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Methods, Tools, and Technologies

Assessing impacts of sulfur deposition on aquatic ecosystems: A decision support system for the Southern Appalachians

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Abstract

With climate change and ongoing impacts from human development and resource extraction, US federal land management agencies are acutely concerned with managing for healthy aquatic ecosystems in the Southern Appalachian Mountain (SAM) Region. Here, we describe development of a spatial decision support application to assess the biological and ecological impacts of atmospheric S and N deposition on aquatic ecosystems of the region. We first summarize foundational published work to predict continuous maps of surface water acid neutralizing capacity (ANC) and soil base cation weathering (BC_w). We use the predicted ANC and BC_w maps to estimate steady-state critical loads (CLs) of atmospheric S and N deposition. We included estimated CLs of atmospheric N to get a complete picture of CLs and potential exceedances. We then present a logic-based decision support model for assessing effects of S and N deposition based on statistically modeled stream ANC and CL exceedance. The model is easily modified for continuous monitoring of CL exceedance patterns as new S and N deposition and ANC data become available. We present mapped model results for the SAM study area and an important subset of the region, the Great Smoky Mountains National Park. ANC modeling results revealed that predicted acid sensitivity was spatially variable, with areas of relatively low stream ANC (<50 $\mu eq \cdot L^{-1}$) and soil BC_w (<50 $meq \cdot m^{-2} \cdot year^{-1}$) predominantly found in certain critical areas. Within the Great Smoky Mountains National Park, evidence for S CL *exceedance* based on an ANC criterion of 50 $\mu eq \cdot L^{-1}$ was strong at locations where ambient S deposition was at least two times the CL. We also predicted likely impacts of CL exceedances on aquatic insect species richness and native fish abundance. Responses for *insect species richness* and *fish impact* showed variability similar to CL exceedance, with increasing impact positively correlated with elevation. Finally, we discuss ways that the decision support system can be used to prioritize management across the region.

KEYWORDS
atmospheric deposition, biological impact, critical load, exceedance, hurdle modeling, spatial decision support

INTRODUCTION

This study details application of a spatial decision support system (DSS) to assess biological and ecological impacts of acidic sulfur (S) and nitrogen (N) deposition on aquatic systems in the Southern Appalachian Mountain (SAM) region of the southeastern United States (US). The first two subsections provide an overview of the acidification issue and introduce the decision support technology used in this study.

Background on stream water acidification

The U.S. Environmental Protection Agency (US-EPA), U.S. Department of Agriculture, Forest Service (USDA-FS), and U.S. Department of Interior National Park Service (USDI-NPS) are concerned with the current and future health of aquatic ecosystems. There have been numerous studies of ecosystem sensitivity to acidification and the effects of acidic S and N deposition on surface water quality (Baker, Kaufmann, et al., 1990; Baker, Bernard, et al., 1990; Bulger et al., 1999; Greaver et al., 2012; Sullivan et al., 2004; Sullivan, Webb, et al., 2007). The main sources of atmospherically deposited S are coal-fired electricity generation and other industrial facilities. Sulfur is the primary determinant of acidic precipitation, and sulfate (SO_4^{2-}) is the dominant anion (Sullivan et al., 2004). Although a portion of atmospherically deposited S is retained in watershed soils, sulfate concentration in many mountain streams has increased because of increased acidic deposition (Sullivan, Cosby, et al., 2007). Nitrogen is a secondary determinant of acidic precipitation, and nitrogen oxides (NO_x) are the dominant anions (Greaver et al., 2012; Sullivan et al., 2004). Main sources of atmospherically deposited NO_x are transportation and home/business heating emissions.

Values of stream water acid neutralizing capacity (ANC) reflect a catchment's ability to neutralize acidic inputs, which derives from the balance among strong bases and acids in soil and water solutions. High ANC values indicate high buffering capacity against acids. ANC is similar to pH, but as defined here, it is neither influenced by dissolved CO_2 nor organic acids. As the rate of acidic deposition increases, stream water ANC can decrease in proportion to the natural resupply of soil base cations (BCs). Streams with low ANC values display reduced pH, and, often, increased mobilization of inorganic aluminum (Al) from soils. Both increased hydrogen (H^+) and aluminum (Al^{3+}) ionic concentrations can be toxic to fish, including native brook trout (*Salvelinus fontinalis*; Baldigo et al., 2007). Specific ANC thresholds are associated with biological effects (U.S. EPA, 2009). For example, moderate effects on macroinvertebrates and fish are associated with concentrations between ~50 and 100 $\mu eq \cdot L^{-1}$ (Cosby et al., 2006; Sullivan et al., 2006), while more substantive effects are observed at concentrations <50 $\mu eq \cdot L^{-1}$ (Cosby et al., 2006; Sullivan et al., 2006; U.S. EPA, 2009). Brook trout are sensitive to concentrations <50 $\mu eq \cdot L^{-1}$, but some aquatic insects they feed on are also sensitive to concentrations between 50 and 100 $\mu eq \cdot L^{-1}$.

The critical load (CL) is the level of atmospheric S and N deposition below which sensitive ecosystem components remain unharmed (Nilsson & Grennfelt, 1988). Any S and N deposition above the CL can be considered an exceedance of the CL. In a monitoring strategy, CLs of S and N are operationally estimated to protect stream resources from damagingly low ANC levels. An important consideration in this context is that some soils derive from parent materials that are ordinarily deficient in BCs (Elwood et al., 1991). As a result, their associated streams naturally exhibit low ANC values due to these catchment-level geochemical characteristics. Hence, it is unreasonable in some areas to generate CLs and evaluate effects on species richness using an ANC threshold that can never be reached. In these cases, management of aquatic conditions is better focused on areas that are amenable to remediation. Here, we estimate CLs and related aquatic ecosystem effects based on ANC thresholds of 50 and 100 $\mu eq \cdot L^{-1}$, recognizing that these values may not be obtainable for all SAM region streams.

The Ecosystem Management Decision Support system

We use a spatially enabled DSS to assess the biological and ecological impacts of acidic S and N deposition on streams. A spatial DSS is enabled by software that organizes, analyzes, and presents spatial information about conditions of a system to facilitate individual or group decision-making. The DSS is helpful in this context because it reveals both the conditions and the trade-offs and synergies among factors that can influence those conditions. The role of a spatial DSS is not to make decisions but to assist human decision-making. All DSSs rely on models, but all models simplify reality; hence, there are always added factors that decision-makers must consider.

The first module of a DSS designed in Ecosystem Management Decision Support (EMDS) evaluates the state of a system; the second module evaluates what to do about the conditions revealed in the first module. Holsapple (2003) broadly defines a DSS as consisting of four components (see also Mintzberg et al., 1976; Simon, 2003):

1. a language system that comprises the conventions (e.g., semantics and syntax) by which the user and software communicate with each other,
2. a user interface, by which the user visually interacts with the system,
3. a body of knowledge (e.g., a model or knowledgebase), on which the system operates, by means of,
4. a software engine (typically, a dynamic link library).

Under this definition, DSSs range from simple tools that perform one specific analysis, such as a multi-criteria decision analysis (e.g., Saaty, 1994), to more complex multicomponent applications. The latter can invoke several different software engines in a variety of analytical sequences to handle large and often complex solutions that have both strategic and tactical components. These can be expressed as frameworks that are used to implement a virtually endless variety of DSS applications. There are many commercial off-the-shelf DSSs available; Borges et al. (2014) provide a global survey of DSSs used for forest management; most of which are multicomponent applications. The EMDS system (Paplanus et al., 2014; Reynolds et al., 2014) used here is a DSS application development framework.

EMDS is open access and designed specifically for integrated landscape evaluation, planning, and decision-making (Reynolds et al., 2014; Reynolds & Hessburg, 2014) and includes a set of tools for building customized applications. At version 8.6, EMDS provides decision support for landscape-level analyses through logic and decision engines integrated with the ArcGIS 10+ geographic information system (GIS; Environmental Systems Research Institute, Redlands, CA) and the QGIS system (http://qgis.org/en/site/, last accessed on 11 April 2022). Representative examples of EMDS applications include DSSs for:

1. evaluating the environmental impact of an extensive road network on the Tahoe National Forest, CA, USA (Girvetz & Shilling, 2003),
2. evaluating wetland management opportunities in the northern Netherlands (Janssen et al., 2005),
3. evaluating the conservation potential of lands in the checkerboard ownership area of the central Sierra Nevada in California, USA (White et al., 2005),
4. evaluating natural resource impacts caused by conventional forest management practices in forest plantations (Stolle et al., 2007),
5. developing an integrated assessment framework and spatial DSS to support land-use planning and forest carbon sequestration decisions in China (Wang et al., 2010),
6. evaluating terrestrial and aquatic habitats across western Oregon, USA, for their suitability to meet defined ecological objectives (Staus et al., 2010),
7. integrated landscape restoration on the Okanogan-Wenatchee National Forest in the State of Washington, USA (Hessburg et al., 2013), and
8. assessing ecological integrity of US National Forest System lands in the continental United States (Cleland et al., 2017).

Each of these examples makes use of the logic processing component of EMDS to assess some aspect of ecosystem state. For example, Hessburg et al. (2013) assess ecosystem departure from a set of historical reference conditions, and Cleland et al. (2017), in a similar fashion, assess ecosystems departure from specified attributes of ecological integrity. Hessburg et al. (2013) go a step further, applying one of the decision analysis components of EMDS (Criterium DecisionPlus [CDP]), to develop strategic priorities for landscape restoration and recommending which landscape patches are the highest priority for restoration, given their degree of altered conditions. In addition to these examples, the EMDS Wikipedia page (https://en.wikipedia.org/wiki/Ecosystem_Management_Decision_Support, last accessed on 11 April 2022) provides a comprehensive list of >85 published EMDS applications that have been developed worldwide since 1997.

In this work, we make use of the logic processing component in EMDS to design a DSS application that assesses aquatic impact of historical atmospheric S and N deposition in the SAM study region and explores ecosystem sensitivity to possible changes in aquatic impact associated with alternative future S and N deposition scenarios.

Objectives

We first summarize foundational published work to predict continuous ANC, base cation weathering (BC_w), and

CL conditions throughout the SAM study region (McDonnell et al., 2014; Povak et al., 2013, 2014). We then specify an EMDS application to inform forest management decisions to address CL exceedances. We illustrate use of this application throughout the SAM region, present a variety of change scenarios for a portion of the region, the Great Smoky Mountain National Park, to highlight model sensitivity, and describe its ongoing utility to inform both forest management and restorative actions within the region. Finally, we discuss how the application can be extended to include other logistical, economic, and social value considerations for prioritizing activities that mitigate acidification effects from atmospheric S and N deposition. We close by highlighting the potential for incorporating additional drivers of aquatic and terrestrial habitat suitability.

We emphasize here that the present work is intended as an example of a general methodology for spatial decision support of interest to landscape modelers, and the model does not comprehensively address all sources of acidifying atmospheric deposition, nor does it comprehensively evaluate all relevant dynamics of BC_w. With a view toward building on the present work, we address the implications of these limitations in some depth in the discussion.

MATERIALS AND METHODS

Study area

The SAM study area spans the region from northern Georgia to southern Pennsylvania, and from eastern Kentucky and Tennessee to central Virginia and western North and South Carolina. The region comprises the Blue Ridge, Ridge and Valley, and Central Appalachian (Omernik, 1987) level 3 physiographic provinces and includes small portions of the Northern Piedmont, Piedmont, and Western Allegheny Plateau provinces (Figure 1) (U.S. EPA, 2009).

In addition to a base analysis covering the entire SAM study region, change detection analysis was conducted under a variety of scenarios in the Great Smoky Mountains National Park in the southwest portion of the SAM.

Overview of the analysis workflow

Regional ANC, BC_w, and CLs modeling

In previous work, we developed machine learning models to predict the ANC of streams across the SAM region (Povak et al., 2013). Models were developed using stream water chemistry data from >900 sampled locations and continuous maps of pertinent environmental and climatic predictors. Environmental predictors were averaged across the upslope contributing area for each sampled stream location and submitted to both statistical and machine learning regression. Predictor variables represented key aspects of the contributing geology, soils, climate, topography, and acidic deposition. To reduce model error rates, we employed hurdle modeling to screen out well-buffered sites and predict continuous ANC for the remainder of the stream network. Models predicted acid-sensitive streams in forested watersheds with small contributing areas, siliceous lithologies, cool and moist environments, low clay content soils, and moderate or higher dry sulfur deposition.

In a second study (Povak et al., 2014), we again used machine learning to model catchment-level BC_w to identify key environmental correlates and predict a continuous map of BC_w within the SAM region. Predictors included aspects of the underlying geology, soils, geomorphology, climate, topographic context, and acidic deposition rates. Random-forest modeling significantly improved model prediction of catchment-level BC_w rates over traditional linear regression. Low BC_w rates were predicted in catchments with low precipitation, siliceous lithology, low soil clay, nitrogen and organic matter contents, and relatively high levels of canopy cover in mixed deciduous and coniferous forest types. Our results reinforced findings from other studies and identified several climatic predictors, interactions, and nonlinearities among the predictors.

In a third study, we linked statistical predictions of ANC and BC_w for streams and watersheds of the SAM region with a steady-state model to estimate CLs and exceedances (McDonnell et al., 2014). Results showed that >20% of the total length of study region streams displayed $\text{ANC} < 100\ \mu\text{eq} \cdot \text{L}^{-1}$, a level below which effects on biota may be anticipated; most were fourth or lower order streams (i.e., streams found at higher elevations in watersheds). Nearly one-third of the stream length within the SAM region exhibited CLs of S deposition $<50\ \text{meq} \cdot \text{m}^{-2} \cdot \text{year}^{-1}$, which is less than the regional average S deposition of $60\ \text{meq} \cdot \text{m}^{-2} \cdot \text{year}^{-1}$. Owing to their geologic substrates, relatively high elevation, and cool and moist forested conditions, the percentage of stream length in CL exceedance was highest for mountain wilderness areas and in National Parks and lowest for privately owned valley bottom land. Input data for CL and exceedance assessment were generated by McDonnell et al. (2014) for a custom, high-resolution set of catchment polygons and assembled for use in the DSS developed here (Figure 2).

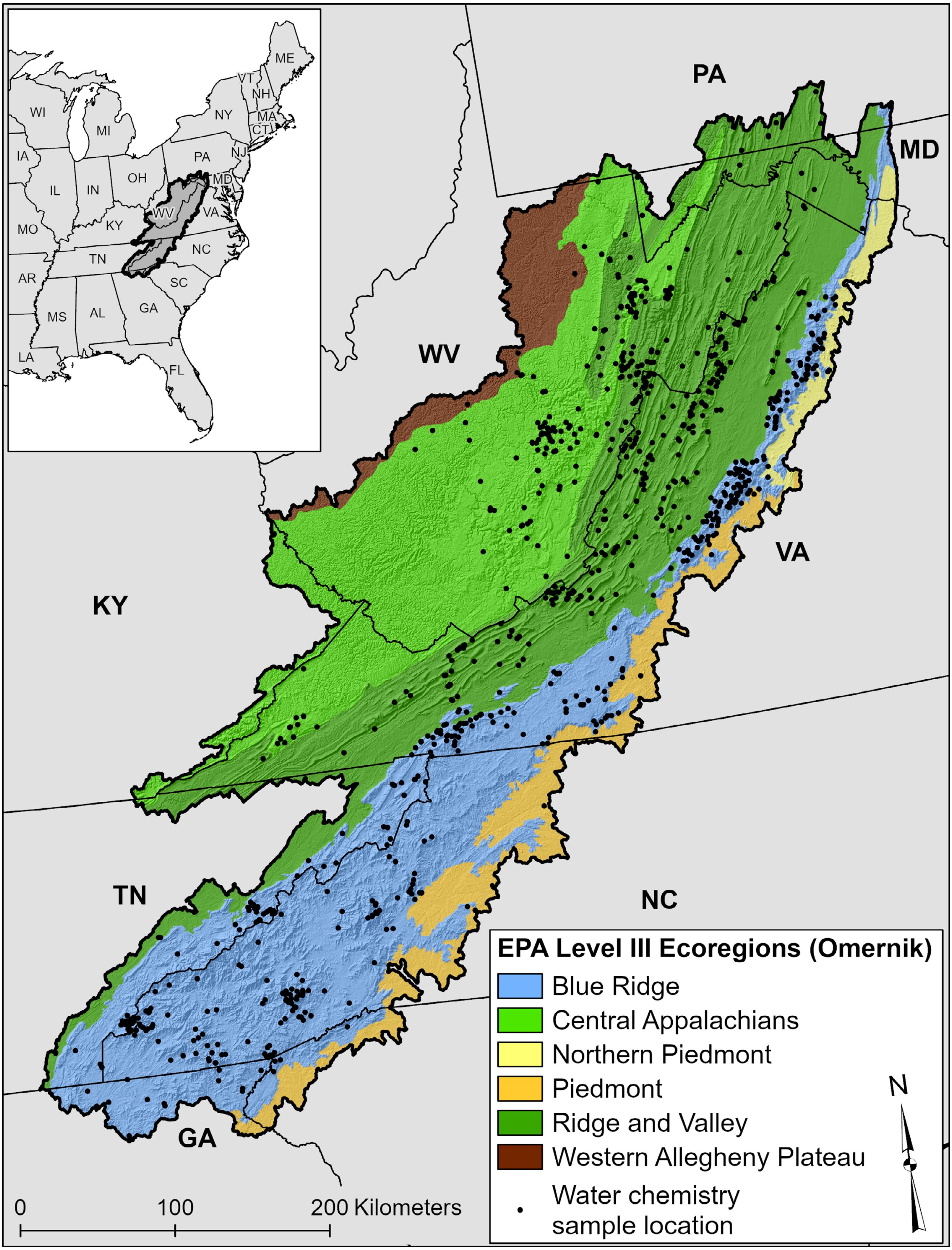

FIGURE 1 Study area boundary and physiographic provinces (Omernik, 1987). EPA, Environmental Protection Agency.

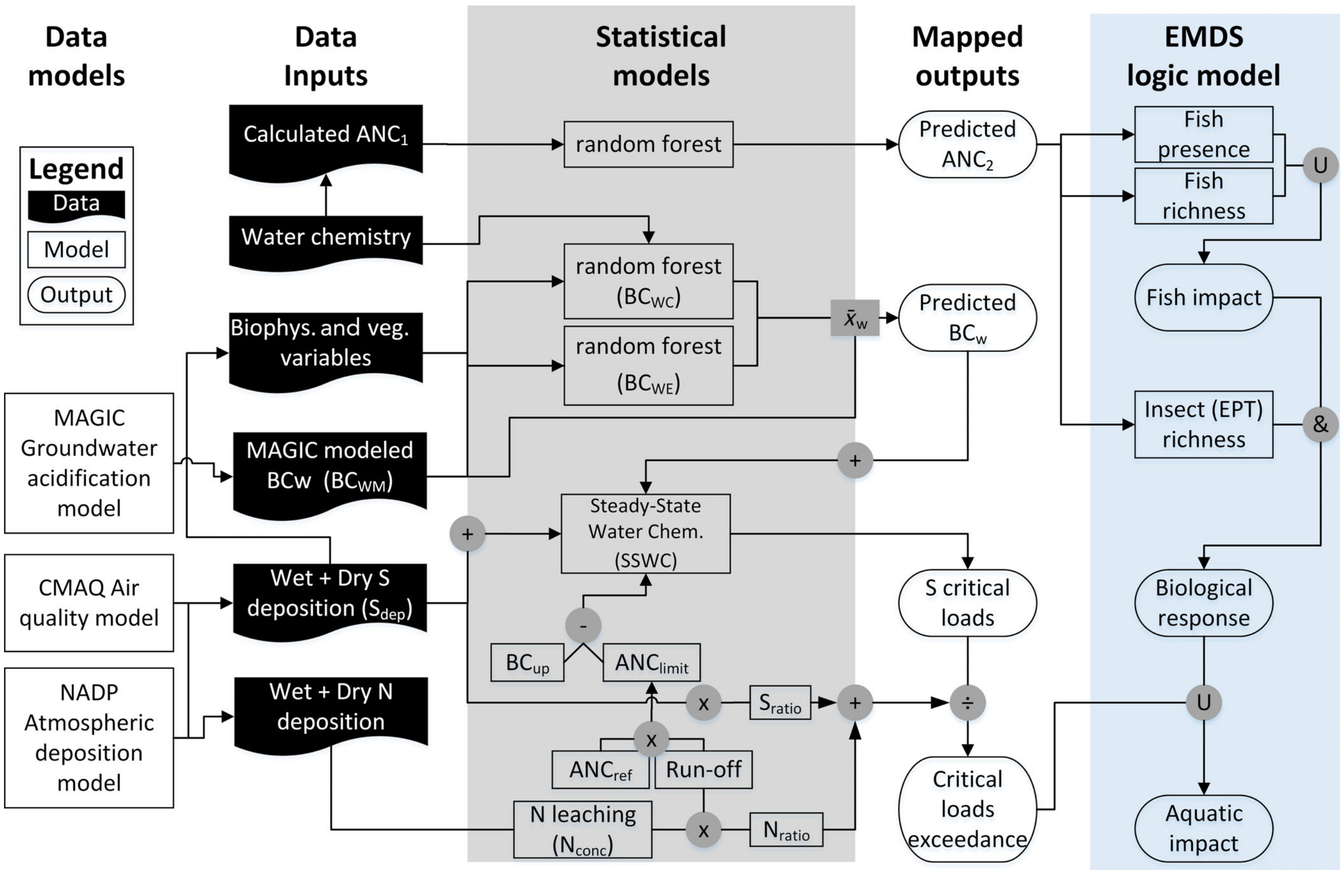

FIGURE 2 Overview of the process workflow for evaluating aquatic impact in the Southern Appalachian Mountain region. ANC, acid neutralizing capacity; BC, base cation; CMAQ, Community Multiscale Air Quality; EMDS, Ecosystem Management Decision Support; EPT, models for insect species richness (Ephemeroptera, Plecoptera, and Trichoptera); MAGIC, Model of Acidification of Groundwater Catchments; NADP, National Atmospheric Deposition Program; U, union.

At the conclusion of the data assembly step, all data required to perform the analyses were organized into a geodatabase table for use in the EMDS project (Archive 1, CLgeodatabase.zip, https://osf.io/5gmwe). The EMDS logic model (see Logic model to interpret aquatic impacts of S and N deposition) was initialized with data that considered current stream water acid sensitivity and parameters that estimate CLs for each stream reach of the SAM study region.

Logic model to interpret aquatic impacts of S and N deposition

The logic for assessing the aquatic impact of S and N deposition at the subwatershed scale is illustrated in Figure 3. The logic model was implemented with the NetWeaver software (Rules of Thumb, Inc., North East, PA; Miller & Saunders, 2002), a knowledge-based model development system.

Overall *aquatic impact* was assessed in terms of CL *exceedance*, which represented a long-term effect of acidification because it is calculated as a steady state (Appendix S1: Foundational Modeling), and *biological response* to ANC, which represented a short-term process. The union (U) logic operator under *aquatic impact* indicated that these two premises of the parent premise, *aquatic impact*, were treated as equally compensating cumulative effects. The first two levels of the logic can be read as "The outcome of *aquatic impact* is low to the degree that the outcomes of its premises (*exceedance* and *biological response*) evaluate to low." *Biological response* also functioned as a conclusion with its own sets of premises, which in this case were combined with the AND (A) logic operator, indicating that the premises were treated as limiting factors.

Except for *fish presence*, topics at the end of each logic path represented elementary networks that read and processed data (Figure 3) and then interpreted results against fuzzy membership functions (Zadeh, 1975a, 1975b, 1976) that returned a continuous metric expressing strength of evidence (SOE) or degree of support for a premise (Miller & Saunders, 2002). To simplify presentation of map products and our discussion, we

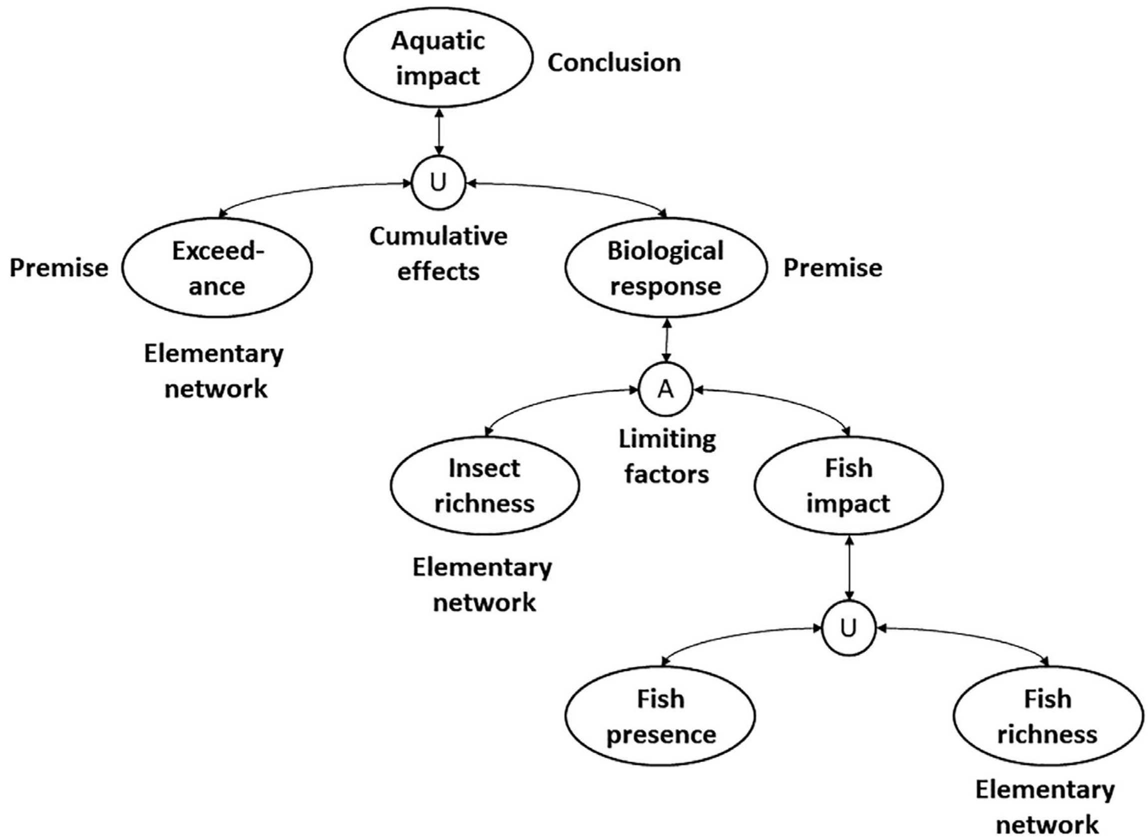

FIGURE 3 Logic to assess S and N deposition impacts. Ovals indicate logic topics, each of which assesses the outcome for the indicated topic. *Aquatic impact* considers both effects of long-term ecosystem response in terms of steady-state critical loads that determine exceedance and effects of acid neutralizing capacity on short-term biological response. Circles indicate logical operators. The Scenarios section provides additional explanation. A, AND; U, union.

linearly translated the underlying SOE metric into a scale expressing impact of outcomes and symbolized maps with categorical outcomes from very low to very high impact. For example, the *exceedance* topic computed the ratio of S + N deposition to the S + N CL calculated for a watershed and then compared that ratio to a fuzzy membership function to evaluate the outcome (Table 1). Ratios lower than 1 were evaluated to an outcome of very low *exceedance*, those higher than 2 were evaluated to an outcome of very high *exceedance*, and those falling on the interval between 1 and 2 were linearly interpolated to a ramp function for the SOE metric. Metrics were then translated to one of the outcome categories, from very low to very high, for mapping. We note that, in the theoretical treatment of exceedance (Henriksen et al., 1999), the CL is a precise threshold that is either exceeded or not. However, in our logical treatment of exceedance, we use the ratio of deposition to CL as a way of expressing uncertainty about the consequences of exceedance to ecosystems through the use of fuzzy membership functions.

As explained in Appendix S1, the major input of BCs to a catchment is through BC_w. BC_w is often modeled with the MAGIC model at the individual catchment level, which is computationally expensive. Povak et al. (2014) developed two random forest models to extrapolate MAGIC BC_w estimates for 140 catchments using (1) biophysical predictor variables for all catchments and (2) biophysical plus water chemistry data for a subset of 933 catchments where stream water chemistry data were available. A weighted average among the three BC_w models was used to assign BC_w estimates to each catchment (Table 2). All missing BC_w data were represented as null in the geodatabase for the EMDS project and ignored in the calculation of the weighted average.

Data inputs for insect and fish species richness were computed using methods given by Cosby et al. (2006):

$$\text{Insect (EPT) richness} = 13.785 + 0.0241 \times \text{ANC} - 0.00005 \times \text{ANC}^2. \tag{1}$$

$$\text{Fish richness} = 2.0812 + 0.0598 \times \text{ANC} - 0.0001 \times \text{ANC}^2. \tag{2}$$

These calculated values were then compared to fuzzy membership functions (Table 1) to determine the extent

TABLE 1 Thresholds defining fuzzy membership functions for data evaluated by elementary logic topics.

Logic topic	Metric evaluated	Full evidence[a]	No evidence[b]
CL exceedance	Ratio[c]	1.0	2.0
EPT richness	Proportion of insect families[d]	1.0	0.9
Fish richness	Proportion of fish species[e]	1.0	0.5
Brook trout presence	Likelihood of presence	1.0	0.5
Sensitive fish presence	Likelihood of presence	1.0	0.5

Note: Values that evaluate to levels between no evidence and full evidence are given an intermediate value, thereby showing the degree of partial evidence for fulfilling the proposition.

Abbreviations: ANC, acid neutralizing capacity; CL, critical load.

[a]The value of the observation at which the fuzzy membership function evaluates to +1, or full evidence in favor of the proposition being tested.

[b]The value of the observation at which the fuzzy membership function evaluates to −1, or no evidence in favor of the proposition being tested.

[c]Ratio of S deposition to S critical load.

[d]Ratio of number of insect families at the predicted ANC to the number of families expected at ANC = 100 $\mu eq \cdot L^{-1}$ (see Equation 1).

[e]Ratio of number of fish species at the predicted ANC to number of species predicted at ANC = 100 $\mu eq \cdot L^{-1}$ (see Equation 2).

TABLE 2 Data inputs to the logic model for assessing aquatic impact.[a]

Data input	Description	Source
ANC_1	Predicted acid neutralizing capacity ($\mu eq \cdot L^{-1}$).	Povak et al. (2013)
ANC_2	Value of stream water acid neutralizing capacity ($\mu eq \cdot L^{-1}$) measured at the nearest downstream water chemistry sampling location.	Sullivan et al. (2004)
ANC_{ref}	Reference value of acid neutralizing capacity ($\mu eq \cdot L^{-1}$) used to compute S + N critical load and biological impacts.	US EPA (2009)
BC_{dep}	Base cations are contributed by atmospheric deposition ($meq \cdot m^{-2} \cdot year^{-1}$). Wet base cation deposition data were obtained from J. Grimm (personal communication) and derived from National Atmospheric Deposition Program (NADP) monitoring. Total base cation deposition was calculated based on dry-to-wet ratios included in Baker, Bernard, et al. (1990).	McDonnell et al. (2014)
BC_{up}	Base cations are lost due to uptake and removal from tree harvest ($meq \cdot m^{-2} \cdot year^{-1}$). Estimates of annualized tree growth rate were used under the assumption that 65% of the bark and bole tree volume is removed from the site during harvest. These uptake terms reflect uptake into woody materials that are removed from the watershed through timber harvest. Base cation uptake was set to zero for areas in which harvesting is not permitted or considered to be unsuitable for harvesting.	McDonnell et al. (2014)
BC_{WC}	Base cation weathering from water chemistry data ($meq \cdot m^{-2} \cdot year^{-1}$).	McDonnell et al. (2012) and Povak et al. (2014)
BC_{WE}	Base cation weathering from statistical predictions (Random Forests) using environmental data ($meq \cdot m^{-2} \cdot year^{-1}$).	Povak et al. (2014)
BC_{WM}	Base cation weathering from MAGIC calibrations ($meq \cdot m^{-2} \cdot year^{-1}$).	McDonnell et al. (2014) and Povak et al. (2014)
Runoff	Stream water runoff ($m \cdot year^{-1}$).	
S_{dep}	Total sulfur deposition ($meq \cdot m^{-2} \cdot year^{-1}$).	US EPA (2005) and McDonnell et al. (2014)

[a]Archive 1, CLgeodatabase.zip (https://osf.io/5gmwe), is a geodatabase that contains all data and parameters used to interpret the data for assessing aquatic impact. Archive 2, NW html.zip (https://osf.io/5gmwe), documents the complete model specification, including all data, model parameters, and associated calculations required to evaluate the logic topics in Figure 3.

to which these premises were satisfied (insect and fish species richness levels are high).

To facilitate sensitivity analysis and explore alternative scenarios, we applied additional computational features into the logic. For sensitivity analysis, we did not fully specify fuzzy membership functions (Table 1) for evaluating logic topics in the NetWeaver logic engine (Rules of Thumb, Inc., North East, PA). Instead, the values for full support were hard-coded as constants directly into NetWeaver, but the values for no support were defined as data inputs to be read from data tables at runtime (Table 1). Thus, system users could alter any database field, as needed, to test the model's sensitivity to parameter choices. To explore alternative scenarios, the calculation of exceedance values requires a specific ANC value as a reference condition, which we also supplied from a database table at runtime (Table 3). Similarly, we designed scaling factors for S and N deposition into the computation of exceedance, which could be used to assess the policy implications of reduced S and N deposition in terms of ecological and biological consequences and their relative importance to future regulatory standards.

In our logic design, the topic *fish presence* evaluated two different levels of fish sensitivity. One was based on the relatively insensitive but socially valued brook trout, and the other was based on more sensitive species, including various dace, darter, and sculpin species (Table 1). The model contained placeholders for including additional fish species as dose/response data became available.

The specific data inputs for the logic model (Figure 3) are summarized in Table 2 and included in the geodatabase used in the EMDS project for this application (Archive 1, CLgeodatabase.zip, https://osf.io/5gmwe). The complete model specification, including all data, model parameters, and associated calculations, is documented in the Archive 2, NW html.zip, https://osf.io/5gmwe. A complete list of all logic topics, data, model parameters, and calculations is also summarized more briefly in Appendix S2: Logic topics and data descriptions.

Scenarios

Four scenarios were developed to illustrate effects of parameter changes on modeled outcomes (Table 3) and to demonstrate model sensitivity to landscape-level changes in conditions in the Great Smoky Mountains National Park, a subset of the SAM region. ANC impact scenarios 1 and 2 test parameter changes that affect biological response (Figure 3). In scenario 1, three parameter changes were introduced simultaneously to evaluate changes to biological response that were related to changes in fish parameters, effectively tightening model requirements for demonstrating good fish response (compare original and scenario values for minimum acceptable values in Table 3). Similarly, scenario 2 considered change to biological response due to tightening model requirements for one parameter for good insect response (compare original and scenario values for minimum acceptable values in Table 3).

Two exceedance scenarios were developed to compare the effects of changing the S and N deposition ratios on exceedance (Figure 3). Exceedance scenarios 1 and 2 tested landscape-scale sensitivity to the effects of reducing or increasing S and N deposition by 50%, respectively (compare the original and scenario values for deposition ratios in Table 3).

Spatial decision support with EMDS

In version 8.6, the EMDS system provides decision support for landscape-level analyses through logic and decision engines integrated with ArcGIS version 10.5 and higher, as well as the open-source QGIS software. The NetWeaver logic engine evaluates landscape data against a formal logic specification (i.e., a knowledge base in the strict sense) designed in NetWeaver Developer to derive logic-based interpretations of ecosystem conditions, such as aquatic impacts associated with S and N deposition. The logic model (Figure 3) was executed in EMDS to provide a baseline spatial assessment of *aquatic impact* for the full extent of the study area, which contained

TABLE 3 Parameter changes for scenarios evaluated in the Great Smokey Mountains National Park.

Scenario	Parameter	Original value	Scenario value
ANC impact 1[a]	Minimum acceptable value for likelihood of brook trout presence	0.50	0.75
ANC impact 1	Minimum acceptable value for likelihood of sensitive fish presence	0.00	0.50
ANC impact 1	Minimum acceptable value for fish richness	0.00	0.50
ANC impact 2	Minimum acceptable value for insect richness	0.90	0.95
Exceedance 1[b]	S and N deposition ratios	1.0	0.5
Exceedance 2	S and N deposition ratios	1.0	1.5

Abbreviation: ANC, acid neutralizing capacity.

[a]Changes to fish (ANC impact 1) and insect parameters (ANC impact 2) affect the impact of ANC on biological response (Figure 3) and are modeled in two scenarios.

[b]Changes to the sulfur deposition ratio affect the evaluation of exceedance and are modeled in two scenarios.

>140,000 hydrologic catchments (Figure 1). We graphically reflected changes among scenarios for the Great Smoky Mountains National Park, an area of significant natural and cultural significance.

Also, within EMDS, the CDP (InfoHarvest, Seattle, WA) engine implements the analytical hierarchy process (AHP; Saaty, 1994) and the Simple Multi-Attribute Rating Technique (SMART; Kamenetzky, 1982), which can be used for both strategic and tactical planning. The AHP and SMART utilities allow application developers to clearly show their decision criteria, relativize weightings amongst criteria, and calibrate decision-making processes.

RESULTS

Machine learning modeling

Continuous ANC and BC_w estimates for the study region are shown in Figures 4 and 5. High CL exceedance varied directly with stream water ANC values <50 $\mu eq \cdot L^{-1}$ and soil BC_w values <50 $meq \cdot m^{-2} \cdot year^{-1}$ across the SAM region. Depending on values of ANC and BC_w, relatively sensitive and insensitive watersheds could occur in close proximity.

Aquatic impacts of sulfur and nitrogen deposition

Mapped outputs from the logic model (Figure 6) parallel the logic structure (Figure 3). Each map is symbolized in terms of strength of impact of S + N deposition. Dark blue indicates a good condition (very low impact), whereas dark red indicates a poor condition (very high impact).

Figure 6 displays overall results for the baseline scenario (i.e., the original data), in which the reference ANC threshold for computing *exceedance* was set to 50 $\mu eq \cdot L^{-1}$. Within the full study area, S CL *exceedance* was often very high (i.e., [(ambient S deposition)/(S CL)] > 2) at higher elevations of the region, even when the ANC reference condition was set to the relatively liberal criterion of 50 $\mu eq \cdot L^{-1}$.

Impact response for *insect species richness* and *fish impact* similarly demonstrated greater impacts (Figure 6),

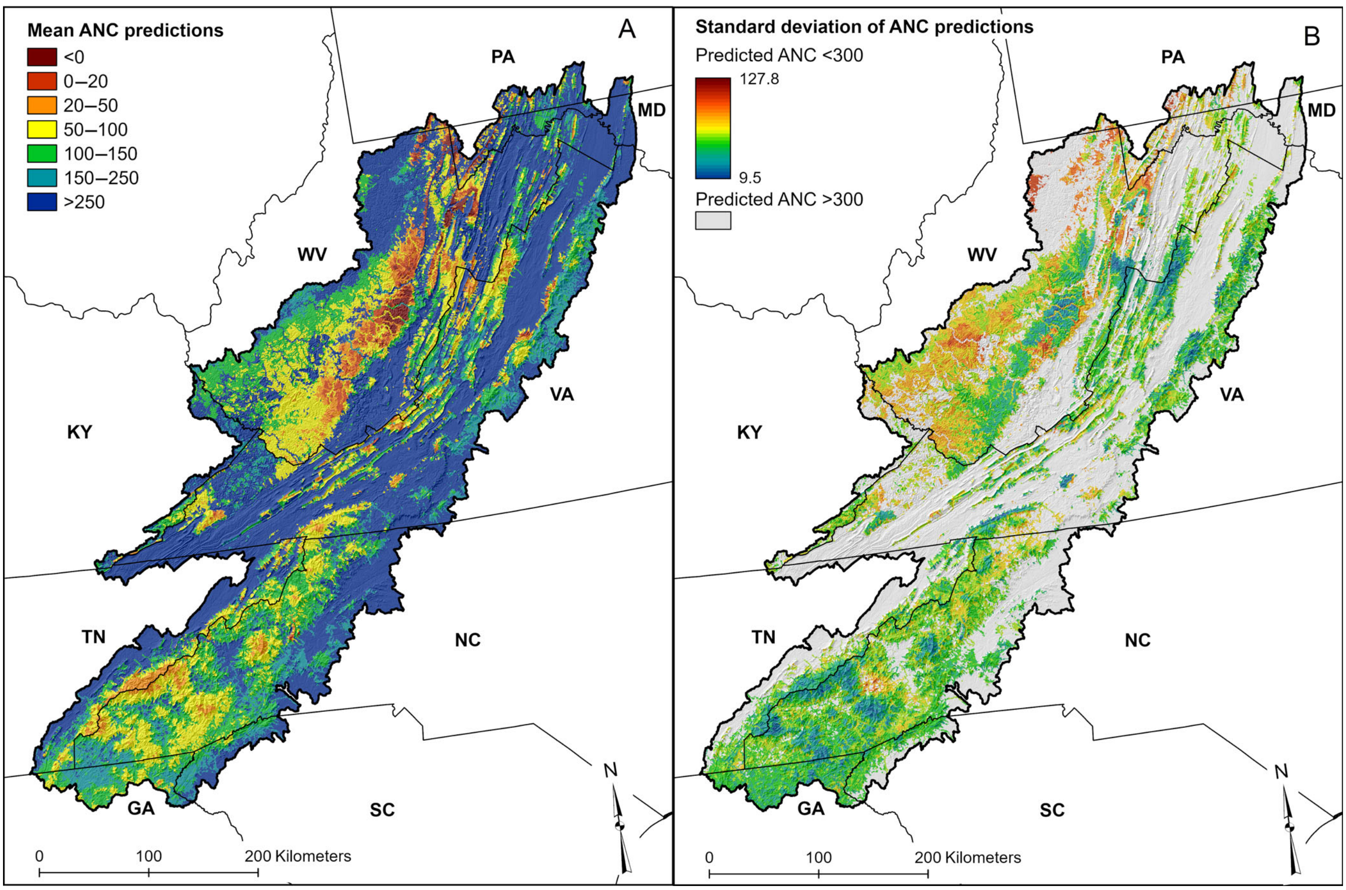

FIGURE 4 Mean and standard deviation of acid neutralizing capacity (ANC) predictions from 1000 regression trees were used to derive the random forest model for the study region.

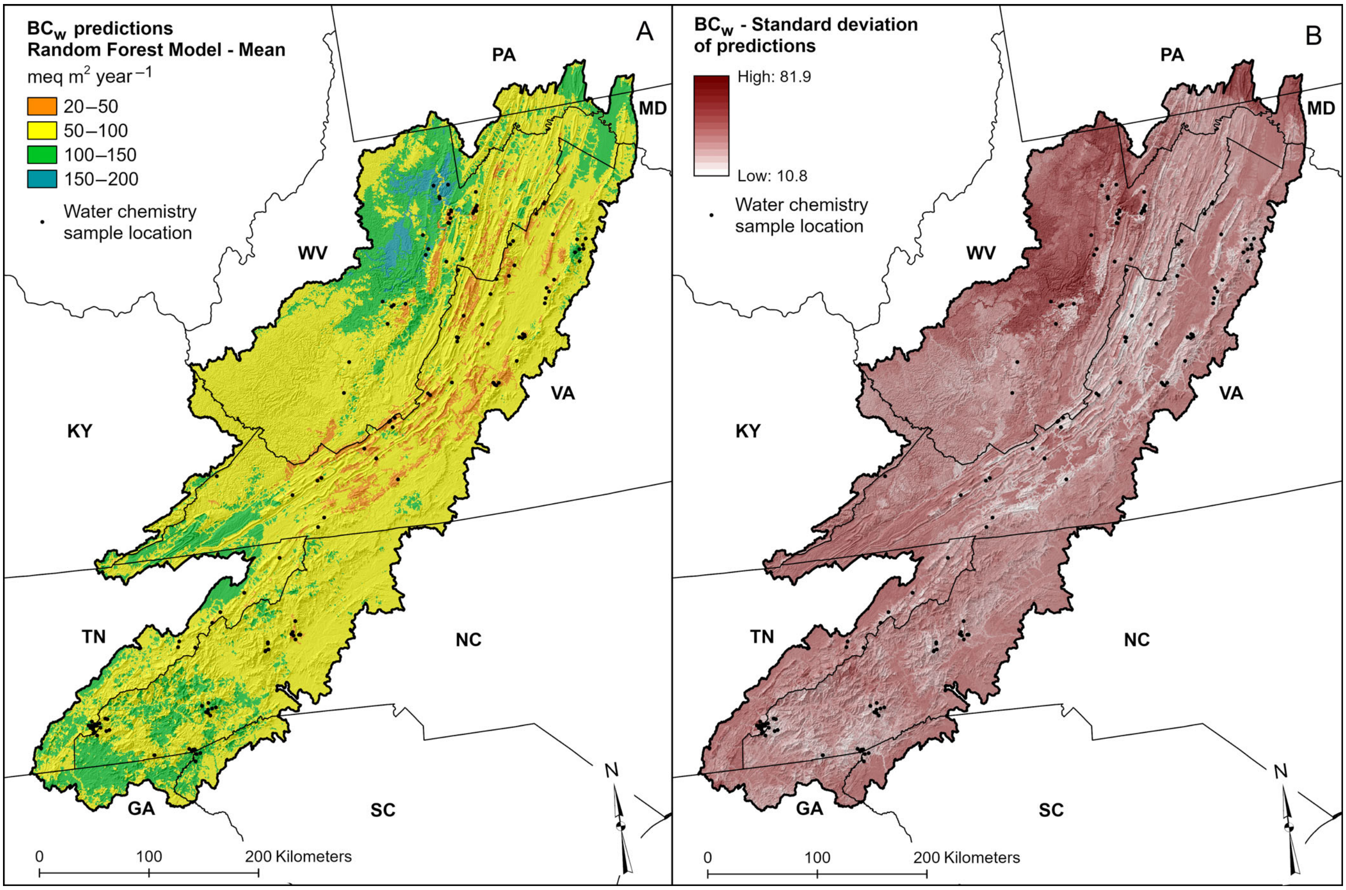

FIGURE 5 Mean base cation weathering (BC_w) and standard deviation of BC_w predictions from 1000 regression trees used to derive the random forest model for the study region.

which were associated with higher elevation environments. The random forest-based machine learning approach used to predict ANC (Figure 4) and BC_w (Figure 5) also generated estimates of the prediction uncertainty (i.e., standard deviations of the predicted response), which were mapped along with *biological response* (Figure 7) and *exceedance* (Figure 8) outputs. Recall that both *insect* and *fish species richness* (Equations 1 and 2, respectively) were functions of ANC. Thus, the SD of ANC could highlight the areas where monitoring *biological response* predictions would be a priority. For example, note that where the strength of impact on *biological response* was predicted to be low, the SD of ANC was generally high. This combined result illustrated that there was high uncertainty about ANC predictions of subwatersheds in these areas. Thus, in such areas, biological response predictions warrant field monitoring to validate and refine these uncertainties. Conversely, where the strength of impact on *biological response* was predicted to be high or very high, the SD of ANC was generally low, which meant that in these areas, watersheds showed a substantial area with low ANC values (Figure 7), and uncertainty surrounding these predictions was low.

The relationship between the uncertainty in BC_w predictions and high impact on *exceedance* is somewhat analogous to the relationship between *biological response* and the SD of ANC (Figure 8). However, in this case, the figure only provides a partial explanation. While BC_w may be the most influential term used to calculate the CL, it is just one of five terms that go into the calculation. Error or uncertainty estimates for the other terms were unavailable for this modeling effort; otherwise, they would have been included. Nonetheless, note that where the strength of impact on *exceedance* is predicted to be high or very high, the SD of BC_w is generally low, and therefore uncertainty for BC_w predictions in these watersheds is also low (Figure 7). Conversely, note that where the strength of impact on *exceedance* is predicted to be low, the SD of BC_w is often high, although the relation is weaker.

Scenarios and change detection in the Great Smoky Mountains National Park

Next, we examine the Great Smoky Mountains National Park. First, we show a detailed view of the higher level logic

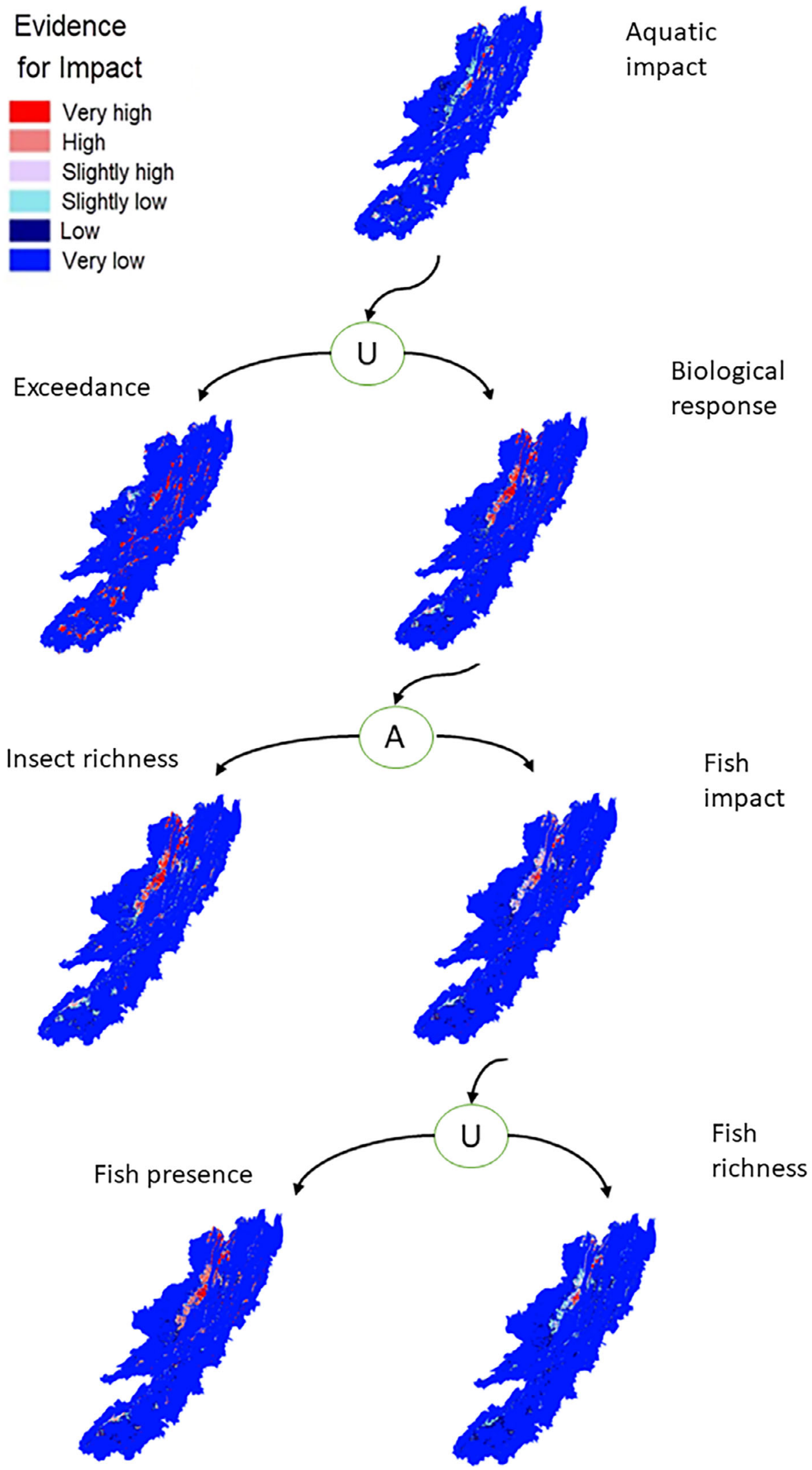

FIGURE 6 Aquatic impacts of acidic S and N deposition in the Southern Appalachian Mountain region, expressed as very low to very high impact. Full-size maps of the thumbnails displayed in this figure are presented in Archive 3, Figure6 full-size images.zip, https://osf.io/5gmwe. A, AND; U, union.

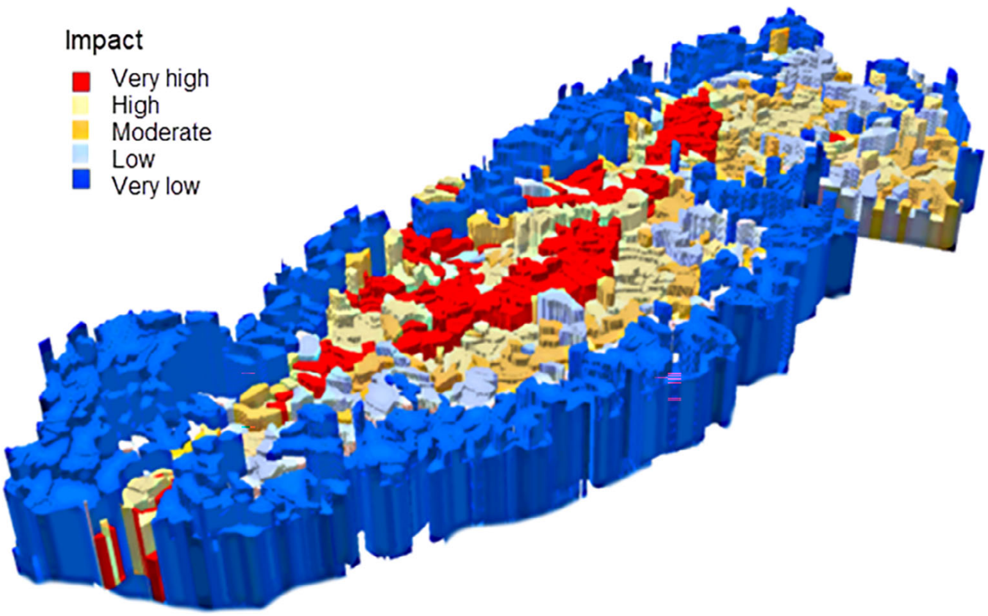

FIGURE 7 Strength of biological response (very low to very high impact) shown with standard deviation of predicted acid neutralizing capacity for the Great Smoky Mountains National Park area.

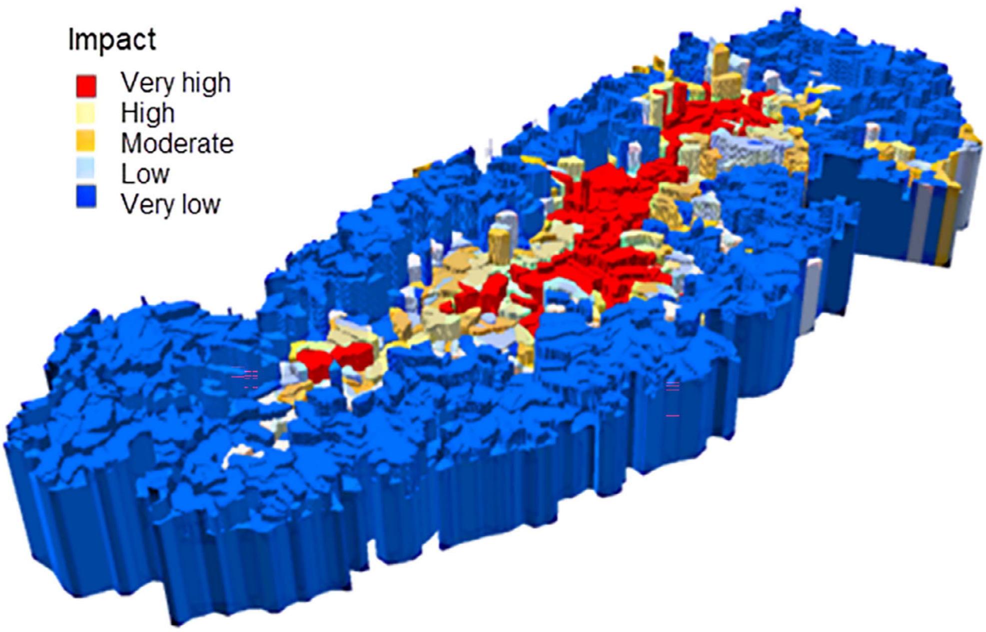

FIGURE 8 Strength of critical load exceedance response (very low to very high impact) shown with standard deviation of predicted base cation weathering for the Great Smoky Mountains National Park area.

components for aquatic impact on the park (Figure 9). Typical of the entire SAM region, the strongest aquatic impact is associated with higher elevations, and this is likewise true for biological response and exceedance in the park.

A change detection map for the ANC impact 1 scenario (change in fish parameters, Table 3) was generated by subtracting the scenario value for strength of biological response from the strength of biological response in the baseline case, for each subwatershed polygon (Table 1), and mapping that value as absolute change for the polygon (Appendix S3: Figure S1). This latter method for calculating change (baseline value minus scenario value) is used throughout all scenarios discussed subsequently. In the case of the ANC impact 1 scenario, scores for biological response were always less than or equal to the scores in the baseline case, so the change metric was

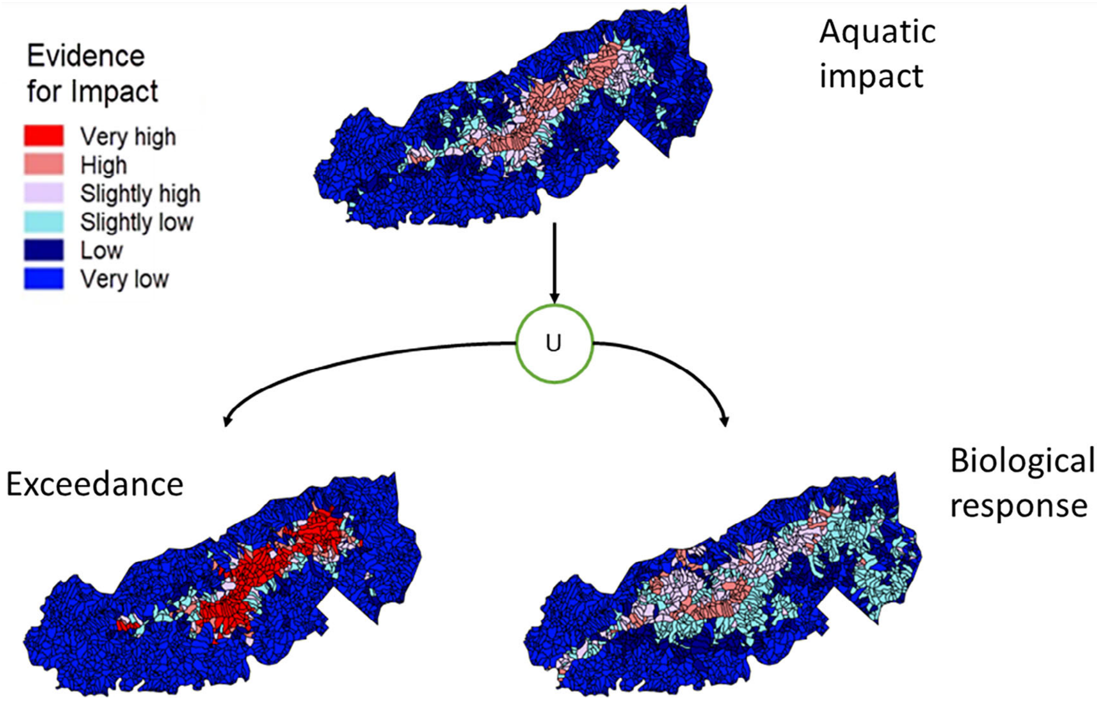

FIGURE 9 Strength of aquatic impact response (very low to very high impact) for the Great Smoky Mountains National Park. U, union.

always positive, indicating movement to a degraded condition (Figure 10A). As seen in the figure, changes due to the scenario were relatively modest, but change was common across the Park.

For the ANC 2 impact scenario (change in the insect parameter, Table 3), the relatively small departure in the minimum acceptable value for insect species richness produced a surprisingly strong response (Figure 10B; Appendix S3: Figure S2), both in terms of the range of response and the high frequency of changed subwatershed responses. As with the previous discussion, here also the change was in a positive direction, so the map of change reflects degraded conditions.

The Exceedance 1 and 2 scenarios tested for change due to 50% reductions (Figure 11A) and increases (Figure 11B) in S + N deposition, respectively. What was readily apparent in both scenarios (Figure 11), however, was that the change in exceedance impact (positive or negative) generally varied with elevation in the park because (1) the changes are proportional to the deposition rate, (2) deposition generally increases with elevation, and (3) higher elevations tend to have lower CLs (Figure 9; Appendix S3: Figures S3 and S4).

DISCUSSION

Our study provides a logic-based interpretation of the aquatic impacts of S + N deposition in the SAM region. The four elementary topics (Figure 3) combine two contrasting perspectives: one is long-term, the other short-term. *Exceedance* represented a potential regulatory and a long-term impact perspective; *insect species richness*, *fish species richness*, and *fish presence* represented shorter term perspectives on biological response of sensitive ecosystem components. The overall model of *aquatic impact* is a synthesis of these perspectives.

In any study of *aquatic impacts* associated with S + N deposition, logic-based map products (Figure 6) provide synoptic views of the spatial assessment. The EMDS system also implements a "surgical" perspective, wherein a user can drill into the derivation steps that produce the model results for individual spatial units via a graphical interface to the logic engine. This capability is useful for understanding and adapting model behavior in the developmental stages of a project (Figure 12).

The four scenarios (Table 3) and associated change analyses (Figures 10 and 11) produced both expected and surprising results. In the baseline analysis (Figure 6), the minimum acceptable value for *insect species richness* was set to a relatively high value of 0.90 (Table 1), based on the premise that insects were critical to fish presence and species richness, and because they played a foundational role in the food web. The relatively strong response (Figure 10B) to set the latter value to 0.95 (a relatively small change) was therefore somewhat surprising. On the other hand, the results for the change analyses of the two exceedance scenarios (Figure 11A) were as expected given the greater

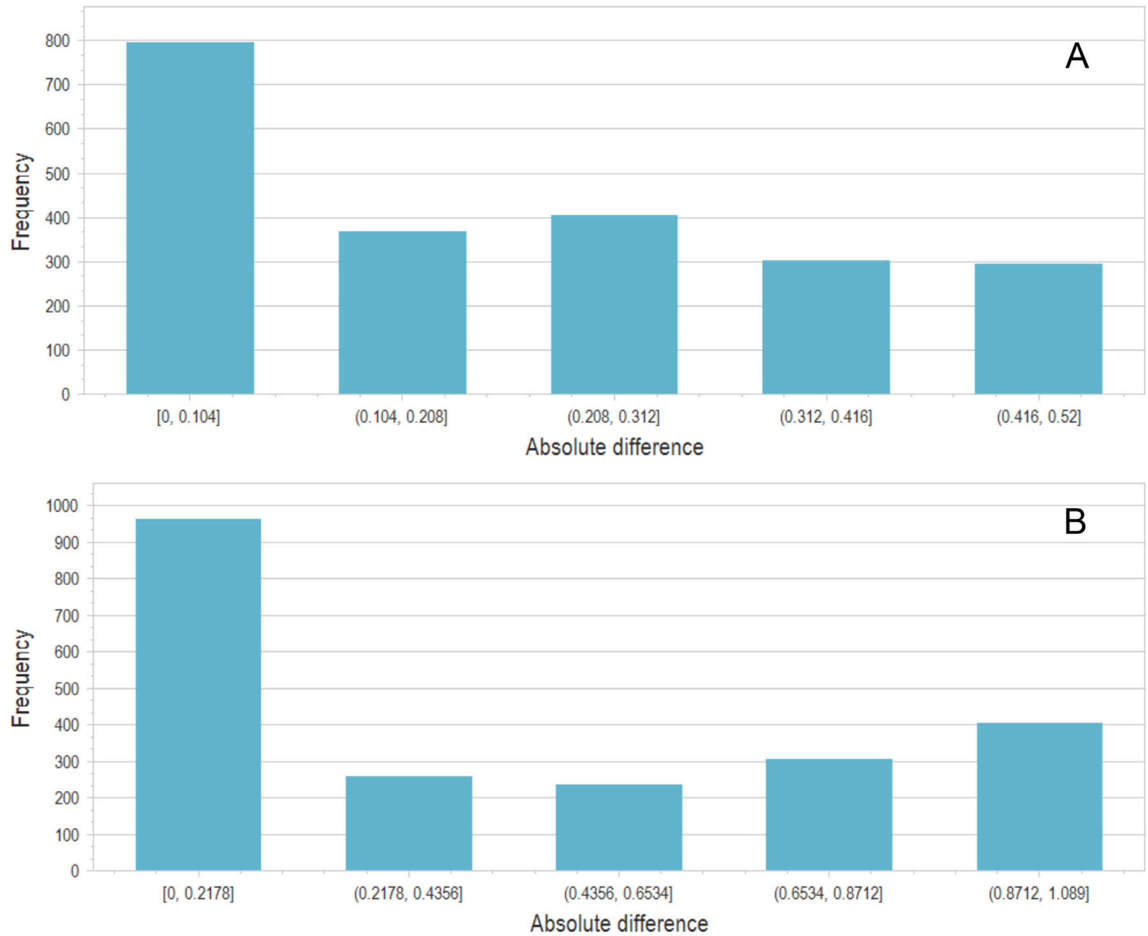

FIGURE 10 Absolute change in biological response impact in response to changes in fish (A) and insect (B) parameters for the Great Smoky Mountains National Park (acid neutralizing capacity [ANC] impact 1 scenario 1 and ANC impact 2 scenario 2, respectively, in Table 3). The change in biological response is calculated as the original NetWeaver score minus the scenario score based on parameter changes in the scenarios. Because the parameter changes in both scenarios represent stricter requirements, the scenarios perform more poorly, so the difference is always positive. Corresponding maps of changes are presented in Appendix S3: Change detection maps for scenarios.

deposition at higher elevations (Figure 9; Appendix S3: Figures S3 and S4) and the change being proportional to S + N deposition rates.

Estimates of S + N CLs and exceedances are of high interest to public land managers in the SAM region. Also, of interest is the ANC value that a stream in any catchment may likely have in the future. Maps of the potential stream ANC for Southern Appalachian National Forests were prepared by Jackson (2015) following numerous EMDS runs that varied the ANC threshold, the amount of S deposition (only S deposition was assessed in this earlier work), and whether the catchment would have timber harvested. If S deposition was reduced by 50% from the 2009 to 2011 average, then 96% or more of the streams would show an ANC suitable for brook trout. The analysis estimated that more streams within the National Forest boundaries would have an ANC of 100 μeq · L^{-1} or greater if there was no timber harvesting and if a 50% reduction in S deposition was realized (Jackson, 2015). Future changes in BC_{dep} and BC_{up}, among other CL model inputs, due to climate change effects may potentially result in future ANC conditions that deviate from expectations based on ambient input data. Furthermore, although NH_4^+ deposition is not the primary component of N deposition in this region, areas in which NH_4^+ deposition is a significant component of N deposition (e.g., downwind from agricultural land use) may experience greater N-induced soil acidification than otherwise estimated by CL models derived based on deposition of oxidized N forms.

The results presented here summarize foundational work on statistical models to predict ANC and BC_w across the SAM Region and then use these predictions to logically evaluate biological and ecological aquatic impacts. The present study only represents the first two steps in a complete decision support process that could more fully address aquatic impacts associated with S + N deposition. In particular, the logic-based assessment characterizes aquatic impacts, providing an important foundation for a planning process, but it does not provide

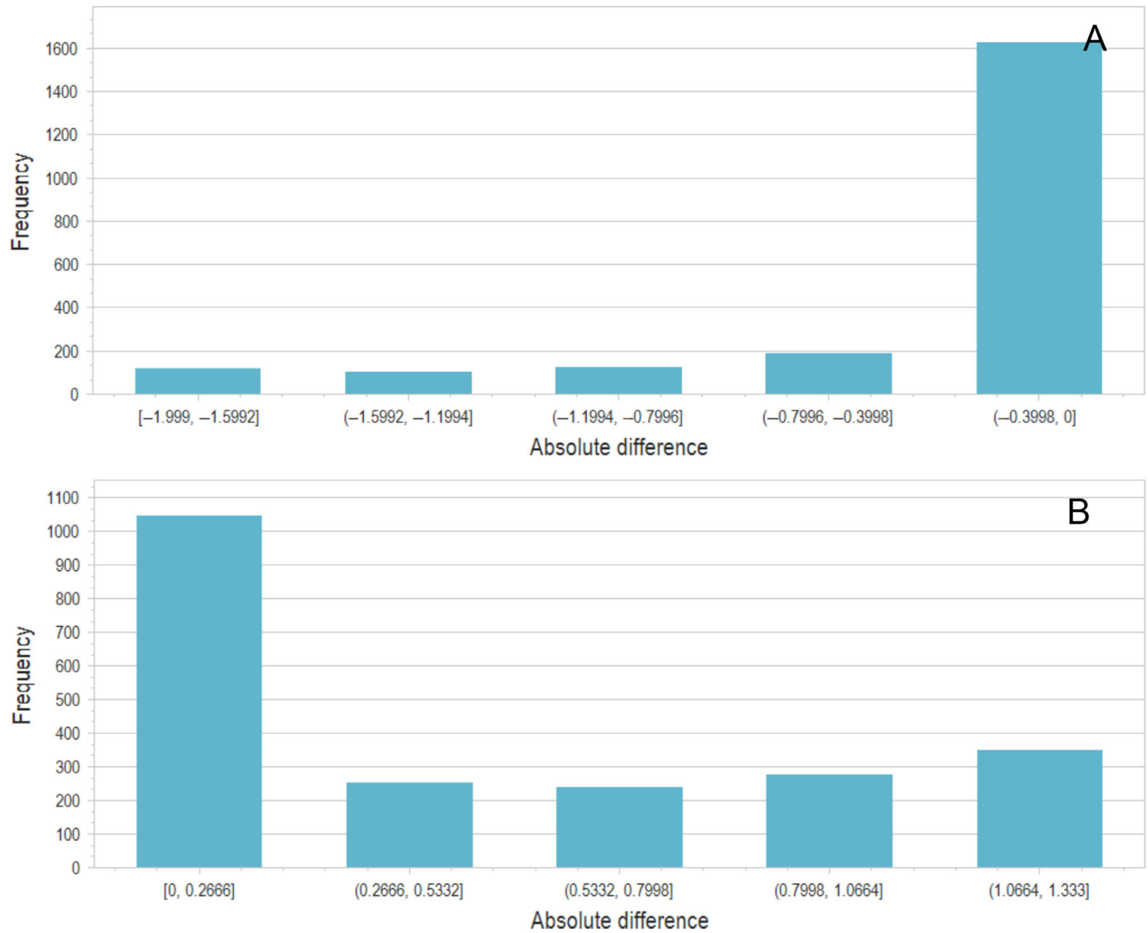

FIGURE 11 Change in exceedance impact due to S and N deposition ratios of 0.5 (A) or 1.5 (B) for the Great Smoky Mountains National Park (Exceedance 1 scenario and Exceedance 2 scenario in Table 3). The change in exceedance response is calculated as the original NetWeaver score for exceedance minus the scenario score based on parameter changes in the scenarios. Scenario 1 represents an improved outcome for exceedance, so the change is negative. Similarly, scenario 2 represents a poorer outcome, so the change is positive. Corresponding maps of changes are presented in Appendix S3: Change detection maps for scenarios.

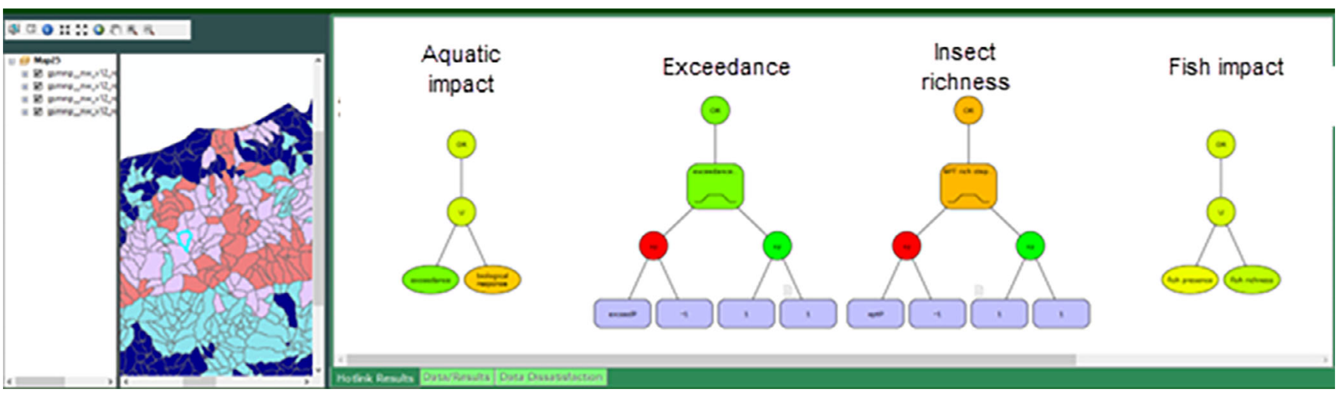

FIGURE 12 Ecosystem Management Decision Support tool for viewing details of NetWeaver logic at the feature level. From left to right, the panes in this figure show: (1) a table-of-contents view of logic topics that have been selected in the tool; (2) a thumbnail map (zoomed in this example) to select a specific feature; and (3) NetWeaver logic topics associated with the table of contents. In the example, a feature has been selected from the map, and the NetWeaver topics are shown in their evaluated state (color coding is for strength of evidence), because the topics are dynamically linked to the selected feature in the map.

explicit support for implementing strategic and tactical planning decisions to address impacts.

In describing EMDS (see The Ecosystem Management Decision Support system), we alluded to decision models as optional components of EMDS applications. Although decision models have yet to be designed for the current application, here we consider how such models can usefully extend the current application with additional functionality.

Potential enhancements to the SAM CLs application

Logic and decision models in EMDS complement one another. A logic model focuses on the state of the system, whereas a decision model focuses on what can be done about the conditions that are found, where ecological concerns are revealed. Logistical and financial limitations to management are not pertinent to the logic model, but they are central to the decision model. An important consequence of separating the overall modeling problem into two complementary models is that each model is rendered conceptually simpler. The logic model evaluates the status of the topics under evaluation, in this case, the *aquatic impact* of S + N deposition (Figure 3). A strategic decision model, implemented in CDP, for example, would not only consider the status of *aquatic impact* in each watershed but could also place it in a management context. Once placed in this context, decision-making is informed by considering practical issues of technical and economic feasibility and efficacy considerations associated with selecting specific watersheds for protection and restoration. These choices would depend on map resources like those provided in Povak et al. (2017, 2020) or Jackson (2015). For example, before stocking brook trout in a stream where they have been extirpated, a manager could evaluate the evidence that they would survive under current acidity conditions.

An additional decision support step might similarly consider tactical choices for high-priority management actions that are most applicable to the specific biophysical and socioeconomic contexts of watersheds. For example, Pascual et al. (2022) applied mixed integer optimization to identify stewardship actions that could be implemented across space and through time to reduce the impact of an invasive species (strawberry guava) on Hawai'i Island. Optimization showed the benefit of clustering treatments over space and time to improve financial efficiency of strawberry guava removal.

Any of the three EMDS decision tools (and their analytical engines), CDP (http://infoharvest.com/ihroot/index.asp, last accessed on 12 April 2022), GeNIe (https://www.bayesfusion.com/, last accessed on 12 April 2022), or VisiRule (https://www.lpa.co.uk/, last accessed on 12 April 2022) might be suitable for this latter tactical decision phase, depending on the questions to be addressed and user preferences as to the choice of modeling tool. For example, a VisiRule decision tree or GeNIe Bayesian network might be designed to recommend specific management actions to mitigate deposition effects, given consideration of specific vegetation, fish, and wildlife species as well as the biophysical context of an affected watershed.

The EMDS system can address multiple aspects of habitat suitability for aquatic species. Factors such as stream temperature and sedimentation could also be incorporated into the current EMDS system to provide greater capacity for evaluating stream conditions related to stressors in addition to acidification. For example, previous work to characterize stream temperature within the SAM region (McDonnell et al., 2015) could be used in conjunction with conditions related to ANC and CL exceedance to identify those conditions that would be most responsive to mitigations. Additionally, CLs for the protection of terrestrial biota, such as trees and herbaceous vegetation, could be incorporated into the EMDS application to expand its utility to a variety of local land management situations.

System enhancements to the SAM CLs application described here are feasibly implemented in a more comprehensive application. Such an application was presented in Marcot and Reynolds (2019), who provided an example workflow for employing all four analytical engines within EMDS in a relatively more complex application for maintaining ecosystem integrity (static) or resilience (dynamic) through time.

Decision support for long-term management of CLs and their associated ecological impacts requires evaluating trajectories of alternative management scenarios over potentially long time frames, where influential conditions may shift. Abelson et al. (2021) present an EMDS application for evaluating the performance of alternative management strategies for maintaining ecological integrity in the Lake Tahoe Basin (Lake Tahoe, CA) over the 21st century, using workflow functionality in EMDS to model time series of predicted system outcomes and associated management effects. Analogous solutions could be developed for CL applications in our SAM project area or other areas where CL concerns are also important. The incorporation of temporally varying conditions in the analysis would allow for an assessment of ecosystem resilience to prolonged exposure to S + N inputs rather than simply a static look at current ecosystem condition or integrity.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflicts of interest.

DATA AVAILABILITY STATEMENT

Data and archived materials (Povak, 2022) are available from the Open Science Framework: https://osf.io/5gmwe.

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SUPPORTING INFORMATION

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