

A Spatially Explicit Model for Estimating Annual Average Loads of Nonpoint Source Nutrient at the Watershed Scale

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Abstract The overloaded nonpoint source (NPS) nutrients in upper streams always result in the nutrient enrichment at lakes and estuaries downstream. As NPS pollution has become a serious environmental concern in watershed management, the information about nutrient output distribution across a watershed has been critical in the designing of regional development policies. But existing watershed evaluation models often encounter difficulties in application because of their complicated structures and strict requirements for the input data. In this paper, a spatially explicit and process-based model, Integrated Grid's Exporting and Delivery model, was introduced to estimate annual in-stream nutrient levels. Each grid cell in this model was regarded as having potentials of both exporting new nutrients and trapping nutrients passing by. The combined nutrient dynamics of a grid is mainly determined by the grid's features in land use/land cover, soil drainage, and geomorphology. This simple-concept model was tested at some basins in north Georgia in the USA. Stations in one basin were used to calibrate the model. Then an external validation was employed by applying the calibrated model to stations in the other neighbor basins. Model evaluation statistics implied the model's validity and good performance in estimating the annual NPS nutrients' fluxes at the watershed scale. This study also provides a promising prospect that in-stream annual nutrient loads can be accurately estimated from a few public available datasets.

Keywords Spatially Explicit Model · Nonpoint Source Pollution · Annual Nutrient Load · Watershed Scale · IGED · Upper Chattahoochee River Basin · Spatial and Temporal Scales

1 Introduction

An overload of nutrients in surface waters, eutrophication, will lead to excessive plant growth and decay, especially favoring certain weedy species. This explosion of plants is capable of disrupting the normal function of the aquatic ecosystem and resulting in a range of ill effects—from diminished soil fertility to toxic algal blooms—and even the emergence of anoxic areas [46]. Aquatic ecosystems in lakes, rivers, and coastal estuaries have suffered nutrient overload across the world. In the USA, eutrophication of surface waters because of the excessive nitrogen and phosphorus inputs has long been of serious concern [14].

A characteristic of nutrient loading is that it is highly correlated with the nonpoint source (NPS) pollution, such as fertilizer application to cropland and the emission of wastewater from urban area. Even in countries where major point source nutrient pollution has been strictly controlled, scientific evidence shows that NPS pollution is still threatening the health of water resources [22, 34]. In the USA, this type of pollution is the leading cause of the deterioration of water quality, according to the US Environmental Protection Agency [44].

Even though the awareness of this issue is increasing, the understanding of NPS pollution is limited. A proper evaluation of its causes and consequences is still difficult because of its complex characteristics.

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Partly because of these limitations, many programs of best management practices have failed to produce measurable improvements in stream water quality despite considerable investments in them [20]. From this perspective, it appears that the dearth of estimation and prediction tools has become a bottleneck for taking effective actions in controlling NPS pollution. As pointed out in [18], the ability to reliably and cost-effectively assess NPS pollutants is of paramount importance. The goal of this study is to develop a conceptually simple and clear, spatially explicit, and process-based model to estimate the annual average NPS nutrient loading at the watershed scale.

On the topic of NPS nutrient production and transport, many studies have been done and a number of models have been developed over the past three to four decades. Deterministic models range from simple empirical regression equations to sets of complex differential equations, while stochastic models range from simple functional models to complicated mechanistic models [17, 18]. In recent years, distributed parameter and process-based models have become widely used to estimate NPS nutrient loading. Reviews for some commonly used models can be found in [8–11].

Although the existing NPS pollution models have some applicability in simulating nutrient production, three restrictive factors may still prevent them from being efficiently used to estimate the annual average nutrient loads along a river. First, the requirements of input can be prohibitive because most models need a significant amount of data and empirical parameters which may further produce difficulties in calibration and calculation. It was noticed that data requirements increase exponentially with the increase in watershed size [31], and this situation limits the applications of the existing models in large watersheds (e.g., [19]). Second, most models have very complicated structures in simulating many physical, chemical, and biological processes and factors. Because the processes controlling nutrient dynamics vary across spatiotemporal scales (e.g., [7]), a model committed to annual load estimation needs to consider processes and factors which are functioning in the appropriate scales. From a practical perspective, including more processes, into a model always produces more uncertainty and increases the possibility of error. It becomes more difficult to depict all processes accurately due to a lack of sufficient monitoring data, inadequate data needed to characterize input parameters, or insufficient scientific understanding [25]. Besides, it is more likely for a complicated model to contain components or submodels that have some inconsistency in concepts and assumptions [15]. Inconsistency such as conflicting assumptions can lead to unreliable but un-

detected simulation outputs [35]. It can also affect the model's predictive power because of the uncertainty emerged during model parameterization [4].

It was pointed out that parsimony should be one of the philosophical axioms that guide model design [29]. A model should have the fewest parameters possible and the parameters should be the easiest ones to infer from the observed data [17]. The complexity of a specific watershed simulation model is determined by its scale and its extent to which important processes are considered [31]. Whereas most models simulate nutrient interactions and processes at rather small scale levels, the scale that many scientific and watershed management problems focus on usually rests on the levels much higher [13, 41]. Approaches to making predictions about large-scale watersheds through recourse to small-scale process dynamics are fraught with significant difficulties [42]. Many low-level processes explicitly addressed in an existing process-based models may be aggregated or simplified if focal scales of an application are large in space and time. For instance, an empirical equation is good enough to estimate the annual nitrate flux in the Mississippi River [36]. In watershed management, it is also desirable to create more generic models that can be run on readily available input data and have the capability to estimate the long-term impact of NPS pollution and serve as a tool to assess the cumulative impacts of proposed land management policies [6, 12, 31].

2 Methodology

2.1 Model Framework

The complete and exact processes which affect nutrient fluxes are numerous and they function at different levels. It is impossible but fortunately not necessary to construct a holistic model addressing all processes. Instead, the key for a successful dynamic model is to appropriately simulate those predominant processes in a given scale. As mentioned above, the existing process-based NPS models usually have too many parameters and require a large amount of input data. Those complicated models are necessary in estimating NPS pollution at a finer spatial and temporal scale. But as scale increases, impact of the complex local and transient patterns is attenuated and other macroscale factors dominate the relationship between nutrient dynamic processes and the corresponding spatial patterns. When considering the annual watershed-scale NPS nutrient loads, many factors that have significant influences in finer scales fade away or need to be addressed in a different way.

The Integrated Grid’s Exporting and Delivery (IGED) model adopts the nutrient source-sink model framework which regards the change of nutrient levels along flow paths as the result of the nutrient exporting process and delivery process. Similar ideas have been found in several studies on this topic (e.g., [27, 33]). Different from the simplest source-sink model, which divides grid cells into two separate groups (source cells and sink cells), in the IGED model, each grid cell plays dual roles in nutrient dynamics. It can be both a source and a sink of nutrient. And the nutrient exporting potential and delivery effectiveness of the grids are attributed to several factors and determined by the relevant parameters which are spatially distributed. On one hand, a grid cell can export nutrients and its potential is mainly determined by the land use/land cover (LULC) type. On the other hand, this grid cell also has the potential to inhibit the nutrient’s creation or trap the nutrient passing by. The effectiveness of this mechanism mainly lies on the physiographic and soil features within this grid. The nutrient level of a grid is the combined result of the two processes above. At a specific grid in the river network, the nutrient level is the sum of upper stream nutrient loads from all flow

paths that reach this grid. Such a relationship can be expressed as follows:

$$L = \left(\sum_{j \in J} L_j + E_{\text{cell}} \right) \times r \tag{1}$$

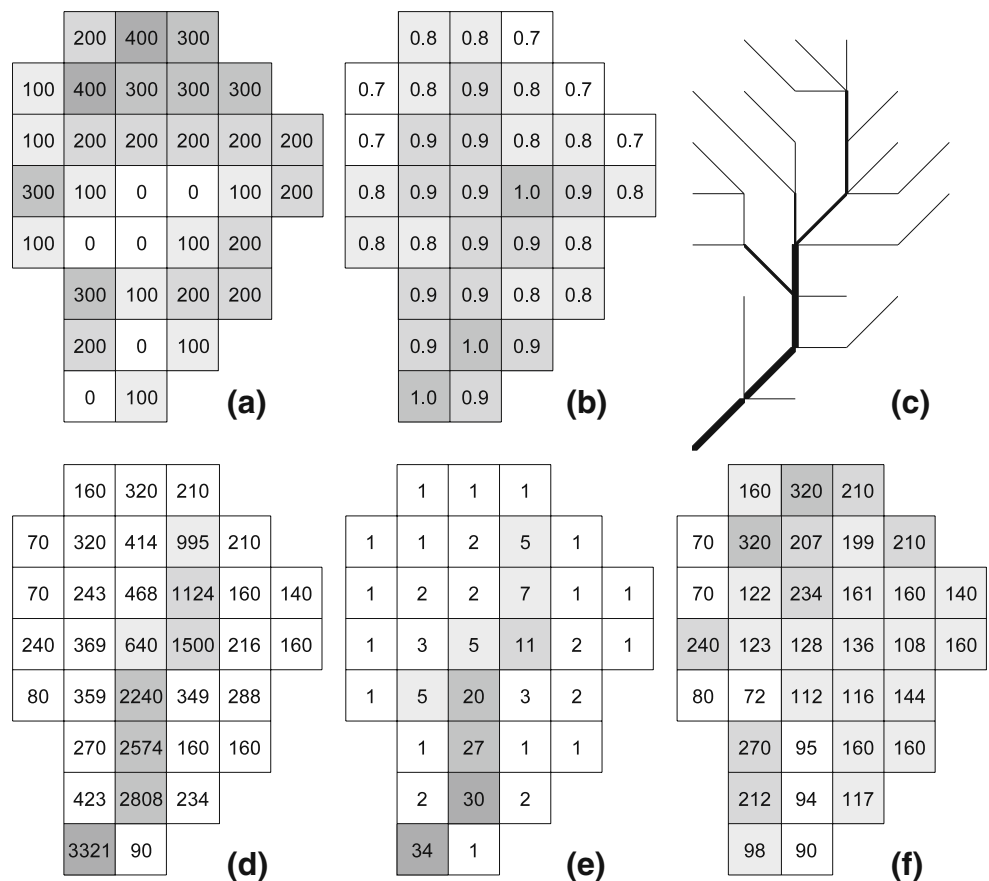
where L is the annual average nutrient load at a given grid. The first summation term represents the nutrient delivered from its neighbor grid cells, the set J . E_{cell} means the nutrient created in this grid cell or the grid’s potential export coefficient (see Section 2.2.1). Taking nutrient delivery process within this grid into consideration, the effective nutrient load is the product of the raw nutrient load and the local delivery ratio at this grid (r). The conceptual model of IGED is illustrated schematically in Fig. 1.

2.2 Model Elements

2.2.1 Export Coefficient

The concept of export coefficient and the relative models have long been used in examining nutrient loading [3, 28, 30, 33]. The export coefficient is always defined

Fig. 1 The conceptual model of IGED. The outline of each *subfigure* is the watershed boundary. **a** Distribution of potential export coefficient of grid cell E_{cell} (kilograms per hectare per year). It is determined by the LULC type of grid cell. **b** Distribution of the local delivery ratio r . It is determined by multiple characteristics of the focal grid cell, including slope, soil drainage condition, flow distance, and flow type. **c** Flow paths in the watershed. **d** Based on the flow path map (c) and the distribution of E_{cell} (a) and r (b), nutrient load level at each grid L is calculated. **e** Catchment area of each grid cell which in this example is in the unit of the cell number. **f** Catchment’s average nutrient load l (kilograms per hectare per year) which in this example is the quotient of L (d) and the cell number of catchment (e)



as the average total amount of pollutant loaded annually into a system from a defined area, usually in the unit of kilograms per hectare per year. Most water quality models used to estimate NPS pollution in watersheds require export coefficients as an important input. Because measuring export coefficients in the field for different LULC types is often cost-prohibitive, the values adopted in those models are normally acquired from the literature. However, it has long been pointed out that nutrient export can exhibit a wide range of variability in export coefficients due to the specificity of individual watersheds in climatology and physiography [3]. Using these values introduces big uncertainty to those models. More importantly, this measurement is scale-related, which means that the values can be largely different with a change in focal scales. For example, Lathrop et al. warned that coefficients derived from short-term or infrequent monitoring of small drainage areas can contribute to predictive variability [32]. While many reference values of export coefficients in the literature were derived from field measurements of plots which were always in irregular shapes and various sizes, it is hard to convert those values into the export coefficient at the cell grid scale.

To overcome the barriers mentioned above, an alternative concept of export coefficient is introduced in IGED, i.e., potential export coefficient. It can be regarded as the highest possible nutrient export of a certain LULC type in a defined area. It is the export coefficient in an environmental condition which is the most advantageous for the nutrient production. In some degree, the concept of potential export coefficient screens out the influence of environmental factors on nutrient exporting. In a region with similar meteorologic and environmental conditions, the value of potential export coefficient is assumed to be only determined by the LULC type. The actual nutrient production of a grid cell (or its opposite, the amount of nutrient retention) is abstracted into the concept of delivery ratio which integrates the influence of soil, slope, flow distance, and flow type on nutrient exporting effectiveness (see Section 2.2.2). Here, the potential export coefficient is coupled with a specific area scale, which in this study is a grid cell of the LULC raster image. For each main LULC type, the potential export coefficient of a grid cell E_{cell} is a model parameter which needs to calibrate.

2.2.2 Delivery Ratio

The traditional definition of delivery ratio is the fraction of nutrients in runoff that reaches surface waters

[21]. Several soil and physiographic factors were proved to be tightly related to its value: soil drainage property, slope, and distance that runoff travels to the stream. In the IGED model, the cumulative delivery ratio at a grid cell R is factored into a set of local delivery ratios of that grid and the grids downstream along the flow path:

$$R = \prod_{[\text{flowpath}]} r \quad (2)$$

The local delivery ratio r can be calculated as follows (adapted from [27]):

$$r = f_{\text{soil}} \times e^{-k_1 \times d \times f_{\text{slope}}} \quad (3)$$

where cell's soil factor f_{soil} addresses the influence of soil drainage characteristics on nutrient delivery effectiveness. It can be regarded as the fraction of nutrients that is not trapped by the soil in that grid cell. d is distance that water has to travel through the grid cell; f_{slope} is the slope factor which accounts for the impact of slope on nutrient exporting. It is calculated as (adapted from [27]):

$$f_{\text{slope}} = f_{\text{min}} + e^{-k_2 \cdot (s+k_3)} \quad (4)$$

where f_{min} is the minimum value for f_{slope} and S is slope gradient of the grid cell. f_{slope} varies between f_{min} (when s is close to 1 or the slope is close to vertical) and 1 (when s is 0 or the landscape is horizontally flat). k_1 , k_2 , and k_3 in these two equations are coefficients. Their values are given in [27]. To reduce the number of model parameters, we take those reference values for k_2 and k_3 (i.e., $k_2 = 16.1$ and $k_3 = 0.057$) and an adjusted value for k_1 (i.e., 0.0104). The adjustment of k_1 's value is because we apply this model to estimate nitrogen, not phosphorus. It is estimated based on the difference of delivery ratio between two nutrient elements mentioned in [47].

f_{soil} in Eq. 3 is a function of soil drainage types which determine the infiltration and resultant runoff. Giasson et al. provided a set of reference values of soil drainage factor for different soil drainage types when they identified and ranked land areas of potential phosphorous export to the New York City watershed [27]. Similar values are adopted in this study (Table 1). But because in their study these numbers were used to address the cumulative effects of soil drainage downstream, a configuration is added in the IGED model to convert them (symbolized by F_{soil} hereafter) into the soil factors of a grid cell, i.e., f_{soil} . Since the soil delivery factors listed in Table 1 are the resultant fraction after runoff flows over a long distance, it is the production of soil factors f_{soil} of the discrete grid cells along the

Table 1 Reference values of cumulative soil delivery factor F_{soil}

Soil drainage type	F_{soil}
Excessively drained	0.1
Somewhat excessively drained	0.2
Well drained	0.3
Moderately well drained	0.4
Somewhat poorly drained	0.7
Poorly drained	0.9
Very poorly drained	1.0

flow path. Suppose the fraction of nutrient approaches to the ratios in Table 1 after the runoff flows over a characteristic distance of D in each soil drainage type. Then f_{soil} can be given by a function of F_{soil} and D , such that:

$$f_{soil} = (F_{soil})^{\frac{d}{D}} \tag{5}$$

where d is the flow length in a grid cell and same as the d in Eq. 3. In our model, characteristic distance D is used as another model parameter that needs to be estimated in model calibration.

2.2.3 Flow Type

The characteristics of nutrient production and transportation in hillslope flow are largely different from those in gully flow. Comparing to the nutrient loss in hillslope flow, the amount of the loss in gully flow is so small that it is negligible in watersheds with a size similar to the ones in our study, i.e., the local delivery ratio for gully flow is 1. This conclusion can also be obtained from other studies (e.g., [1]). In the IGED model, two different flow types are defined by a catchment area threshold: When the catchment area is larger than the threshold value, the flow type is regarded as gully flow. Because the threshold value is always controversial and an arbitrary selection of threshold may influence the accuracy of a model’s estimation [2], we leave it as another model parameter to calibrate. It is defined as the number of grids N of the threshold catchment area.

2.3 Study Area and Data Sources

In this study, the Upper Chattahoochee River Basin (HUC 03130001) is chosen as the study area to calibrate the parameters in the model (Fig. 2). It covers the head-

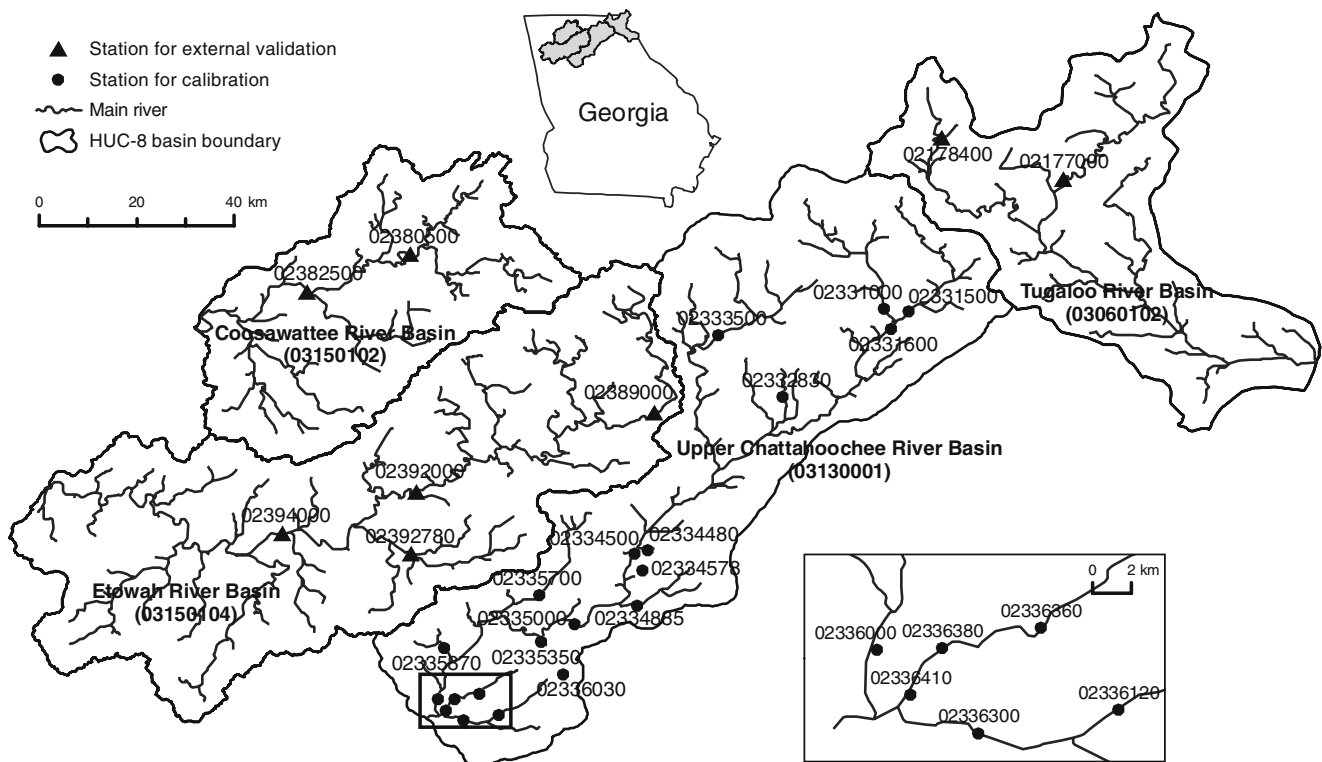


Fig. 2 Map of the study area. The stations in the Upper Chattahoochee River Basin are used for model calibration. The stations in the other three basins are used for model validation

waters of the Chattahoochee River down to the junction with Peachtree Creek. It is a part of the Chattahoochee River Basin and the larger Apalachicola, Flint, and Chattahoochee River basins. The Chattahoochee River originates from the Blue Ridge Mountains in the northeast corner of Georgia and flows southwest to Lake Sidney Lanier, then to the metropolitan Atlanta region where the southwest boundary of this basin is located. The area of this basin is about 4,040 km². It contains various landscapes, including the highly human-disturbed Atlanta metropolitan areas, remote wildness areas, and agricultural and pasture areas. As the major source of nutrient loading, NPS nutrient pollution in this basin has become of substantial concern because of the rapid population growth in this region and the importance of the Chattahoochee River in the state of Georgia. Nutrient overenrichment phenomena were found in some places of this basin, such as Lake Sidney Lanier and the Atlanta region. Studies also showed that in-stream nutrient concentrations and yields of this basin are tightly linked with the relevant land use types [24].

Three neighbor basins are used to test the model's validation. The basins include the Tugaloo River Basin (HUC 03060102), the Coosawattee River Basin (HUC 03150102), and the Etowah River Basin (HUC 03150104; Fig. 2). Comparing with the Upper Chattahoochee River Basin, these three basins have higher forest coverage and less developed areas. But the meteorologic and socioecological conditions are similar in all these basins.

The LULC data used to evaluate potential export coefficient is from the 1992 USGS National Land Cover Dataset (NLCD) for Georgia which was produced

mainly from Landsat TM images taken during 1989 to 1993 with a resolution of 30 m. There are 15 LULC types within the study area (Table 2). The DEM data with 1 arc sec resolution is from the USGS National Elevation Dataset. It is used to calculate the surface flow direction and construct the river network in the basins. The slope gradient raster data are also derived from this DEM data. Soil drainage-type data are obtained from the Soil Survey Geographic (SSURGO) database which was compiled at 1:12,000 scale by the Natural Resources Conservation Service of USDA. For convenience, the raw county-based polygon data are converted into raster format with the same resolution as the LULC data.

2.4 Model Calibration

The parameters in IGED are calibrated using the annual average nutrient loads during 1989 to 1993 at some stream monitoring stations in the Upper Chattahoochee River Basin (Fig. 2). To estimate the annual average nutrient loads of each station, a nonbias log-linear model [16] and its relevant FORTRAN program LOADEST [40] are adopted. LOADEST uses records of instantaneous stream flow and the corresponding nutrient concentration of a station to construct regression models. Then, ideally, with periodic stream flow measurements during a specific period, the regression models can estimate the average load of that station rather accurately. In this study, the stream flow and nutrient concentration data come from the USEPA STORET database. And we choose the unfiltered inorganic nitrogen, i.e., the sum of ammonia and nitrite–nitrate as the nutrients (with parameter codes of P00610 and P00630 in STORET, respectively) to test the performance of our model. They were the most frequently measured nutrient components at the stations and their sum (hereafter, nitrogen) can be regarded as a rough estimate of the total nitrogen data that was much less available in the database. Within the basin, stations with continuous and abundant measurement records are not plentiful. As shown in Fig. 2, only 20 monitoring stations meet the basic requirements of estimating annual nitrogen flux. They are used to calibrate the parameters in the model.

Besides the unknown potential export coefficients (E_{cell}) for all LULC types at the grid scale, two other parameters, characteristic distance of soil drainage D in Eq. 5 and the number of grids for gully flow threshold N , are estimated for the model. The best-fitting parameter set is obtained by the following procedure: Different sets of D and N distributed over a meaningful

Table 2 LULC types within the study area

NLCD code	Type
11	Open water
21	Low intensity residential
21	High intensity residential
23	Commercial/industrial/transportation
31	Bare rock/sand/clay
32	Quarries/strip mines/gravel pits
33	Transitional
41	Deciduous forest
42	Evergreen forest
43	Mixed forest
81	Pasture/hay
82	Row crops
83	Small grains
91	Woody wetlands
92	Emergent herbaceous wetlands

wide range are constructed. N varies from 20 to 1,000 and D varies from 50 meters to 500 m. For each set of D and N , the simulated annealing optimization method is applied to find the set of E_{cell} values that gets the minimum root of mean squared error (RMSE) with the restriction that all E_{cell} values are nonnegative. RMSE is defined as follows:

$$RMSE = \sqrt{\frac{1}{n} \times \sum_{i=1}^n (l_i - \hat{l}_i)^2} \tag{6}$$

where n is the number of the qualified stations, 20 in our case. l_i (in kilograms per hectare per year) is the annual average load estimated for the watershed of each station, and \hat{l}_i (in kilograms per hectare per year) is the simulated annual average load based on the given parameter set. The parameter set with the lowest RMSE is adopted in the calibrated model. The performance of IGED is then tested in the external validation procedure.

2.5 Model Validation

To test IGED’s validation, we search for all other adequate stations in the basins nearby which are in the same meteorologic and socioecological conditions as the Upper Chattahoochee River Basin. Eight stations located in three other neighbor basins are identified and used for external validation (Fig. 2). The annual average loads for these stations are estimated using LOADEST program same as described above. These values are then compared with the results of the calibrated IGED model.

Some commonly used model evaluation statistics are reported. Besides the RMSE, another one is the Nash–Sutcliffe model efficiency coefficient NSE:

$$NSE = 1 - \frac{\sum_{i=1}^n (l_i - \hat{l}_i)^2}{\sum_{i=1}^n (l_i - \bar{l})^2} \tag{7}$$

Two other recommended model evaluation statistics [37] are also reported. They are percent bias PBIAS and RMSE observations standard deviation ratio RSR:

$$PBIAS = \frac{\sum_{i=1}^n (l_i - \hat{l}_i)}{\sum_{i=1}^n l_i} \times 100\% \tag{8}$$

$$RSR = \sqrt{\frac{\sum_{i=1}^n (l_i - \hat{l}_i)^2}{\sum_{i=1}^n (l_i - \bar{l})^2}} \tag{9}$$

3 Results

Parameter sets with the lowest ten RMSEs in the calibration procedure are reported in Table 3. The lowest RMSE (1.302 kg/ha/year) is found when N is 100 and D is 200 m. In other words, when the catchment area contains more than 100 grid cells, the surface flow is regarded as a gully flow. And the cumulative soil delivery factors listed in Table 1 are based

Table 3 Parameter sets with the lowest RMSEs

Flow-type threshold N^a	Characteristic distance D (m)	Potential export coefficient E_{cell} (kg/ha/year)							RMSE (kg/ha/year)
		LULC21	LULC23	LULC33	LULC81	LULC82	LULC85	Others	
100	200	30.3	155.3	230.4	163.0	420.3	74.7	0.0	1.302
100	300	37.6	133.7	177.8	135.3	377.0	26.8	0.0	1.309
75	200	20.8	139.0	191.9	149.3	339.5	122.6	0.0	1.309
100	400	40.3	122.2	155.5	124.1	340.8	13.2	0.0	1.320
800	500	46.4	340.1	380.1	166.6	1,550.9	409.1	0.0	1.322
900	500	0.0	459.0	368.3	157.1	1,699.8	586.7	0.0	1.325
50	200	7.3	130.8	148.3	123.1	296.8	151.1	0.0	1.326
100	500	41.1	116.3	145.9	118.2	309.3	0.0	0.0	1.329
800	400	47.1	349.4	406.6	173.5	1,651.2	424.9	0.0	1.329
900	400	0.0	471.9	397.9	165.0	1,797.2	595.5	0.0	1.334

^aIn the unit of the number of grid cells

on a characteristic flow distance of 200 m. As expected, Table 3 indicates that row crops and transitional land use type (LULC codes 82 and 33, respectively) have the highest inorganic nitrogen potential export coefficients, followed by pasture/hay, and commercial/industrial/transportation types (LULC codes 81 and 23, respectively). The high value for transitional areas implies that deforestation and urbanization have a serious influence on nitrogen levels in the river, with possible disastrous consequences. For forest land covers (LULC codes 41, 42, and 43) and water-dominated land covers (LULC codes 11, 91, and 92), the nitrogen export is negligible. Nitrogen levels created from residential areas with LULC codes of 31 and 32 are also too low to affect the nitrogen levels in a river.

The calibration results for the 20 stations in the Upper Chattahoochee River Basin are plotted in Fig. 3 and listed in Table 4. The external validation results are shown in Fig. 4 and Table 5. The raw RMSE for the validation stations is 1.337 kg/ha/year. However, among the eight external validation stations, there is an obvious outlier (ID 02392780) for which the simulated load level is much higher than the estimated value (Fig. 4). This big residual probably results from the existence of a large wastewater treatment plant only about 2 miles away above the station in Woodstock, Georgia. Because the plant may have significantly reduced the fluxes of pollutants in the river, this station is not suitable for use as a validation sample. When taking

Table 4 Stations used to calibrate the model and the calibration results for the annual average nitrogen load

Station	Drainage area (km ²)	Measured ^a (kg/ha/year)	Simulated (kg/ha/year)
02331000	388.5	1.45 (0.25)	1.96
02331500	404.0	5.01 (0.33)	5.80
02331600	815.8	3.99 (0.20)	3.86
02332830	47.4	9.99 (0.42)	7.71
02333500	396.3	3.65 (0.12)	2.69
02334480	24.2	4.51 (0.62)	3.45
02334500	2,745.4	2.29 (0.10)	3.86
02334578	13.1	2.83 (0.12)	3.74
02334885	121.7	4.73 (0.22)	3.67
02335000	3,030.3	2.92 (0.20)	3.89
02335350	23.0	3.00 (0.13)	4.73
02335700	186.5	3.73 (0.11)	5.59
02335870	75.6	3.94 (0.18)	3.41
02336000	3,755.5	4.08 (0.24)	4.03
02336030	3.7	11.18 (2.81)	11.09
02336120	90.1	8.37 (1.69)	6.07
02336300	224.8	5.11 (0.13)	6.74
02336360	68.9	7.92 (1.73)	5.97
02336380	90.1	4.06 (0.34)	5.43
02336410	97.6	5.23 (0.68)	5.41
RMSE (kg/ha/year)			1.302
R^2			0.73

^aThe standard error is given in parenthesis

out this outlier, the RMSE reduces to 0.393 kg/ha/year and the NSE statistic, as an equivalent of R^2 for a linear regression model, equals 0.77 (Table 5). Compared with

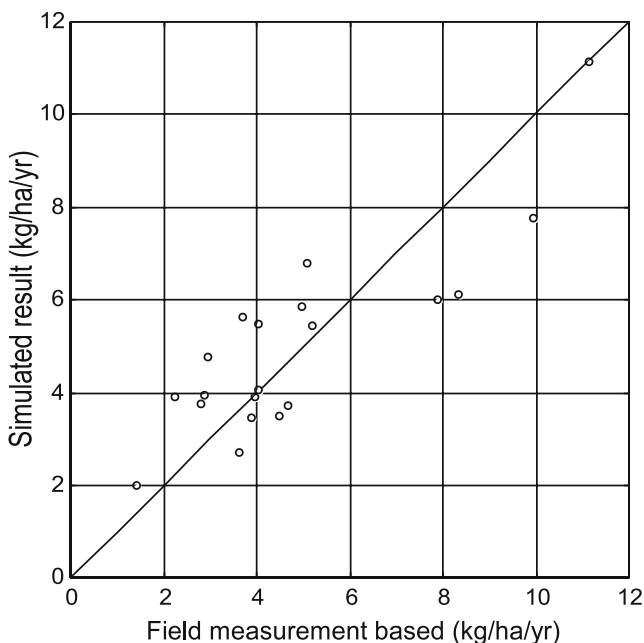


Fig. 3 Model calibration result

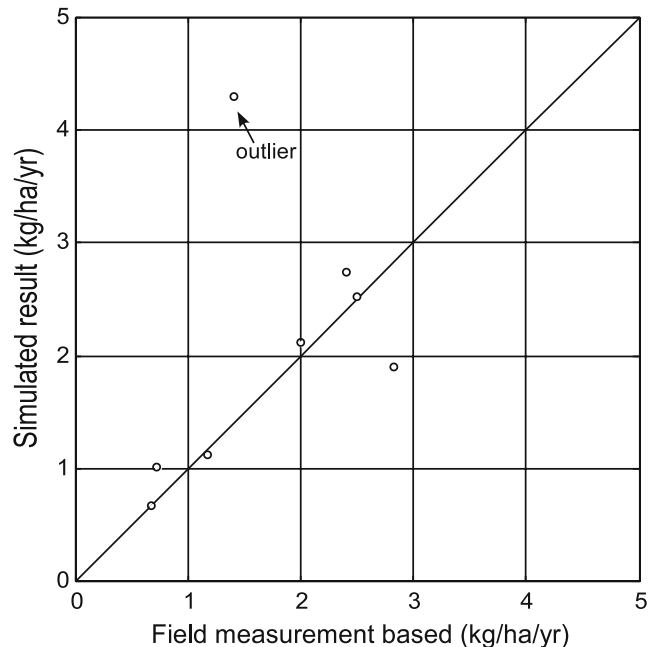


Fig. 4 Model external validation result

the performance of some other process-based models (e.g., [9, 37]), the IGED model shows a promising potential in predicting and estimating nutrient’s annual average load. NSE, PBIAS, and RSR all imply that the performance of this model can be rated as “very good” for the designed applications according to the rating standards in [37] for monthly nutrient load estimation (no standard available for annual load estimation). Furthermore, the stations used in this validation process are outside of the basin where the calibration-used stations locate. The total area of the basins they represent is 9,564 km² (Table 5). It implies that a calibrated IGED model may be applicable for a much larger area if it is under the similar meteorologic and environmental conditions to the calibration-used basin.

Among the six nitrogen-source land use types, the two agricultural types (LULC codes 81 and 82) have the lowest cumulative delivery ratios while the two residential types (LULC codes 21 and 23) are the highest in cumulative delivery ratio (Fig. 5). It is apparent that this difference is due to the different spatial distribution patterns and different hydrological characteristics of nitrogen transportation between the impervious surface of urban areas and the soil or vegetative surface of agricultural regions. The cumulative delivery ratio also varies within each LULC type, ranging from 0 to 1. The distribution of cumulative delivery ratio in each LULC type has a similar positive skew pattern (Fig. 5).

Table 5 Stations used in external validation and the results of external validation for the annual average nitrogen load

Basin Station	Drainage area (km ²)	Measured ^c (kg/ha/year)	Simulated (kg/ha/year)
03060102			
02177000	536.1	0.74 (0.12)	0.99
02178400	146.3	0.70 (0.34)	0.65
03150102			
02380500	611.2	2.84 (0.13)	1.88
02382500	1,349.4	2.01 (0.40)	2.10
03150104			
02389000	277.1	1.20 (0.26)	1.10
02392000	1,587.7	2.51 (0.21)	2.50
02392780 ^a	360.0	0.65 (0.12)	4.29
02394000	2,898.2	2.43 (0.07)	2.73
RMSE (kg/ha/year) ^b			0.393
NSE ^b			0.77
PBIAS ^b			3.7%
RSR ^b			0.48

^aOutlier

^bAfter the outlier is removed

^cThe standard error is given in parenthesis

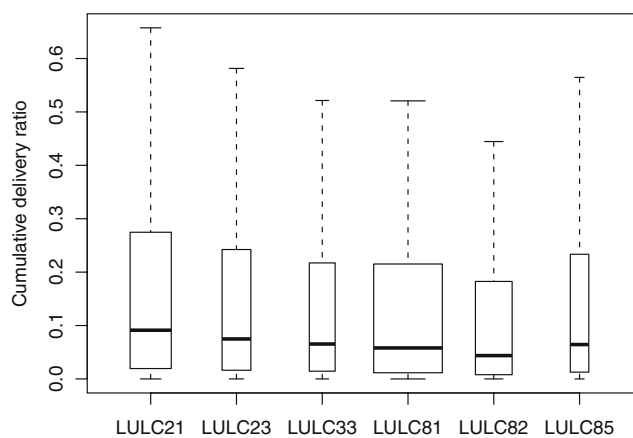


Fig. 5 Box plots of the cumulative delivery ratios by six nitrogen-source LULC types. The end of upper whisker in each plot is 1.5 interquartile range (IQR) of the upper quartile. The extreme values are not shown for virtual purpose. The width of the boxes represents the amount of grid cells of that LULC type. The statistics is based on the entire Upper Chattahoochee River Basin (HUC 03130001)

4 Discussion

In some predictive regression models of NPS nutrient loads, landscape composition information or the proportions of different LULC types are the main predictors, such as the pollutant budget estimation model in the WATERSHEDSS system [39], the export coefficient model adopted in the PLOAD model [43], and the method of estimating nutrient influx from headwater catchment in the SPARROW model [1]. Comparing with a complex, data intensive, spatially distributed mechanistic model, this type of models can offer a quick estimation of lumped basin nutrient loads and therefore is usually used as scoping models [23]. However, the effectiveness of nutrient production and transportation is affected by many environmental factors along the flow path. To better predict the loads or to estimate spatial distribution of loading intensity, heterogeneity within each land cover needs to be considered and a spatially explicit model is more appropriate.

The concept of cumulative delivery ratio introduced in the IGED model is equivalent to a weight of the potential export coefficient for each grid cell. The weighting is based on several spatially distributed soil and physiographic factors. As a result of weighting, the effective nitrogen contribution from a grid cell is greatly different from its potential export coefficient in amount (Fig. 6). From this perspective, the total nitrogen loads at an outlet depend on the amount of grid cells, the potential export coefficient, and the mean weight for each nitrogen-source land use type.

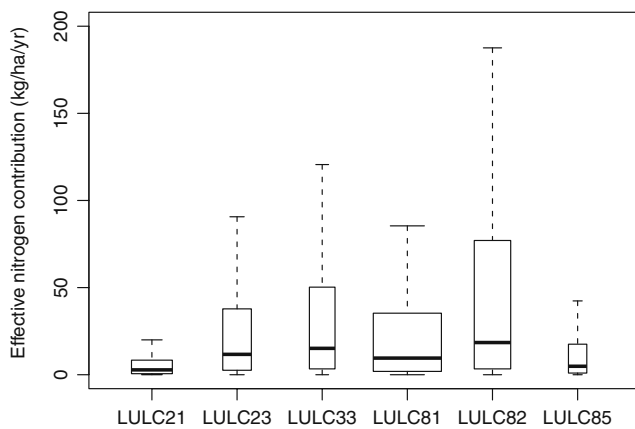


Fig. 6 Box plots of the effective nitrogen contribution at the scale of grid cell by six nitrogen-source LULC types. The end of *upper whisker* in each plot is 1.5 IQR of the upper quartile. The extreme values are not shown for virtual purpose. The width of the *boxes* represents the amount of grid cells of that LULC type. The statistics is based on the entire Upper Chattahoochee River Basin (HUC 03130001)

Although IGED shows a satisfactory estimation and predictive power, the potential export coefficients for some LULC types appear not to be consistent with common experiences. More specifically, E_{cell} s for high intensity residential and quarries/strip mines/gravel pits (LULC codes 22 and 32, respectively) are both zero while E_{cell} of high intensity residential type is even lower than that of cells with low intensity residential land use (LULC code 21; Table 3). For the type of quarries/strip mines/gravel pits, the reason that produces this calibration result is because this classification in all the watersheds is so small that no convergent value is acquired for its E_{cell} in the numerical optimization process. So its E_{cell} value of zero may not reflect the reality.

Regarding the high intensity residential type, its low E_{cell} value is believed to be reasonable. In those areas, most nutrient outputs is conducted into the municipal sewer systems and then to the wastewater treatment plants. In many cases, the nutrient pollutants have been largely removed by the time the treated water is discharged into rivers and the discharge sites may be far from the source areas. Same as many other nutrient loading estimation models, this factitious factor is not explicitly considered in the IGED model; but its effect is reflected by the zero value of E_{cell} for high intensity residential grid cells.

The IGED model developed in this study is based on several simple concepts which have long been discussed and tested. Two special configurations in IGED make it applicable to a wider area and have a rather high predictive power. First, rather than directly adopting

reference values from other literature, we used a numerical optimization method to calibrate the model's parameters before applying the model to predicting. This is not only because of the large range of each parameter found in the literature and the environmental specificity of the study area but more fundamentally because some parameters, including the soil drainage factor and nutrient export coefficient, are scale sensitive, but their scale effect was not fully discussed in the literature. Under different scales, values of these parameters are incommensurable, e.g., the potential export coefficients in Table 3 and the values found in [33]. Scale-specified values of the parameters have to be calculated from scratch.

Secondly, every parameter calibrated in IGED corresponds to a definite notion in the conceptual model. No additional scalar or intercept parameter is included in the model. This setting excludes uncertainty which comes from any unclear source and ensures the model's robustness and parsimony to some degree. By contrast, complex distributed models are often difficult to parameterize, interpret, and verify [5, 7].

On the other hand, as Table 3 shows, parameters such as the gully flow threshold and the soil drainage characteristic distance have significant impacts on the optimization results of the potential export coefficients and the overall RMSE. Because their influences on the estimation results are nonlinear and sensitive to the river network structure, theoretically only spatially distributed models are suitable to simulate their impacts. Simple linear regression models or spatially lumped models may yield incorrect predictions or inferences if the landscape heterogeneity is apparent in a watershed [45].

Because the nutrient dynamics involve numerous factors and processes, many models and methods of estimating in-stream nutrient loads coexist and compete with each other. Studies from different disciplines have been done to examine the processes and factors from their own perspectives. To construct a process-based model, one of the most important tasks is to identify processes that are most relevant to the specific application and find out essential factors that determine the behaviors of these processes. Taken as a whole, the processes and factors identified in different studies have suggested a hierarchical structure of the nutrient dynamics issues. A certain process or factor usually functions just in a limited range of scale. For the processes and factors at a lower level, their roles can always be integrated into one or more processes and factors at a higher level. The issue of spatial scale in NPS pollution assessment is extremely important [6], as is the temporal scale. From a practical perspective,

whether including a process or a factor into a process-based model largely depends on the scale in which this process or factor functions. A model needs to represent the key processes expected to occur at the scale for which the model is applied [38]. Including trivial processes or factors is not only unnecessary and making simulation much more complicated, it is also misleading and may bring in more uncertainty.

This study focuses on the nutrient fluxes among watersheds from rather small scales up to an HUC-8 basin. Its focal temporal scale is the annual average level. In this case, a factor or process that does not vary within these specific spatial and temporal scales can be neglected. For example, the temperature and atmospheric nitrogen deposition have important impacts on the nutrient yields in a regional, continental, and global scale or over a long-term period. However, because the variability of these factors is not large and does not have a significant influence within an HUC-8 basin in a few years, it can be regarded as an implicit environmental constant instead of a functional factor. Similarly, daily precipitation condition can be a decisive factor for the daily nutrient fluxes and its variability within a basin can be great. However, if the variance of annual precipitation is stationary over years and across the study area, the precipitation factor can also be considered as an environmental constant. In future studies, additional work on validating the model's capabilities is needed to test the performance of IGED in other different types of basins. Because of its simple framework, IGED is flexible in taking more factors into consideration. For example, the effect of varied precipitation across a study area may be quantified as a factor of potential export coefficient.

The major limitation of the IGED model is that it assumes that the NPS nutrient loading mainly comes from overland flow. Contributions of nutrient loading from the groundwater flow and interflow are not considered in the model. This simplification is reasonable for the basins in our study areas because the surface watersheds are essentially coincident with the ground watersheds and they can be considered as a single and inseparable system [26]. If the spatial variability of these contributions is improperly ignored, especially in the area where the amount of nutrient loading from those sources becomes comparable to or even exceeds the amount from overland flow, the bias of this model could become large. Another limitation of this model is that the current calibration method is a combination of numerical optimization approach (for potential export coefficients) and enumeration (for gully flow threshold and characteristic distance of soil drainage). It is not very efficient and it does not guarantee that the para-

meter set result is the real optima, but in the proximity of the optima.

5 Conclusions

Estimating the NPS nutrient loading is always the prerequisite for optimizing management practices in the reduction in-stream nutrient levels. However, the accuracy and the availability of input datasets are always two barriers to applying complicated spatially explicit and process-based models of the NPS nutrient loading. The IGED model uses only a few of public available datasets and some simple concepts about nutrient dynamics in the runoff to estimate the in-stream nutrient flux with an acceptable accuracy. This model is designed for specific spatial and temporal scales, namely the annual average load levels at the watershed scale varying from rather small catchments up to HUC-8 basins. Under these scales, the IGED model considers the LULC conditions, soil drainage conditions, and several physiographic features as dominant factors affecting the nutrient exporting and delivery efficiency in a grid with a resolution of several tens of meters.

The calibration results in the Upper Chattahoochee River Basin indicate that row crops, transitional, pasture/hay, and commercial/industrial/transportation areas are the dominant potential sources of inorganic nitrogen in the study area. Due to the spatial variability of some factors including physiographic, soil drainage features, and the distance to gully flow streams, actual contribution to the river network from each grid may not be proportionate to its potential export coefficient. The low RMSE value and high NSE value in external validation results imply that the factors considered in the IGED model are appropriate and a calibrated model has a satisfactory performance in estimation and prediction. The IGED model also shows a promising potential in applicability because the calibrated model can be applied to a wider range of watersheds within the same environmental conditions as the calibration-used basin.

Overall, the IGED model is simple and clear in concept and structure. And it does not have a high requirement for input data. It offers a rapid, efficient, and economic method to estimate the distribution of annual nutrient outputs in basins. It is also possible to use this model as a simulation tool to evaluate the role of landscape spatial patterns on nutrient loading and the relationship between LULC change and in-stream nutrient enrichment. The model's performance highly depends on the optimization results of the parameter set in the model calibration stage. Improving

the calibration algorithm will be an important work in future studies. It is also recognized that more model validation work in different basins is needed to confirm the applicability of IGED. This study does not imply that this model can replace the existing models or is superior to others, but indicates the promising prospect of using a model with simple structure and concepts to estimate NPS nutrient dynamics in a high scale level.

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