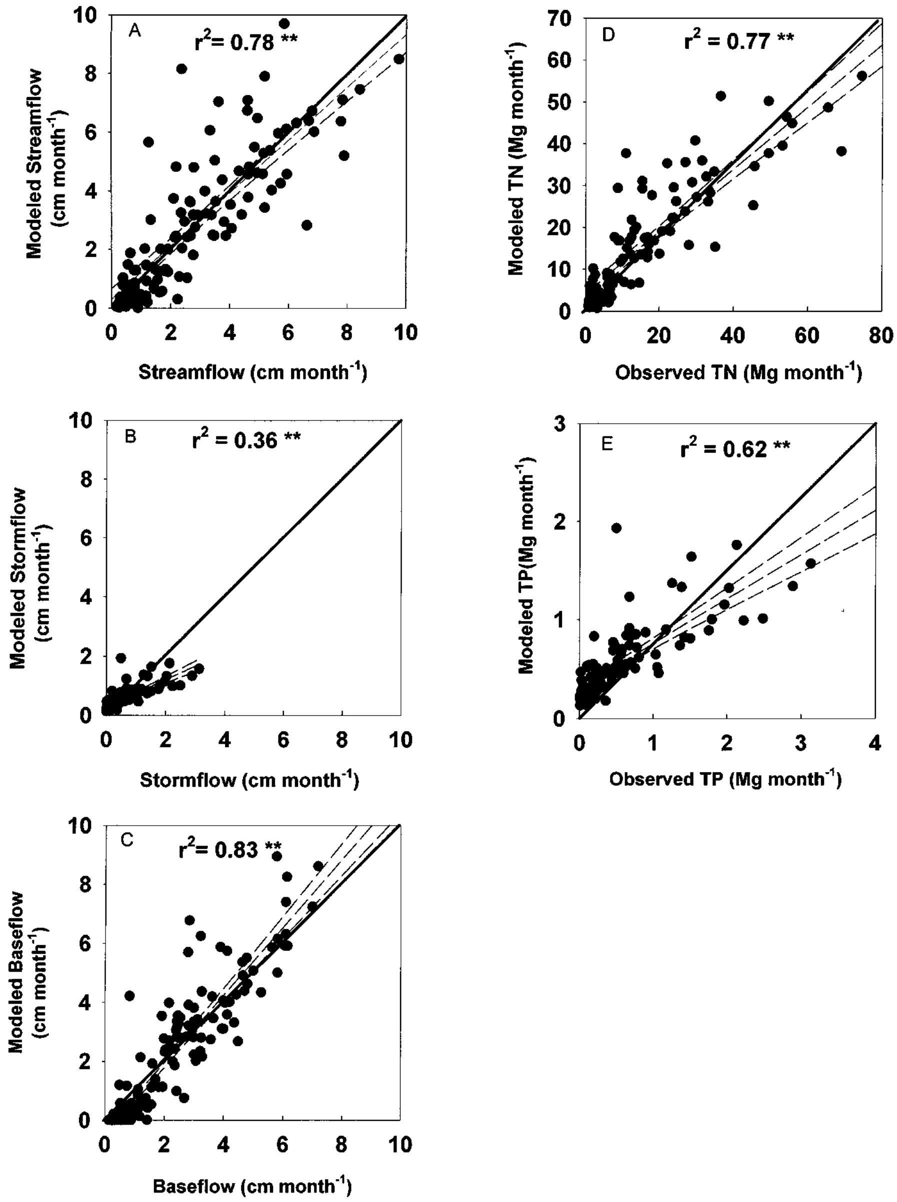

Figure 5. Correlations between modeled and observed monthly measurements during the calibration period from WY1980–WY1990 at the Greensboro watershed. Solid line is the 1:1 line; dashed lines represent the line of best fit with 95% confidence limits.

Table 3. Summary of model predictions, observations and errors for GWLF during the calibration period at the Greensboro watershed (WY1980–WY1990). Cumulative and RMS errors (predicted – observed) for annual and monthly time scales were computed and expressed both in absolute units and as a % of the annual or monthly mean.

	Stream	Base	Storm	TN	TP
WY80–90	cm	cm	cm	mg	mg
USGS/Fisher et al. 1998	422.38	304.59	117.79	1701.56	57.65
GWLF	422.37	304.58	117.79	1701.56	57.65
Cum. error	−0.01	−0.008	−0.002	0.0001	−0.0001
% Cum. error	−0.003	−0.002	−0.001	−0.000005	−0.00018
Annual					
RMS error (year^{-1})	4.46	2.78	5.00	38.50	2.36
% RMS error	11.63	10.03	46.47	17.15	37.69
Pred. vs obs. r^2	0.93**	0.91**	0.44*	0.98**	0.82**
Slope = 1?	<1	NS	<1	<1	<1
Intercept = 0?	>0	NS	>0	>0	>0
Monthly					
RMS error (month^{-1})	1.44	0.97	1.15	7.88	0.43
% RMS error	44.87	42.29	129.24	48.64	77.48
Pred. vs obs. r^2	0.78**	0.83**	0.36**	0.77**	0.62**
Slope = 1?	NS	>1	<1	<1	<1
Intercept = 0?	NS	<0	>0	>0	>0

error of the observations (∼5% for water, 10% for N and P). At the annual time scale, streamflow can be predicted to within 4.5 cm or 12%, and N and P export can be predicted to within 20–40%, with some flow-dependent model bias. At the monthly time scale, streamflow predictions are ±1.4 cm or 45%, and N and P export are predicted ±40–80%. GWLF, calibrated locally, can therefore be expected to make accurate and precise predictions at time scales >1 y, within 50% for a given water year, and within a factor 2 (50–100%) for a given month.

Model validation

Validation was performed to test the model under conditions outside of the calibration period and location with independent data. There were two kinds of validation: (1) we used USGS discharge and chemistry data from WY1991 through WY1996 at Greensboro (same location, different time) and (2) we used hydrochemical measurements of Jordan et al. (1997) from WY1991 to WY1995 for the German Branch watershed (within the Choptank Basin, but a different location and time). Monthly TN and TP export at the Greensboro gauge were obtained from USGS for WY1991 to WY1996. These monthly export values estimated by USGS were based on continuous hydrology observations and 2–5 water chemistry measurements per month. The USGS chemistry data are independent of, but correlated with those reported by Fisher et al. (1998). For German Branch, continuous measurements of discharge and weekly composited, flow-weighted TN and TP were obtained from Jordan et al. (1997). These data were transformed to monthly values by summing weeks or fractions of a week for comparison with GWLF output.

Validation at Greensboro

For the validation test at Greensboro during WY1991–WY1996, there were no adjustments of calibrated parameters. Using observed weather data, we compared model predictions with USGS measurements (streamflow and nutrient export) during WY1991–WY1996. The model captured the seasonal and interannual variation (Figure 6), consistent with performance during model calibration (WY1980–WY1990). TP transport during the largest storm flows was again underestimated (compare Figures 3 and 6). During this 6 water-year validation period, the model produced cumulative errors of -5 to 2% for streamflow, baseflow and stormflow (Table 4). The simulation for N and P produced cumulative errors of -5% to -36% over the 6 water years.

At the annual time scale, observed streamflow, baseflow, and stormflow were predicted well by the model ($r^2 = 0.93^{**}$, 0.99^{**} and 0.69^{*}, respectively, Table 4). The predicted and observed data points scattered about the 1:1 line, with no model bias (Figure 7 (A)), and average RMS errors were 6–35% (Table 4). TN was predicted well by the model ($r^2 = 0.96^{**}$, Table 4), with no significant model bias (Figure 7(B)) and an average RMS error of $\sim$10%. However, TP was severely underpredicted in wet years (Figure 7(C)), and the average RMS error was $\sim$50%.

Modeled and observed values of monthly discharge for WY1991–WY1996 at Greensboro (streamflow, baseflow, and stormflow) were strongly correlated ($r^2 = 0.74^{**}$, 0.75^{**}, and 0.62^{**}, respectively, see Figure 8(A–C)). Monthly % RMS errors were 54–115% for streamflow, baseflow and stormflow (Table 5). At this time scale, baseflow was predicted well without model bias; streamflow and stormflow can be predicted within 50–120% with some model bias.

The modeled nutrient export at the monthly time scale was good for TN and weaker for TP. Figure 8(B, C) shows that model simulation of TN export

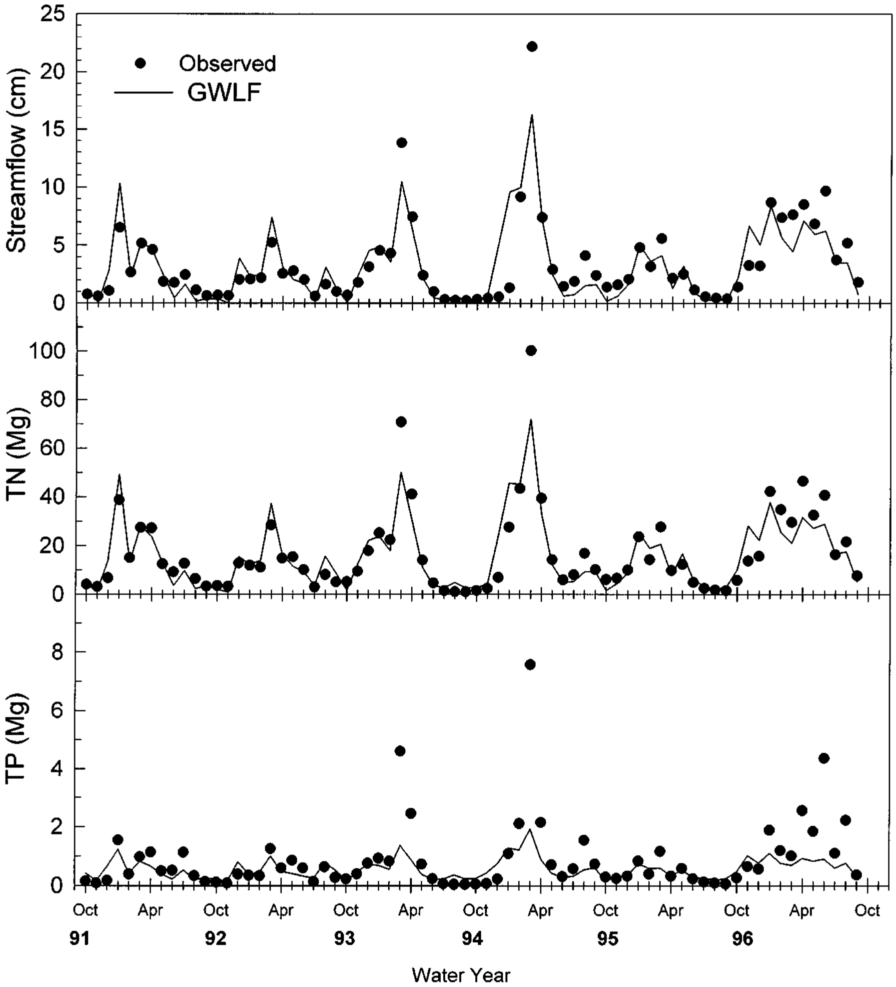

Figure 6. Model validation: time series comparisons of measurements by USGS at Greensboro compared with streamflow and export of N and P modeled with GWLF.

agreed with observed measurements (r^2 = 0.84** with no bias); however, P export was consistently underestimated at the highest flows. Monthly RMS errors for TN and TP export during validation were similar in magnitude to those obtained during calibration (42 or 49% for N, 110 or 77% for P, respectively; Tables 3, 4).

Validation at German Branch

Model simulation for German Branch was considered the most rigorous validation procedure due to the different location. We had two different

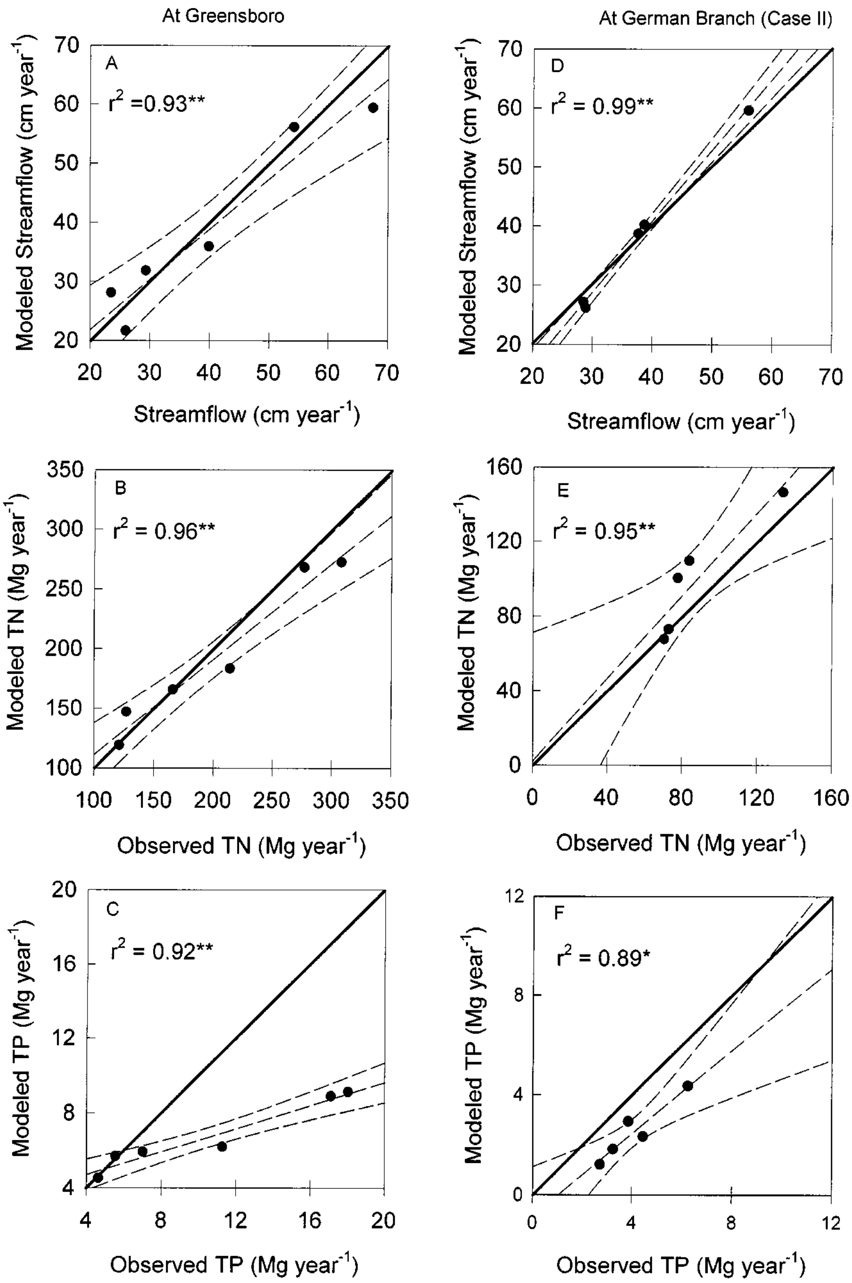

Figure 7. Correlations between modeled and observed annual measurements at Greensboro from WY1991–WY1996 and at German Branch 310 from WY1991–1995 (Case II). Solid line is the 1:1 line; dashed lines represent the line of best fit with 95% confidence limits.

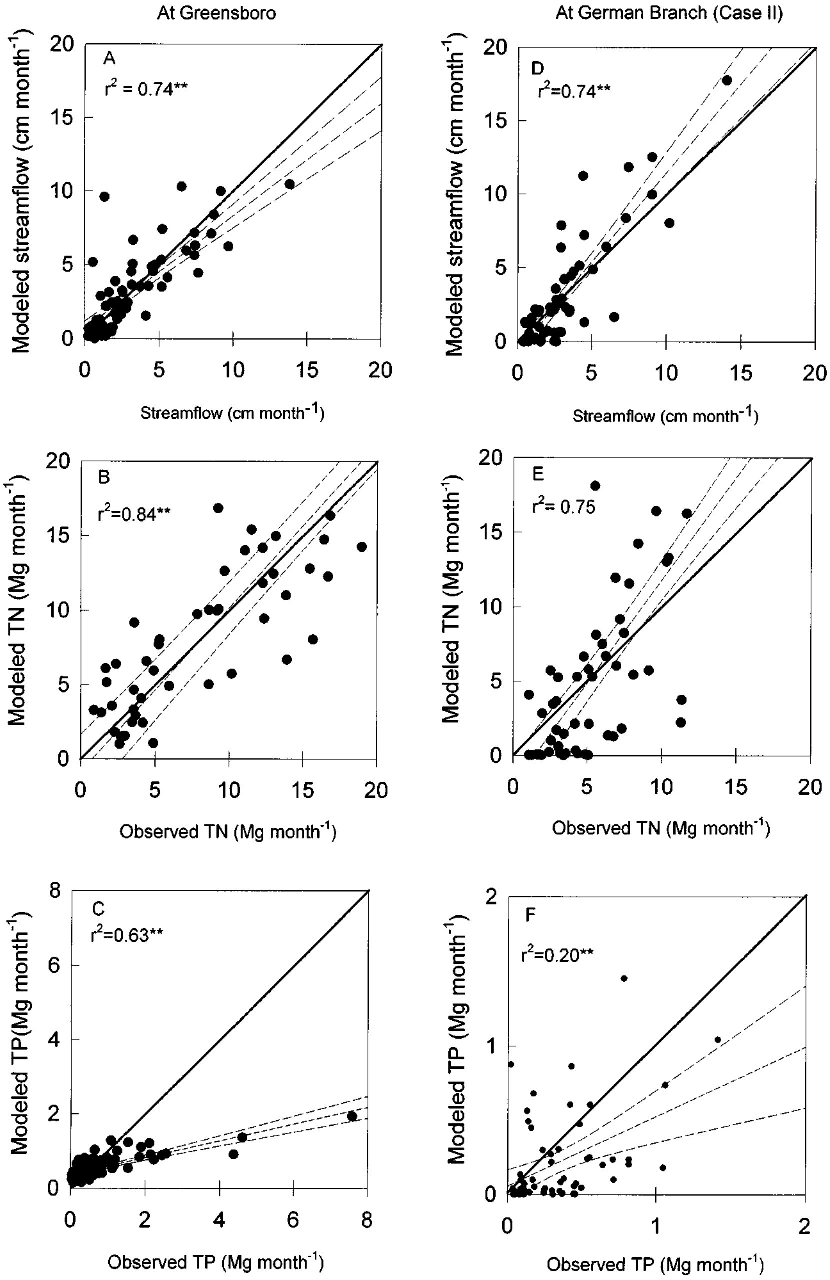

Figure 8. Correlations between modeled and observed monthly measurements at Greensboro from WY1991–WY1996 and at German Branch 310 from WY1991–1995 (Case II). Solid line is the 1:1 line; dashed lines represent the line of best fit with 95% confidence limits.

Table 4. Summary of model predictions, observations, and errors for GWLF during the validation period at the Greensboro watershed (WY1991-WY1996).

	Stream	Base	Storm	TN	TP
WY91-96	cm	cm	cm	Mg	Mg
USGS/Fisher et al. 1998	240.33	170.49	69.84	1212.7	63.59
GWLF	233.21	162.29	70.92	1155.7	49.78
Cum. error	−7.12	−8.20	1.08	−56.61	−23.17
% Cum. error	−2.96	−4.81	1.54	−4.70	−36.50
Annual					
RMS error ($year^{-1}$)	4.63	1.76	4.05	21.01	5.38
% RMS error	11.55	6.20	34.85	10.39	50.76
Pred. vs obs. r^2	0.93**	0.99**	0.69*	0.96**	0.92**
Slope = 1?	NS	NS	NS	NS	<1
Intercept = 0?	NS	NS	NS	NS	>0
Monthly					
RMS error ($month^{-1}$)	1.81	1.12	1.11	7.07	0.99
% RMS error	54.47	47.37	115.30	41.96	112.42
Pred. vs obs. r^2	0.74**	0.75**	0.62**	0.84**	0.63**
Slope = 1?	<1	NS	<1	NS	<1
Intercept = 0?	>0	NS	<0	NS	>0

modeling approaches for this watershed. In case I, we initially used the values of the model parameters calibrated at Greensboro, but used site-specific data for basin area, land use %, and population. In the second approach (case II), we adjusted the groundwater recession coefficient using the local discharge data (r = 0.097±se 0.009, n = 5), and we also adjusted the dissolved N concentration in agricultural stormflow and total N in groundwater based on the land use characteristics of German Branch. This adjustment was based on observations of Mayers and Fisher (in press), in which N concentrations in stream waters of the Choptank Basin increased exponentially with linearly increasing agricultural land use (see discussion). Applying this observed relationship, we increased the N concentrations in agricultural stormflow by a factor of 2.5, corresponding to an increase in agricultural land use at Greensboro of 49% to 72% at German Branch.

For case I (no site-specific parameter adjustments), the model slightly underestimated water discharge, and performed poorly for N and P export (Figure 9(A–C)). The model underestimated N and P export, although it

Table 5. Summary of model predictions, observations, and errors for case I & II during the validation period at the German Branch 310 watershed (WY1991-WY1995). For case I, no local adjustments in parameters were made other than area, landuse, and population. For case II, other adjustments were made to improve model performance (see text).

	Case I (no local adjustments)			Case II (adjusted locally)		
	Stream	TN	TP	Stream	TN	TP
WY91–95	cm	Mg	Mg	cm	Mg	Mg
Jordan et al. 1997	189.91	438.52	20.51	189.91	438.52	20.51
GWLF	169.31	148.99	12.30	191.84	497.66	12.67
Cum. error	−20.59	−289.53	−8.21	1.92	59.14	−7.84
% Cum. error	−10.84	−66.02	−40.01	1.01	13.4	−38.23
Annual						
RMS error ($year^{-1}$)	4.25	59.49	1.69	2.26	16.52	1.62
% RMS error	11.21	67.84	41.33	5.95	18.84	39.53
Pred. vs obs. r^2	0.99**	0.95**	0.89*	0.99**	0.84*	0.89*
Slope = 1?	>1	<1	NS	>1	NS	NS
Intercept = 0?	<0	NS	NS	<0	NS	NS
Monthly						
RMS error ($month^{-1}$)	1.61	6.14	0.35	2.02	5.25	0.34
% RMS error	50.79	83.97	101.00	63.72	71.77	100.50
Pred. vs obs. r^2	0.73**	0.75**	0.17**	0.74**	0.76**	0.20**
Slope = 1 ?	NS	<1	<1	>1	>1	<1
Intercept = 0 ?	NS	NS	NS	NS	<0	NS

mimiced the pattern of seasonal changes and inter-annual variation. As shown in Table 5, cumulative errors during WY1991–WY1995 were −11% to −66%, considerably larger than during calibration. At the annual and monthly time scale, model errors increased still more (11–68%, and 51–101%, respectively). Due to the poor performance for case I, we applied site-specific model parameters.

For the case II simulation, parameters were adjusted for the local recession coefficient and the exponential effect of the high agricultural land use in the German Branch watershed (Table 1). As a result, the model's performance improved, particularly for N export. The model more closely simulated the observed pattern of seasonal changes of water discharge over the 5 water years (Figure 9(D)) with a cumulative error of +1% (Table 5). For N and P (Figure 9(E–F)), the model output exhibited a cumulative error of +13% for N and −38% for P (Table 5).

At the annual time scale, observed streamflow was predicted very well by the model (r^2 = 0.99**), with some model bias (Figure 7(D)). RMS errors

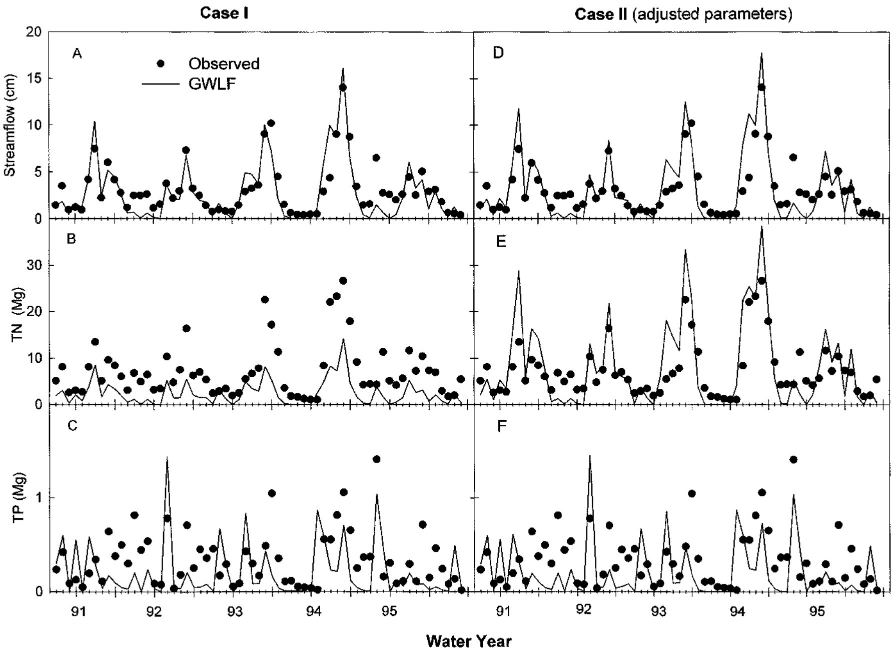

Figure 9. Model validation: time series of measurements at German Branch 310 with streamflow and N and P modeled with GWLF. Export modeled with GWLF is shown as solid lines; measurements from Jordan et al. (1997) are points. Simulations without local adjustments are shown in panels A, B, C (Case I); simulations with adjustments for local characteristics are shown in panels D, E, F (Case II).

were 6% (Table 5). Modeled N and P were predicted well ($r^2 = 0.84^*$ and 0.89^*, Figure 7(E, F)), with no significant bias. Average RMS errors were 19% for N export, and 40% for P export.

In the scatter plots of monthly model output and observed measurements (Figure 8(D–F)), there were significant correlations ($r^2 = 0.74^{**}$, 0.76^{**}, and 0.20^{**}) for water, N, and P, respectively. Monthly water, N and P were predicted with bias (slope >1 or <1), although the intercepts were not significantly different from 0 in some cases (Table 5). RMS errors were 63% for water, 72% for N, and 100% for P.

The results from the validation of GWLF suggest that GWLF has good performance for water and N export, and weaker predictive ability for P. At annual time scales, GWLF is able to predict streamflow with 6–12% errors and to predict N with 10–20% errors, although P export is underestimated by 40–50% (Tables 4 and 5). These errors are similar to those encountered during calibration at this time scale. At the monthly time scale, errors are increased to $\sim$50–100%, or within a factor of 2 of observations. We also found that the use of locally based parameter values was essential to maintain this level of accuracy (i.e. Case I errors are > Case II, Table 5).

Discussion

We have explored the ability of GWLF to predict export of water, N, and P from two gauged areas in the Choptank Basin. At interannual time scales, the model's predictions were quite good, generally less than 10%, except for P export, which was generally within 30–40% of observed values. At shorter time steps, the models' cumulative and RMS errors increased, but even predictions at the monthly time scale were generally within a factor of two of observations (Tables 3–5). We have attempted to characterize these inherent errors in GWLF to understand its limitations; however, it is also apparent that GWLF is a good loading function model for long-term simulation (e.g., Figures 3, 6, and 9), although for any particular month (especially, in summer) or year (especially wet years), GWLF may provide predictions only within 50–100% of measured values.

Our validation at German Branch showed that it is important to use as many local characteristics as possible for simulations. When we did not adjust for the effects of basin area on the recession coefficient and used only GWLF's linear extrapolation for agricultural land use from the gauged area at Greensboro (Case I simulation), we obtained model predictions with large negative cumulative errors for water (−10%) and N export (−66%). When we adjusted the groundwater recession coefficient locally and also adjusted the N parameters based on the observed exponential effect of increasing agricultural land use in this basin (Case II simulations), the model's performance for water and N export improved markedly (Table 5). Thus, model parameters are very site-dependent, and it is necessary to calibrate and verify model parameters locally for the most accurate applications.

Application of GWLF to other areas

GWLF is a lumped-parameter model, in which an empirical equation was employed to average spatial heterogeneity (Beasley 1986; Novotny & Olem 1994). Therefore, the effects of the spatial structure of land use, the continuity of riparian zones, and the thickness of buffer zones along streams were not considered during model calibration. These factors have been shown to be important controls on nutrient losses in empirical studies (Johnston et al. 1984; Jacobs & Gilliam 1985; Vought et al. 1994; Emmett et al. 1994; Hill 1996). For example, TN and TP can be removed by up to 84% and 50%, respectively, within riparian wetlands (Peterjohn & Correll 1984).

These removal mechanisms are via denitrification, microbial immobilization, and particle deposition (Johnston et al. 1984; Jacobs & Gilliam 1985; Hill 1996). These could have a substantial effect on the calibration of parameters, and consequently, on the model performance at different locations. Another consideration when extrapolating this model to different locations is that [TN] and [TP] in groundwater may originate from intermediate (or regional) systems (Jordan et al. 1997). This could easily lead to under- or over-estimates of the nutrient concentrations in groundwater.

Of all the hydrological parameters in GWLF, the groundwater recession coefficient, *r*, is one of the most important. There is usually no information available to estimate *r* for ungauged areas. Here we provide an empirical relationship showing a correlation between *r* and watershed size, based on USGS Water Resources Reports and the standard hydrograph separation techniques described above. This relationship is modeled as an hyperbolic relationship in Figure 10. The watersheds that we chose for Figure 10 varied from 3 to 901 km^2, and all are located in the mid-Atlantic coastal plain and piedmont. For watersheds >100 km^2, the groundwater recession coefficient declines slowly with watershed size from $\sim$0.07 to $\sim$0.04. However, for small watersheds <100 km^2, *r* increases rapidly from $\sim$0.07 to $>$0.4 and becomes quite variable (Figure 10). When applying GWLF to other areas, a calibration procedure is highly recommended for a gauged watershed, although the function in Figure 10 can provide an initial estimation of *r* for coastal plain watersheds.

Another important parameter for application of GWLF to other areas is the value of N concentrations in agricultural stormflow. In the Choptank Basin, we used the relationship between agricultural land use and stream TN reported by Mayers and Fisher (in press, Figure 11) to adjust the optimized value from the Greensboro watershed when we applied GWLF to the German Branch watershed. This exponential relationship is probably the result of losses of forested areas or other N-trapping landscape features as agricultural land use increases. Application of this exponential relationship corrected the linear assumption of GWLF and significantly reduced both the cumulative and RMS errors of model output. Although the relationship shown in Figure 11 does not necessarily apply to all coastal plain settings, adjustments to GWLF similar to the ones described above appear to be important for the most accurate estimates.

We have grouped the parameters of GWLF (Table 2) into 3 classes for application to other areas. Essential parameters (group 1) are those that must be locally adjusted to achieve model performance similar to that reported here. These are curve number (CN, based on land use and soil drainage), sediment delivery ratio, the groundwater recession coefficient (*r*),

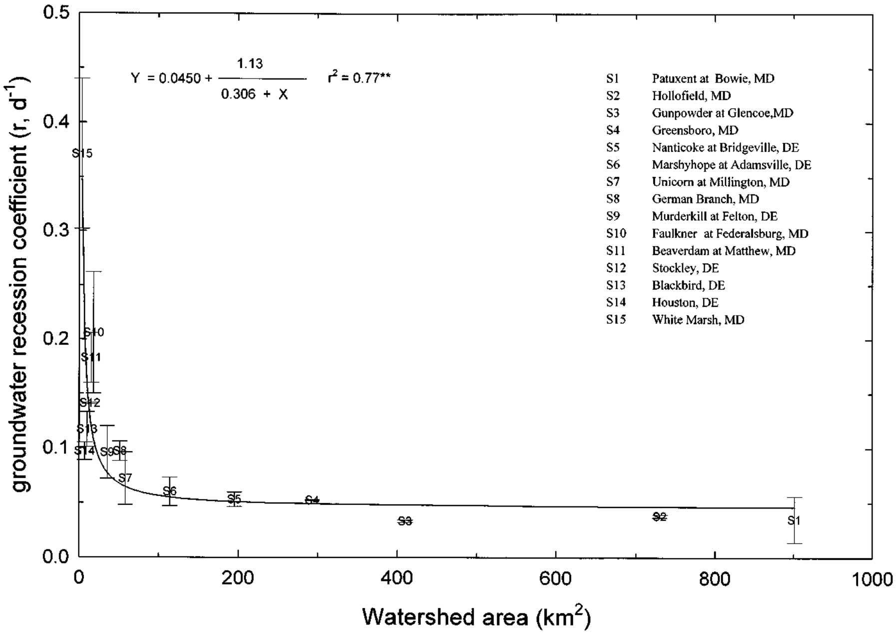

Figure 10. Hyperbolic relationship between the groundwater recession coefficient (r, d^{-1}) and watershed size (km^2) for selected watersheds in the mid-Atlantic coastal plain region. Three hydrographs were analyzed for each watershed; data source = USGS.

the seepage coefficient (s), unsaturated available water capacity (UAWC), dissolved and particulate nutrient concentrations associated with each land use, point sources, and population. These are indicated as group 1 parameters in Table 2. The second group of parameters (useful but not essential) are those which can improve the model's performance. These are KLSCP, crop coefficients for evapotranspiration (KU), tank effluent and uptake rates for N and P (Table 2, group 2). The nonessential parameters (group 3) are those which can be set to default values because they influence the model output only for the first few months. The effects of these variables can be avoided by running the model for a year prior to the time period of interest. These parameters are unsaturated (IUS) and saturated storage (ISS), initial snow (IS), and 5-day antecedent precipitation.

For future applications, there are other processes (e.g., atmospheric deposition, fertilizer application rates, population density, and land use change) which need to be considered or incorporated into this model. It was assumed that both population density and fertilizer applications did not change during the simulation periods. In fact, historically there has been exponentially increasing use of commercial fertilizers in North American

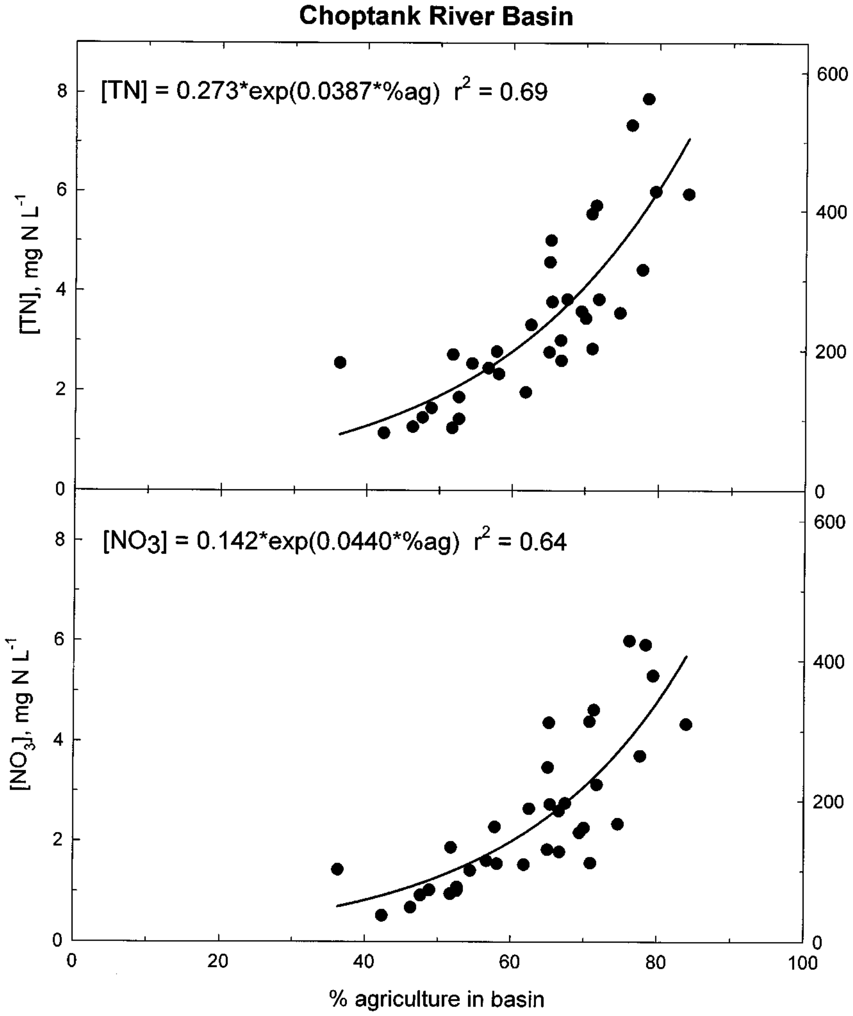

Figure 11. Exponential relationships between N concentrations in streams and % agriculture in subbasins within the Choptank River Basin. Data were from Mayers and Fisher (in press).

(Nixon & Pilson 1983) as well as increasing deposition of atmospheric N (Jordan & Weller 1996; Paerl 1997). Land use change should be considered as well, and we are currently applying this model to historical changes in land use in the Choptank Basin to evaluate the effects on water, N and P export over the previous 150 years.

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