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Patuxent Landscape Model. III. Model Calibration

A. Voinov, R. Costanza, T. Maxwell, and H. Vladich

Gund Institute for Ecological Economics, University of Vermont 590 Main Street, Burlington, VT 05405-0088
e-mail: alexey.voinov@uvm.edu

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Abstract—Using the LHEM/SME the Patuxent Landscape Model (PLM) was built to simulate fundamental ecological processes in the watershed scale driven by temporal (nutrient loadings, climatic conditions) and spatial (land use patterns) forcings. The model addresses the effects of both the magnitude and spatial patterns of land use change and agricultural practices on hydrology, plant productivity, and nutrient cycling in the landscape. The spatial resolution for the full Patuxent watershed is 1 km^2, while subwatersheds are analyzed at a 200×200 m resolution to allow adequate depiction of the pattern of ecosystems and human settlement on the landscape. The temporal resolution is different for various components of the model. We used a modular, multiscale approach to calibrate and test the model. Model results show good agreement with data.

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INTRODUCTION

Large drainage basins are composed of multiple smaller catchments. Each of these catchments contains a heterogeneous collection of land uses, which vary in composition and spatial pattern (structure) and thus differ in functions such as nutrient retention. Two problems arise from this heterogeneity that present major challenges to both research and management. First, variation in structure and function inevitably prevents true replication in intensive field studies that attempt to relate landscape function to landscape structure. Second, variation among land uses within watersheds makes it difficult to directly extrapolate among spatial scales. Even though drainage basins can be broken down hierarchically into smaller catchments based on topography, "scaling up" from intensive catchment studies is not a linear additive process because of differences among catchments and interactions between adjacent land uses. Management of water quality over large drainage basins must address both problems with innovative methods synthesizing data from intensive experimental studies on a few watersheds, then extrapolating important generalizations to larger drainages using modeling techniques.

The Patuxent Landscape Model (PLM) was designed to serve as a tool in a systematic analysis of the interactions among physical and biological dynamics of the Patuxent watershed (Maryland, USA) (Fig. 1), conditioned on socioeconomic behavior in the region. A companion socioeconomic model of land use dynamics in the region is developed to link with the PLM to provide a means of capturing the feedbacks between ecological and economic systems (Fig. 2). By coupling the two models and exchanging information and data between them the socioeconomic and ecological dynamics can be incorporated. Whereas in most ecosystem models, the socioeconomic development is fed into the model in the form of scenarios or forcing functions, a coupled model can explore dynamic feedbacks, adjusting the socioeconomic change in response to the ecological perturbations.

To run the ecological and economic modules in concert, we need to account for specifics of both modules in their design and make assumptions about how the information will be exchanged. In particular, the spatial representation of both should be matched such that land use or land cover transformations in one module can be communicated to the other one directly inside the model. In this case it would be difficult to employ the approach based on spatial aggregation to larger units, called elementary landscapes, elementary watersheds, elementary areas of pollution or hillslopes [1–4], which are considered homogeneous and form the basis for the hydrologic flow network. In these models the boundaries between spatial units are fixed and cannot be modified during the course of the simulation. A more mechanistic approach seems to be better suited when the landscape is aggregated as a grid of relatively small homogeneous cells and process-based simulations are run for each cell with relatively simple rules for material fluxing among nearest neighbors [5–9]. This fairly straightforward approach requires extensive spatial data sets and high computational capabilities in terms of both storage and speed. However it provides for quasi-continuous modifications of the landscape, where habitat boundaries may change in response to socioeconomic transformations.

The economic component for the PLM was presented elsewhere [10–13]. Here we focus on describing the construction of the ecological component, paying special attention to those aspects of the model that were stipulated by the integrated fashion of the entire

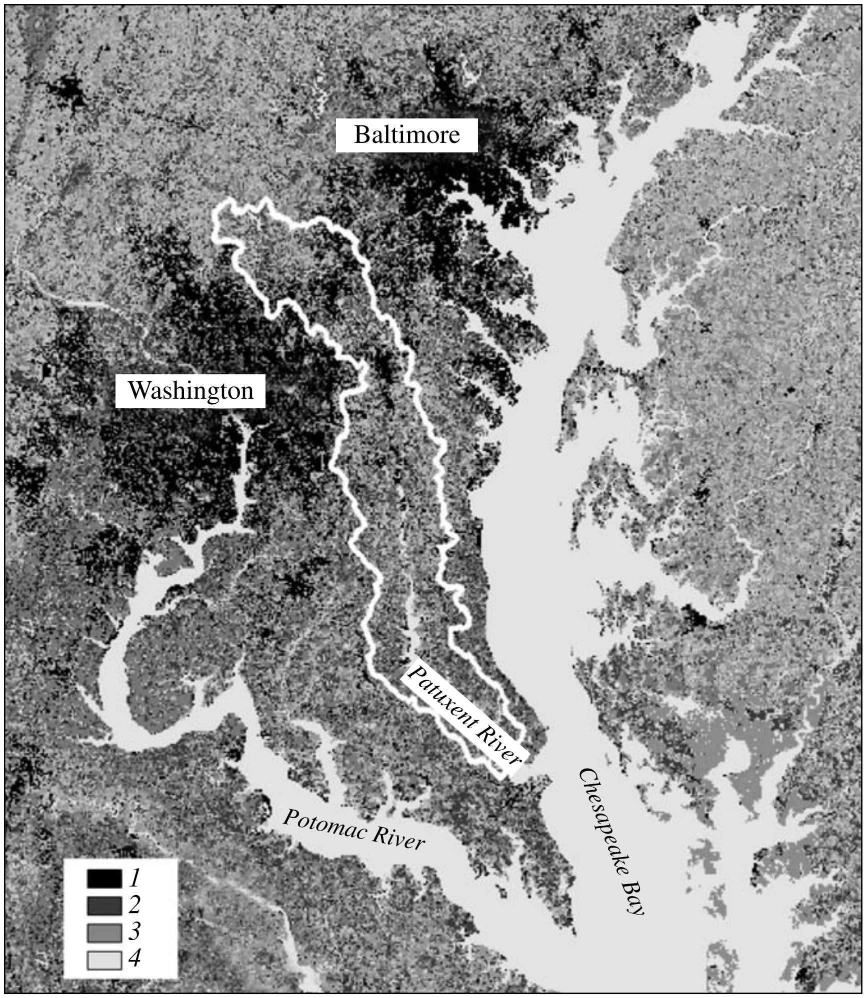

Fig. 1. Location of the Patuxent watershed. Background map is based on NOAA C-CAP land cover data of Chesapeake Bay Watershed 1988/89. Resolution is 30 m. (*1*) Urban territories; (*2*) agriculture; (*3*) forest/marsh; (*4*) water.

research effort. We first outline the overall model design in terms of its spatial, temporal and structural organization. Then we look at the single-cell (local) ecological processes. Next we consider the spatial implementation of the model and discuss some aspects related to scale and resolution. We conclude with a review of the results and potential applications of the model.

MODEL STRUCTURE

The PLM may be considered as an outgrowth of the approach first developed in the Coastal Ecosystem Landscape Spatial Simulation (CELSS) model [5, 6], and later applied to a series of wetland areas, the Everglades clearly being the most sophisticated example [14, 15]. The modeled landscape is partitioned into a spatial grid of square unit cells (ranging in this application from 2352 to 58905 square unit cells). The model is hierarchical and modular in structure, incorporating the ecosystem-level unit model that is replicated in each of the unit cells representing the landscape (Fig. 3). With this approach, the model builds on the format of a raster-based geographic information system (GIS), which is used to store all the spatially referenced data included in the model. Thus, the model can be considered an extension of the analytical function of a GIS, adding dynamics and knowledge of ecological processes to the static snapshots stored in a GIS.

Although the same unit model runs in each cell, individual models are parameterized according to habitat type and georeferenced information for a particular cell. The habitat-dependent information is stored in a parameter database, which includes initial conditions, rate parameters, stoichiometric ratios, etc. The habitat type and other location-dependent characteristics are referenced through links to GIS files. In this sense, the PLM is one of several site-specific ecological models that are process-based and are designed to apply to a range of habitats. Some other models within this category are CENTURY [16], TEM [17], and BIOME-BGC [18]. All these models can be adapted to a partic-

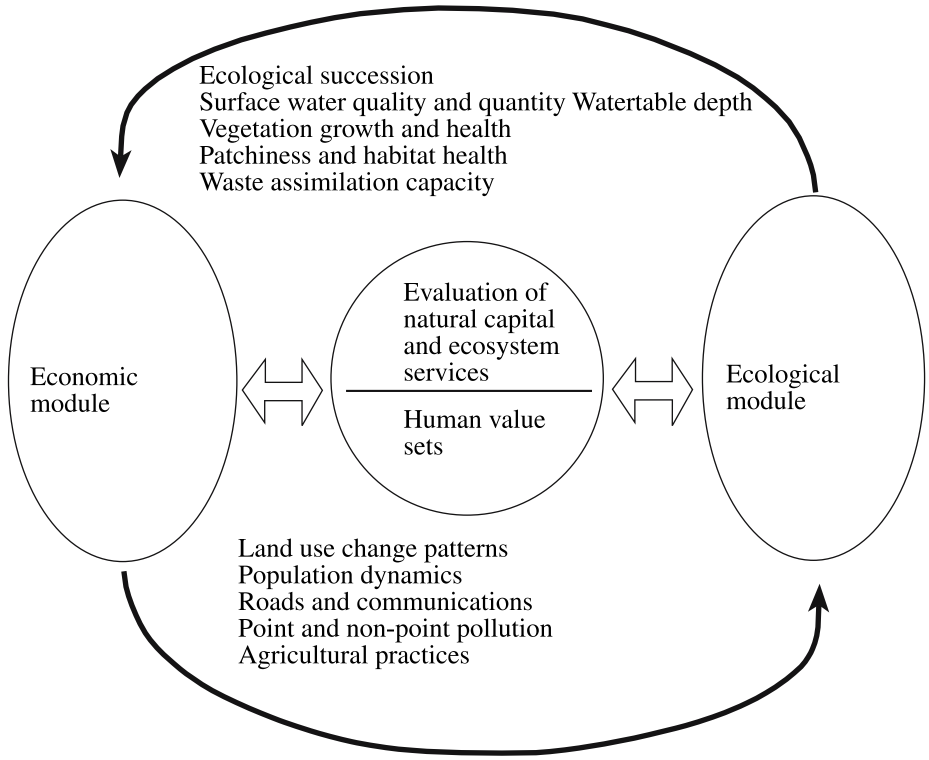

Fig. 2. Relationships and linkages between the economic and ecological subsystems. The ecological and the economic modules provide essential feedbacks that are instrumental to create a realistic system of values and to learn to measure these values.

ular site through parameterization of initial stocks and flux rates among various ecosystem components. These models vary in complexity and capabilities, which makes one model more suitable for certain applications than others. As a rule of thumb, more complex models will resolve issues in more detail, but are more difficult and time-consuming to calibrate, run, and interpret [19]. The PLM aims for an intermediate level of complexity so that it is flexible enough to be applied to a range of ecosystems but is not so cumbersome that it requires a supercomputer.

The unit models in each cell exchange matter and information across space. The horizontal fluxes that join the unit models together are defined by surface and subsurface hydrology. Alternative horizontal fluxes could be movement of air, animals, and energy such as fire and tidal waves although at this stage the PLM fluxes only water and entrained material. The spatial hydrology module calculates the amount of water fluxed over the surface and in the saturated sediment. The fluxes are driven by cell-to-cell head differences of surface water and saturated sediment water, respectively. Water fluxes between cells carry dissolved and suspended material. At each time step, first the unit model updates the stocks within each cell due to vertical fluxing and then cells communicate to flux matter horizontally, simulating flows and determining ecological condition across the landscape.

Figure 4 presents how the various modeled events are distributed in time when simulated in the PLM. The model employs a time step of 1 day so that most of the ecological variables are updated daily. However certain processes can be run at longer or shorter time steps. For example some spatial hydrologic functions may need an hourly time step, whereas certain external forcing functions are updated on a monthly or yearly basis. This explicit spatial and flexible temporal design of the PLM ecological module is instrumental for a linkage with a companion economic model that predicts the probability of land use change within the seven counties of the Patuxent watershed [11]. The economic model allows human decisions to be modeled as a function of both economic and ecological spatial variables. Based on empirically estimated parameters, spatially heterogeneous probabilities of land conversion are modeled as functions of predicted land values in residential and alternative uses, and costs of conversion. Land value predictions are modeled as functions of local and regional characteristics. The predictive model of land use conversion generates the relative likelihood of conversion of cells, and thus the spatial pattern of greatest development pressure. To predict the absolute amount of new residential development, the probabilistic land use conversion model is further combined with models of regional growth pressure. As a result a new landuse map is generated and fed into the ecological model on a yearly basis.

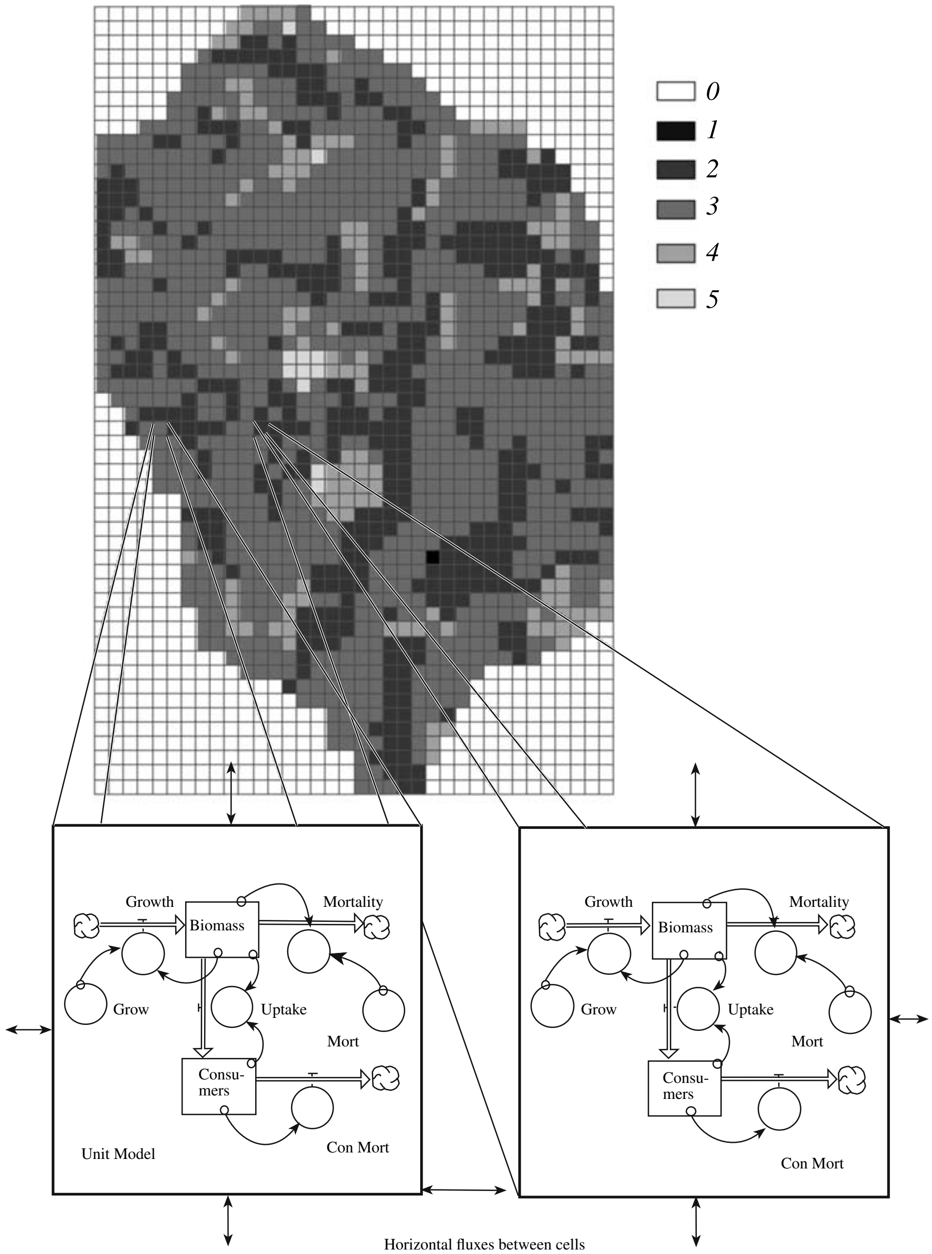

Fig. 3. Spatial organization of the Patuxent watershed model. The unit model is replicated in each of the cells on the study area. Different habitat types are characterized by different parameters in the unit model. Hydrological fluxes connect the unit models horizontally. (1) water; (2) forest; (3) agricultural; (4) rural resident; (5) urbanized;

GEOGRAPHIC AND TIME SERIES DATA

A variety of spatially and temporally disaggregated data is required to develop and calibrate the model. The database we have assembled is partially described in Appendix 1. The model database contains the data, which drive the model forcing functions, parameterize equations, and provide calibration and verification data for adjusting model parameters and comparing model output to the real system. The database was developed from extensive data sets collected for the Patuxent watershed by various governmental agencies, academic institutions, and research programs ([20–22, 23]) . Existing data for the local region were supplemented with broader regional databases where appropriate.

Much of the available data is at a temporal or spatial resolution that is different than we would like, so we sometimes employed data aggregation or interpolation techniques to adjust the data. For example, maps of model driving forces such as precipitation are created as the model runs by interpolating time series data from the set of 7 meteorological stations distributed throughout the area. Land use data are aggre-

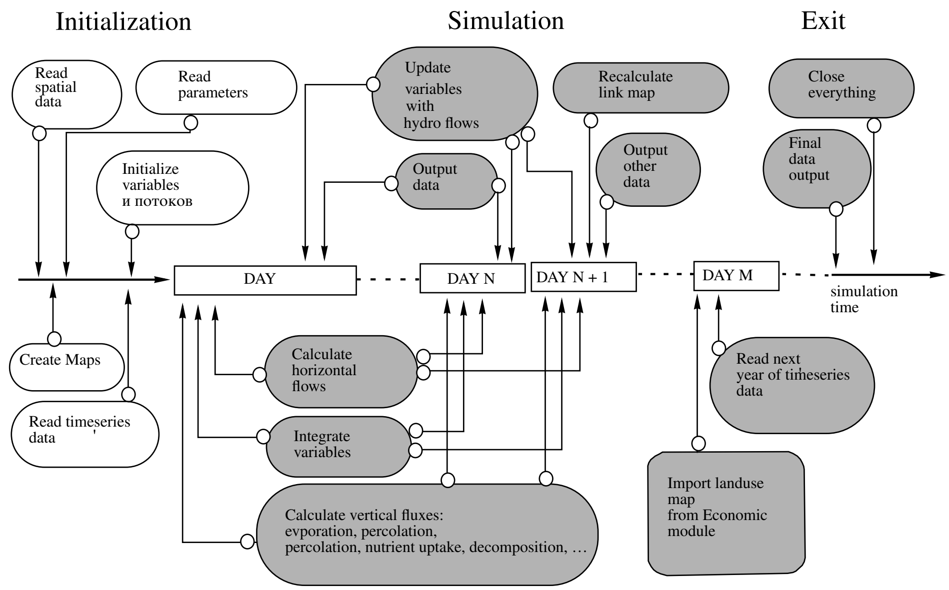

Fig. 4. Temporal course of events in PLM. SME offers certain flexibility in scheduling simulation events. Individual time steps can be assigned to different modules.

gated from higher resolution maps with more categories than we need. Another example is our use of elevation data (1 : 100000, with 1-m vertical resolution) combined with river network data (Maryland Office of Planning) to improve the watershed boundary and shoreline delineation.

Spatial (GIS) data include several types of data sets. One set of maps describes initial conditions, such as land cover, elevation, soil type, bathymetry, and groundwater elevation. Other spatial data developed from satellite images provide a time series of estimated ecological conditions, which are used for calibration purposes (e.g. Normalized-Difference Vegetation Index (NDVI, [24])). Watershed boundary, slope, aspect, and study area map layers were developed with the watershed basin analysis program in GRASS—Geographic Resources Analysis Support System [25], and later refined using similar functionality in ArcInfo@. Figure 5 shows the basic spatial coverages that have been employed in the PLM and some of the derived layers that were also essential for the hydrologic module. Spatial fluxes of surface water in watershed models are predominantly driven by the elevation gradient.

In addition to the meteorological time series data, which are used to map daily weather conditions, time series data are used to provide other information at specific points in the landscape. For example, point source discharges are used to introduce materials at specific points in the landscape. Hydrologic point time series data (stream flow, surface and ground water quality) are used for calibration in the non-tidal portions of the streams.

Specific rate constants are generally functions of spatial or habitat characteristics, such as soil or vegetation type. Habitat-dependent parameters include growth coefficients, uptake rates, and seasonal controls. About half of these data are specific to the Patuxent watershed with the remainder derived from a more general database or literature sources.

ECONOMIC LAND USE CONVERSION (ELUC) MODEL

Spatially explicit data on property sales and many of the economic and ecological characteristics of areas in spatial proximity to these sales was available for the seven counties encompassing the Patuxent watershed. This allowed land use change to be empirically modeled in a spatially disaggregated way. The model estimates probabilities of land conversion from forest or agriculture to different densities of residential use within each spatial cell in the seven-county area of the Patuxent basin [11, 12, 13, 26].

The model consists of two stages. The first stage estimates the value of land parcels in different uses. The assessed value of any structures was subtracted from data on the selling price to get the residual value of the land in residential use. This land value was used as the dependent variable and spatial variation in land prices were explained by an extensive array of features of the location, including: distance to employment centers, access to public infrastructure (roads, recreational facilities, shopping centers, sewer and water services), and proximity to desirable (e.g. waterfront) and undesirable (e.g. waste dumps) land uses. Also included were some less obvious explanatory variables that describe the nature of the land uses surrounding a parcel. The estimation techniques used were maximum

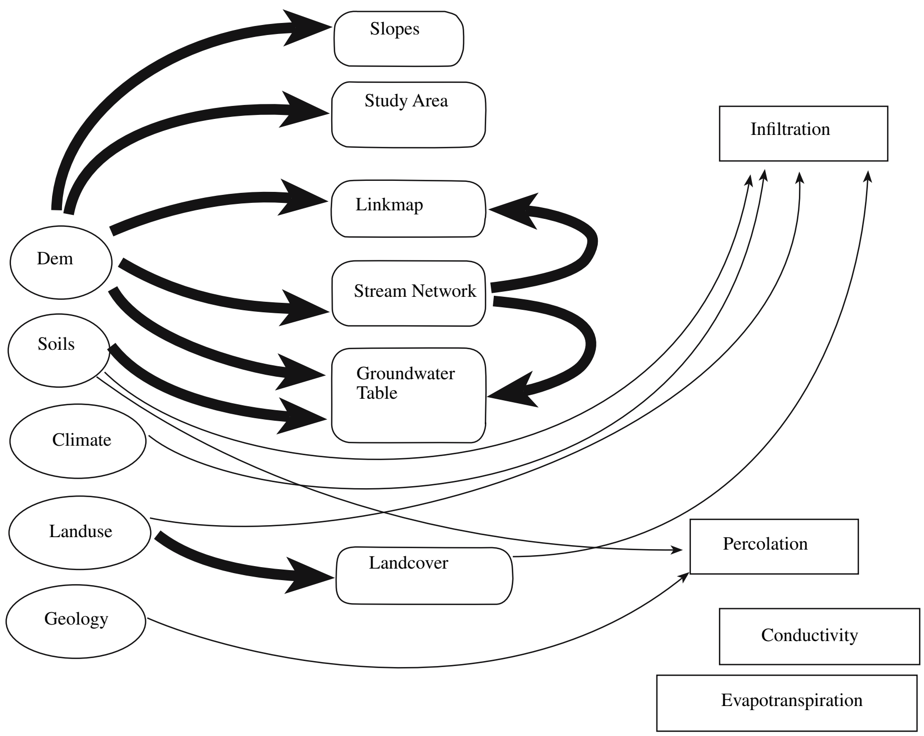

Fig. 5. PLM spatial coverages. There are 6 basic coverages. Additional maps are created during preprocessing and model initialization. Other spatial parameters and variables are calculated and updated during model runs.

likelihood and generalized method of moments, the latter being an approach that allows for treatment of the obvious spatial autocorrelation in the model

The second stage involved estimating "qualitative-dependent variable" models (i.e. discrete choice models) of historical land use conversion decisions. In this stage, historical decisions as to whether or not to convert a parcel in an agricultural or forest use to residential use are modeled as functions of their value in original use, predicted value in residential use (derived from the first stage model), and proxies for the relative costs of conversion. The purpose of this stage was to determine what factors affect land use conversion and to estimate parameters of those conversion functions.

Once the parameters of the two stages of the model were estimated, it was used to generate the relative likelihoods of conversion of different parcels in the landscape. A spatial pattern of relative development pressure was obtained as a function of the characteristics of the parcels and their locations. Since the explanatory variables used to predict the values in residential and alternative uses and the costs of conversion are all functions of ecological features, human infrastructure, and government policies, the effects of changes in any of these variables can be simulated. Total growth pressures in the region were then used to estimate the spatial patterns of new residential development into the future. For example, to generate the scenarios used in this paper, a projection of 28000 new dwelling units in the 5 years from 1997 to 2003 in the 7 counties that include the Patuxent watershed was used. Other alternatives for growth pressure could also be analyzed, but this seemed to be the consensus opinion on growth pressure in the near term. The new dwelling units were then distributed in the watershed in the "most likely" locations based on the results of the stage 1 and 2 modeling exercises described above.

CALIBRATION AND TESTING

Much of the time involved in developing spatial process-based models is devoted to calibration and testing of the model behavior against known historical or other data [6]. To adequately test model behavior and to reduce computational time, we performed the calibration and testing at several time and space scales, and for the unit model independently of the full spatial model. To calibrate the model we have followed the multi-tier calibration strategy (Fig. 7). This was a step-wise process that started with the calibration of individual modules, moving then to spatial implementations of modules and groups of modules at several scales, until finally the full ecological model was calibrated for the whole watershed. The obvious benefit of this was a much simpler model to calibrate at each step. Clearly the aggregate of several modules does not necessarily behave similarly to the individual modules taken separately. Therefore recalibration was needed every time we went from simple individual modules to their com-

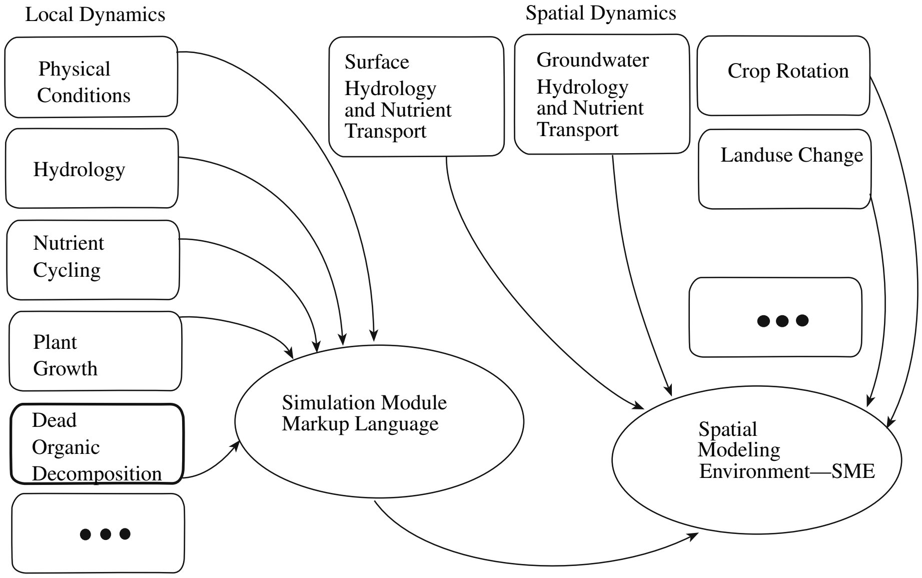

Fig. 6. The Library of Hydro-Ecological Modules used to build the PLM. The modules can be run as stand-alone models or combined together using the SME.

binations, both locally and spatially. However, it was always much easier to fine-tune the already performing modules, than to do a full-scale calibration of the full model in its overall complexity.

MODULE CALIBRATIONS

We start with a series of calibrations of the unit modules and then the full unit model [27]. Next we add the spatial dimension and start calibrating individual modules for smaller subwatersheds. Calibrating and running even the hydrologic module of this level of complexity and resolution requires a multi stage approach [28]. We first identified two spatial scales at which to run the model—a 200-m and 1-km cell resolution. The 200-m resolution was more appropriate to capture some of the ecological processes associated with landuse change but was too detailed and required too much computer processor time to perform the numerous model runs required for calibration and scenario evaluation for the full watershed. The 1-km resolution reduced the total number of model cells in the watershed from 58905 to 2352.

Secondly, we identified a hierarchy of subwatersheds. The Patuxent watershed has been divided into a set of nested subwatersheds to perform analysis at three scales (Fig. 8). The small (23 km^2) subwatershed of Cattail creek in the Piedmont northern part of the Patuxent basin was used as a starting point. Another small subwatershed, Hunting Creek, was selected to calibrate the model for the different hydro-ecological conditions of the coastal plain area. The next larger watershed was the upper non-tidal half of the Patuxent watershed that drained to the USGS gage at Bowie (940 km^2). And finally we examined the whole Patuxent watershed (2352 km^2). The number of total model cells grew from 566 cells initially, to 23484 cells for the half watershed, and then to 58905 cells for the entire study area at the 200-m resolution.

In this stage of the calibrations, we ran only the hydrologic component of the model, without links to the plants and nutrients. While transpiration by plants and the influence of nutrients on plant productivity and transpiration are obviously important influences on hydrology, we excluded them at this stage: (1) for simplicity; (2) for direct comparison to other hydrologic models; and (3) to test the effects of adding the plant and nutrient dynamics later (see below).

We staged a set of experiments with the small Cattail creek subwatershed to test the sensitivity of the surface water flux. Three crucial parameters controlled surface flow in the model: infiltration rate, horizontal conductivity and number of iterations per time step of the unit model. Riverflow peak height was strongly controlled by the infiltration rate. The conductivity determined river levels between storms and the number of iterations modified the width of the storm peaks.

Surface water flow was calibrated against the 13 USGS gaging stations in the area that have data concurrent with the climatic data series (1990–1996). In this calibration, the model results for the Cattail subwatershed (Fig. 8a) are in fairly good agreement with the data and may be considered as a partial model verification, because none of the parameters had been changed after the initial calibration using 1990 data. Some of the flow statistics are presented in table, where we have also included calibration results from the Hydrologic Simulation Program—Fortran (HSPF) [29], that has been previously applied to the Patuxent watershed [30]. We

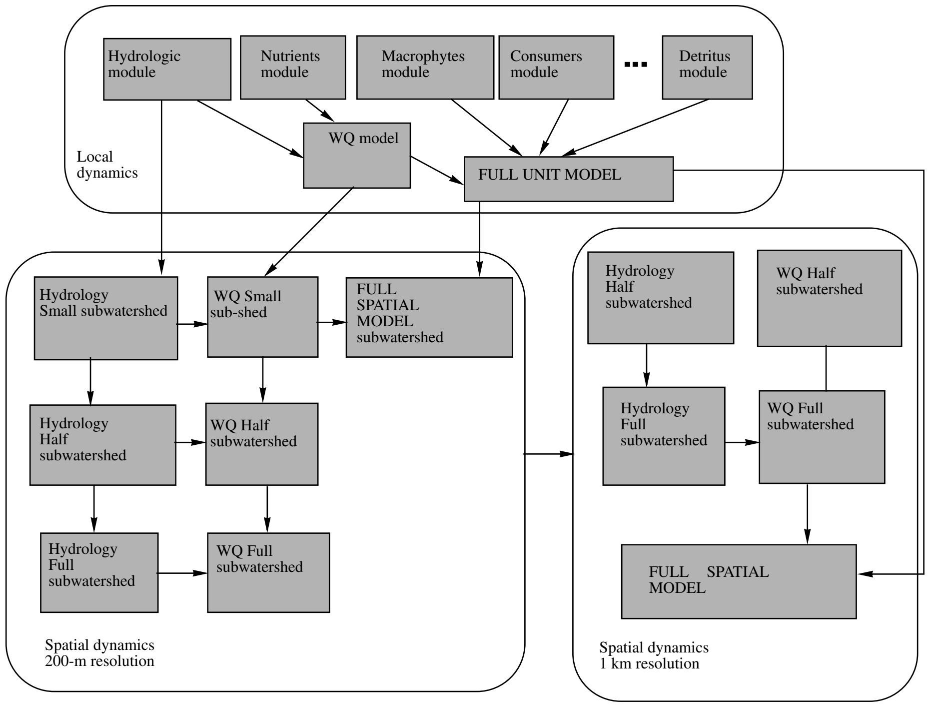

Fig. 7. The multi-tier calibration strategy, when we perform the model calibration by calibrating individual modules and groups of modules in different types of spatial representations. We start with local modules and then gradually increase the spatial domain of the model. Each time we have to recalibrate the model, however the complexity of the full spatial implementation would be overwhelming and prohibitive for analysis and interpretation.

attained a better fit to the data with our model, than with HSPF. HSPF is a more empirically based model that uses high temporal resolution input data (e.g. hourly rainfall data), but low spatial resolution (e.g. aggregated subwatersheds). Much more of the behavior in HSPF is embedded in the parameters of the model than in the PLM, (which uses the pattern of land use to drive much of the behavior). Thus the effects of changes in the spatial pattern of land use (one of our key questions) cannot be adequately addressed using HSPF, since it would require recalibrating the model for the new land use pattern, and empirical hydrologic data for this new, hypothetical, land use pattern obviously does not exist.

Next we performed a spatial scaling experiment, which involved varying the spatial resolution of the model. In this experiment we were mainly looking at the effects of changing the *model* resolution, not the *data* resolution. Using GIS operations we aggregated the model, switching from a 200-m to a 1-km cell resolution. Model runs for the 1-km resolution were remarkably close to the results from the 200-m model. This finding was especially promising for analysis of the other modules of the full ecological economic model. Since most of the horizontal spatial dynamics is governed by the hydrologic fluxes, the coarser 1-km resolution should be sufficient for the spatial analysis of the integrated model of the watershed in this case.

Overall, the model of the half watershed (Fig. 8b) showed less precise model results (Fig. 9) than the Cattail subwatershed, as predicted from theory [19]. The calibration statistics for the half watershed area are summarized in table. In general, the increased spatial extent of the model presented more heterogeneity that was not fully accounted for in the calibration. Specific reasons for this include: the spatial resolution of the input climatic data, the greater complexity of groundwater flows at this scale (which are handled in a very simplified way in the model), and the need to recalibrate some of the hydrologic parameters at the larger scale.

One parameter that needed to be adjusted was the number of iterations N in the hydrologic module. At the larger watershed scale, it turned out that a better fit could be obtained if the number of iterations was further increased. Apparently this was because at this larger scale we needed to move water further and faster to better simulate the short-term high peaks that were observed in the data. This was a clear illustration of the fact that different scales present new emerging behavior of the system, and that rescaling is an important process that can usually not be done mechanically. The best fit to data was obtained when running the model with the self-adjusting method for N with the maximum number of iterations $m = 100$ [28]. Interestingly, the Cattail subwatershed still performed as well as before with this value of m. This could be expected since the previous analysis showed that there was no sensitivity of subwatersheds to increases in N beyond 20 ($m = 20$).

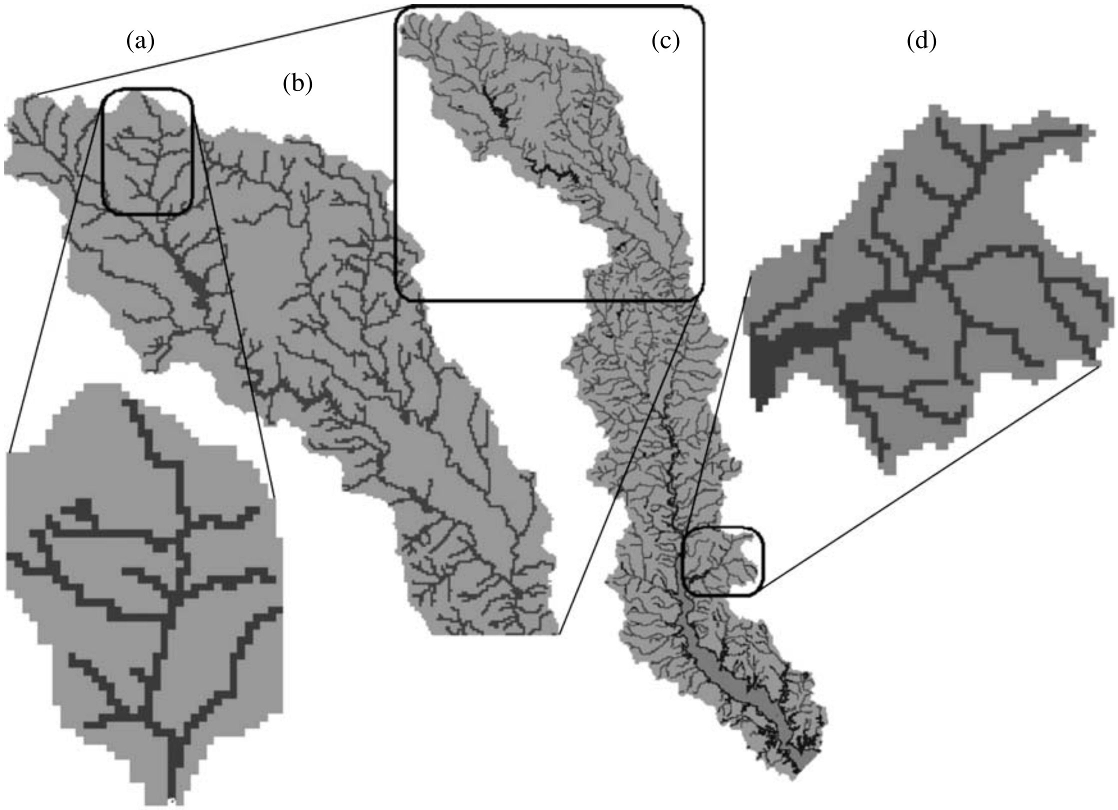

Fig. 8. Hierarchy of subwatersheds in the Patuxent drainage basin used to calibrate and analyze the model. (a) 23 km^2 Cattail Creek; (b) 940 km^2 Upper Patuxent draining at Bowie; (c) 2352 km^2 Full study area, (d) 70 km^2 Hunting Creek.

Within the subwatershed we assumed that the groundwater dynamics closely follows the surface water flows and confined the groundwater to the subwatershed area. This is probably not accurate even for Cattail Creek, and at larger scales the groundwater patterns are even more complex.

The spatial rainfall and other data were interpolated from daily records of 7 stations distributed over the

PLM testing and comparison to the HSPF model statistics for the Cattail Creek and Unity subwatersheds and the Half subwatershed draining at Bowie

Summary Statistic	Cattail				Unity				Bowie			
	Data	Model	PLM % error	HSPF % error	Data	Model	PLM % error	HSPF % error	Data	Model	PLM % error	HSPF % error
Total Flow	2510.41	2527.58	0.7	8.2	3950.54	3981.31	0.8	–2.1	36617.43	37978.78	3.6	9.7
Max 10%	930.2	925.79	–0.5	4.9	1410.15	2148.13	41.5	2.3	12497.58	16546.70	27.9	15.1
Min 50%	587.3	596.25	1.5	–14.7	826.76	626.78	–27.5	–12.1	7917.98	6582.62	–18.4	9.0
Total												
1986	326.16	282.24	–15.6		484.52	446.30	–8.2		4752.94	4352.84	–8.8	
1987	472.83	469.25	–0.8	–0.7	816.48	942.00	14.3	–11.6	6446.08	7041.22	8.8	–2.6
1988	482.01	414.22	–16.4	–	819.30	792.10	–3.4	–	6751.99	5841.62	–14.5	–
1989	660.62	748.29	11.7	+18.1	960.30	949.45	–1.1	+8.0	10507.98	11881.88	12.3	+25.3
1990	568.78	611.31	6.9		869.94	851.47	–2.1		8158.45	8861.23	8.3	

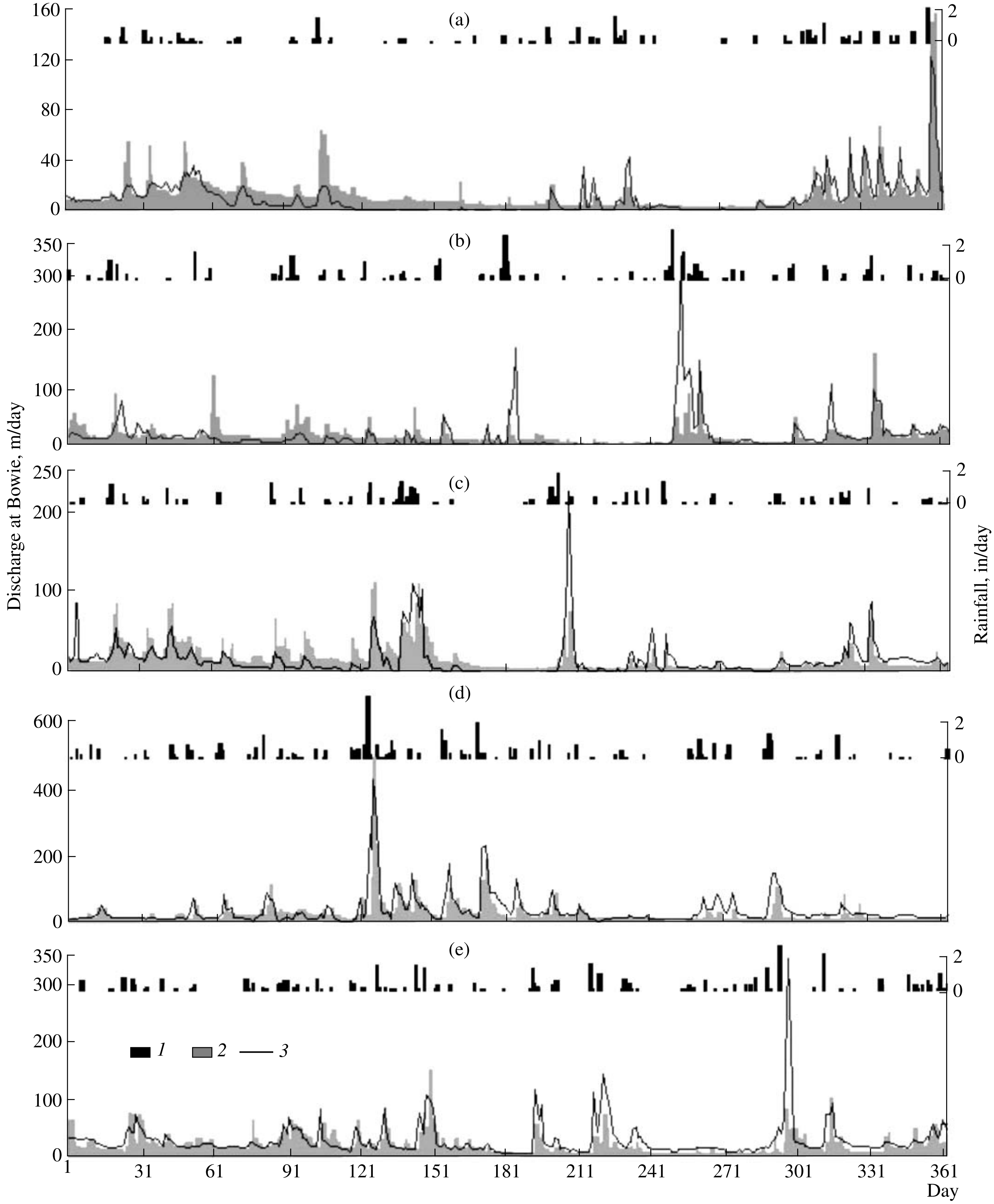

Fig. 9. Comparison of output from the hydrologic component of the model with the data for Upper Patuxent at Bowie for 1986–1990. Calibration was performed for 1986–1987 data. The other years present a partial verification of the model. (1) Rainfall, (2) data; (3) model run.

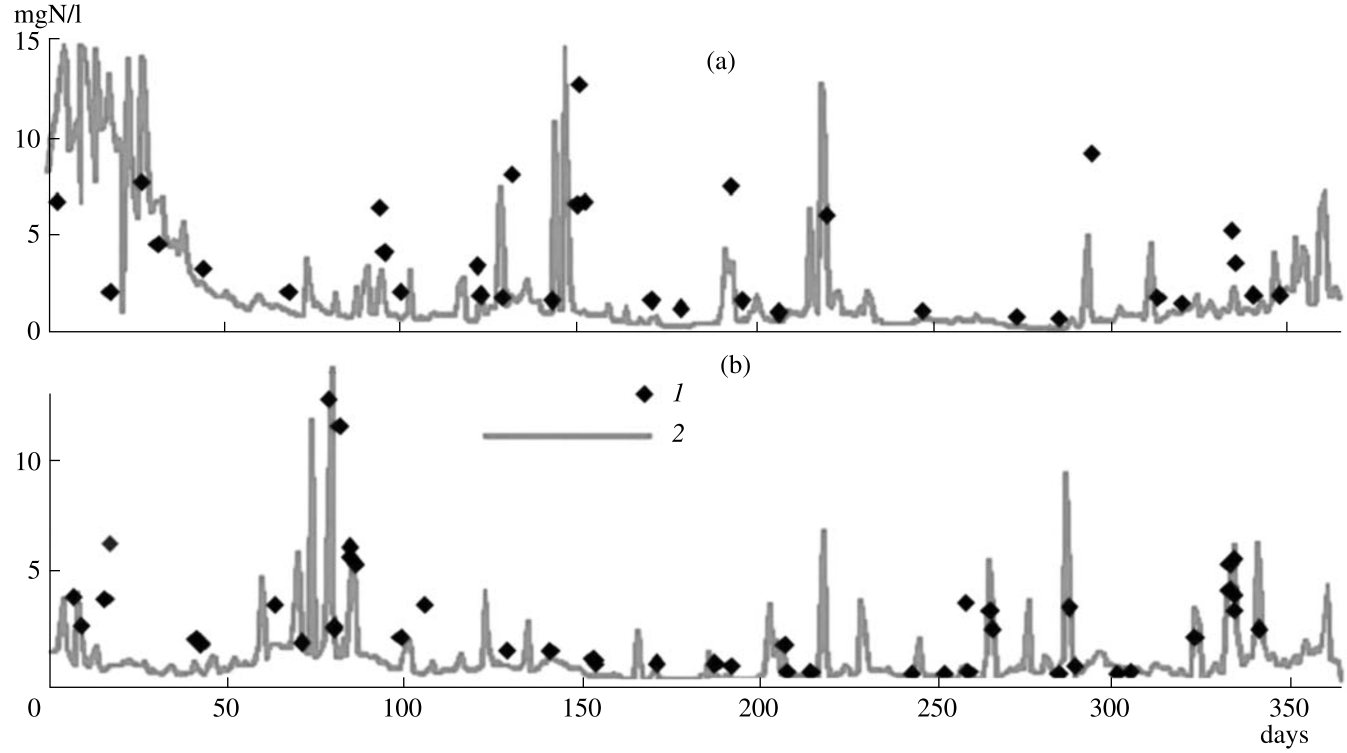

Fig. 10. Calibration results for flow weighted nitrogen concentrations in the Patuxent River at Bowie for 1990 and 1991. (*1*) USGS data, (*2*) model results.

study area. The Cattail subwatershed hydrology was driven by one climatic station and the half-watershed model incorporated data from 3 stations. The lack of data on the true variability of the meteorological data in space and time hinders the model's ability to accurately represent short term or localized responses in river flow. However, the model is able to consider antecedent moisture and runoff-generating areas in a spatially realistic manner based on topography, land use and soil type, giving the simulation a fairly high degree of precision. The general hydrologic trends seem to be well captured by the model and allow us to expand the study to other modules [31].

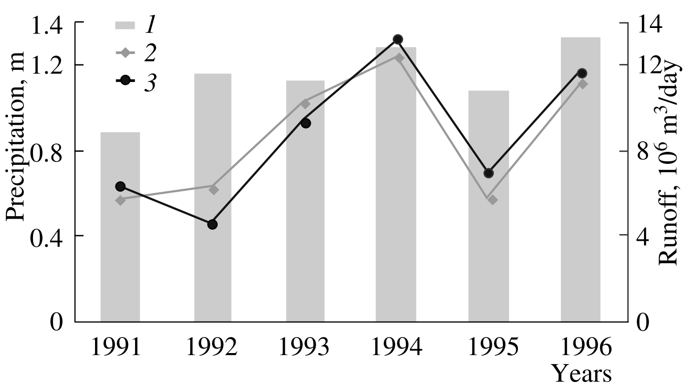

Fig. 11. Calibration results for flow weighted nitrogen concentrations on the annual basis. (*1*) Precipitation, (*2*) gage data, (*3*) model output.

We also refer the reader to our web page at http://giee.uvm.edu/PLM, which further describes the model.

FULL ECOLOGICAL MODEL CALIBRATION

The full spatially explicit ecological model was run for several years using historical climate inputs for calibration purposes. In this case we ran the model at a 1-km spatial resolution. We used two methods to compare the model performance to the available data.

Certain modeled variables, or indices that aggregate model variables, were compared to point time series data such as streamflow, nutrient concentration in the streams, and historical tree-ring data for the region. The inclusion of plant and nutrient dynamics improved the model's hydrologic performance in comparison to the output reported above. The spatially explicit representation of plant and nutrient dynamics modifies the evapotranspiration and interception fluxes in the model, making the model performance more realistic. It was also essential for scenario runs that take into account land use and cover changes, in which these changes modify the hydrologic fluxes in the watershed.

A sample of calibration for flow weighted nitrogen concentrations in the Patuxent River at Bowie is presented in Fig. 10. Data is available to calibrate longer-term runs of the model with these data sets. Model output was compared to field data by visually inspecting superimposed graphs and comparing annual mean and total values. For example, the long-term trend of nitrogen dynamics in Hunting Creek—a small subwatershed in the Coastal Plain area—shows good correlation with the annual dynamics calculated from the data (Fig. 11).

Comparison of raw spatial data is a much more difficult and less studied procedure. Spatially explicit data is scarce and rarely matches the spatial extent and resolution produced by the model. Some example spatial output from the model can be found on the project web page at http://giee.uvm.edu/PLM [31]. In particular it shows the typical pattern of seasonal plant growth in the region, which has a significant impact on hydrology through transpiration. Data derived from AVHRR satellite images, the NDVI or "greenness" index, were used to calibrate the full model's predictions of primary production for intra-annual effects. We created indices from the NDVI data, and the model output so that we were comparing the timing and pattern of NDVI change to the timing and pattern of NPP change in the model. A visual comparison shows fairly good agreement between the model output and the data currently available.

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