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Cokriging to Assess Regional Stream Quality in the Southern Blue Ridge Province

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Cokriging is used to predict stream chemistry at unsampled locations with the use of spatial and intervariable correlation. The technique is used in this study to predict the acid neutralizing capacity (ANC) of streams in the Southern Blue Ridge Province (SBRP). ANC measurements between pairs of streams surveyed in this region were found to be spatially correlated over distances up to around 40 km. Predictions were improved by including elevation in the analysis to represent the combined influence of elevational gradients in climate, geology, soils, hydrology, and vegetation on stream ANC. The cokriging analysis identified specific stream reaches predicted to be most sensitive to acidification and located areas of high uncertainty. Stream ANC levels below 50 μeq/L were predicted for one-fifth of the upper nodes associated with digitized headwater reaches in the SBRP. The majority of these were located in the higher elevations of the Great Smoky Mountains National Park, in the vicinity of Mount Mitchell, and in the Blue Ridge Mountains in southern North Carolina.

INTRODUCTION

As concern for large-scale environmental problems, such as acid rain, global warming and climate change, ozone depletion, nonpoint-source pollution of surface waters, and air pollution, has grown in recent years, the need for regional impact assessment has increased. It is anticipated that future efforts to detect and ameliorate the effects of large-scale environmental problems will require the development of new monitoring and assessment methods [*Science Advisory Board*, 1988]. The key features of these large-scale problems are spatial variability and geographic extent. Consequently, assessment techniques are needed that explicitly deal with environmental data in a spatial context. Spatial statistical methods are well suited to the assessment of spatially explicit environmental data and deserve special attention in the development of new assessment methods. This paper demonstrates two valuable roles for spatial statistics in regional assessment: (1) the location of specific problem areas or resources at risk and (2) the estimation of regional distributions for environmental attributes from spatially extensive survey sample data.

Future efforts to study or ameliorate impacts on specific lakes and streams will require identification of individual surface waters that are likely to be susceptible to acidification. Since it is generally not feasible to take chemical samples of all stream reaches within a region, methods are needed for locating susceptible streams based on limited survey data. Kriging can provide estimates of stream chemistry at desired locations based on available survey data. These estimates can then be used to pinpoint environmental problem areas for study or remediation.

A second role of spatial methods is to produce refined regional population estimates from survey data. Recent large-scale environmental surveys have identified large regions of the eastern United States that contain surface waters characterized by low buffering capacities, making these systems sensitive to impacts from acidic precipitation [*Omernik and Powers*, 1983; *Landers et al.*, 1988; *Schindler*, 1988]. In response to the Acid Precipitation Act of 1980, the United States Environmental Protection Agency (EPA) has conducted synoptic surveys of lakes and streams in these potentially sensitive areas [*Linthurst et al.*, 1986; *Kaufmann et al.*, 1988]. To date, analysis of survey data has successfully characterized the chemical status of surface waters in many regions of the United States with a statistical approach that requires no assumptions about resource attributes. However, this approach removes the resources from the spatial context in which they occur, and, in general, does not benefit fully from the resource information gained by sampling. The spatial statistical approach presented here produces refined regional population estimates that take advantage of the spatial context of the population.

Spatial Autocorrelation in Stream Acid Neutralizing Capacity

Kriging techniques make use of the fact that many natural phenomena exhibit spatial autocorrelation. Streams that are close together tend to share similar soils, geology, climate, vegetation, atmospheric deposition rates, and other environmental factors that influence surface water chemistry. Kriging methods construct a regional model of spatial autocorrelation to estimate variables, such as water chemistry, at unsampled locations based on data measurements at sampled locations. Cokriging methods use not only the spatial autocorrelation information but also spatial correlations with other environmental variables. Cokriging can improve prediction of surface water chemistry with the addition of covarying geographic variables. An important feature of both techniques, from both a scientific and policy point of view, is that variance estimates are provided that quantify

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the uncertainty associated with predictions at each location. These estimates can be used to display the spatial patterns in uncertainty throughout a region and to identify localized areas where additional sampling efforts should be directed.

In this study, we use the spatial statistical technique of cokriging to predict the acid neutralizing capacity (ANC) of streams in the Southern Blue Ridge Province (SBRP), one of the regions studied by the EPA synoptic surveys [*Messer et al.*, 1986, 1988; *Kaufmann et al.*, 1988]. The SBRP is of particular interest because of its exposure to relatively high levels of atmospheric deposition and the existence of low ANC surface waters in the region [*Church*, 1989]. ANC measures the ability of a stream to neutralize or buffer acidic inputs and is therefore a good indicator of sensitivity to acidification. We demonstrate in this paper that SBRP stream ANC, measured as part of the National Stream Survey (NSS), exhibits spatial autocorrelation over distances up to approximately 40 km and is therefore well suited to the cokriging approach. Elevation is used as a covariate in the cokriging analysis because of its correlation with ANC and because it is also a spatially autocorrelated attribute of streams.

This application of kriging is unconventional in that streams do not exist everywhere in the two-dimensional landscape, suggesting that stream distance or connectedness between stream reaches might be a more appropriate distance measure than euclidean distance. On the other hand, there are many influences on stream ANC that operate in the full two-dimensional landscape. *Church* [1989, p. 801] emphasized the fact that streams should not be divorced from their watersheds, noting that "although surface waters can be affected by acidic deposition originating from emissions many miles distant, the importance of the watershed as a unit remains crucial to the understanding of current and future aquatic effects. Indeed, for drainage lake and reservoir systems in the Northeast, Upper Midwest, and Southern Blue Ridge Province of the U.S., a vast majority of ANC production occurs as a result of biogeochemical processes within the surrounding watershed."

The spatial associations between directly linked streams in a network may be superimposed on the field of spatial autocorrelation caused by watershed processes and other two-dimensional factors. The approach used here restricts attention to euclidean distances in studying the spatial autocorrelation among stream reaches.

Effects of Elevation on ANC in Streams

The Great Smoky Mountains and Southern Blue Ridge Mountains occur in the SBRP. The elevational range among sampled NSS streams in this region is 728 m (see Figure 1) and the correlation between elevation and $\log_e$ (ANC) among sampled NSS reach nodes is -0.51 ($p = 0.0001$). The next-highest correlation between ANC and any geographic variable measured by the NSS was with stream grade, which correlates well with stream elevation. This suggested that including elevation as a covariate would improve ANC predictions.

A decreasing trend in buffering capacity along an elevational gradient has been noted in other surface waters and areas as well. Both *Winger et al.* [1987] and *Silsbee and Larson* [1982] report a significant negative correlation between elevation and alkalinity in the SBRP. Lakes in the Adirondack Mountains show a strong negative correlation (-0.63) between ANC and elevation [*Hunsaker et al.*, 1987; *Brakke et al.*, 1988]. *Turk and Adams* [1983] report a much stronger association in the Flat Tops Wilderness Area of Colorado, with elevation accounting for 76% of the variance in lake alkalinity.

Elevation is a complex gradient that represents the combined influence of other environmental gradients such as geology, soils, vegetation, and climate [*Whittaker*, 1973]. Several of these factors contribute to the tendency for stream and lake ANC to decrease at higher elevations.

Average annual precipitation tends to increase with elevation [*Dingman et al.*, 1988] and ranges from about 140 cm to 250 cm in the Great Smoky Mountains National Park [*Silsbee and Larson*, 1982]. Increased precipitation, combined with lowered temperature and evapotranspiration, leads to an average stream discharge at high elevations that is approximately double that at low elevations [*Silsbee and Larson*, 1982]. Streams at high elevations drain watersheds that spend a larger percentage of time in the clouds, which generally have a low pH. Higher wind velocities result in greater interception and deposition of aerosols. *Swank and Waide* [1988] report that sulfate deposition showed a measurable increase at higher elevations in Coweeta, North Carolina, with sulfate replacing bicarbonate as the dominant anion in stream water. These orographic effects result in increased deposition of sulfate and hydrogen ion with elevation.

In addition to increased deposition, the amount of buffering of precipitation accomplished by cation exchange interactions with soils is likely to decrease with elevation. Steep slopes and shallow soils lead to a lower soil water contact time (quick flow), lowering the potential for sulfate adsorption by soils and decreasing the potential for release of base cations through weathering and ion exchange. *Swank and Waide* [1988] measured a greater fraction of precipitation discharged as quick flow in high-elevation catchments. They postulate that lowered temperatures reduce overall biological activity, causing a decrease in the rates of sulfate adsorption and microbial incorporation of sulfate into organic sulfur at higher elevations.

The geology of a site in the SBRP sometimes determines its elevation, with more-resistent, slow-weathering formations at higher elevations. In valley regions with limestone geology the streams tend to run in limestone-bearing faults or windows. Limestone weathers quickly and provides buffering capacity to streams. Resistant sedimentary rocks make up the Great Smoky Mountains, while metamorphic and granitic rocks characterize the Blue Ridge Mountains to the southeast [*King et al.*, 1968]. Neither of these bedrock complexes weather easily or provide much buffering capacity to streams. In addition, a sulfur-bearing Anakeesta formation occurs at high elevations in some areas of the Smoky Mountains and is a natural source of acidity. In general, the contribution to streams from groundwater buffered by contact with bedrock decreases with elevation, leaving a larger fraction contributed by more-acidic surface flow.

The relationship between ANC and elevation can be modeled as a stochastic and/or a deterministic relationship. In the cokriging approach used here, the relationship between the two variables was modeled as a statistical association, with no deterministic component other than a constant unknown mean. More deterministic alternatives to cokriging

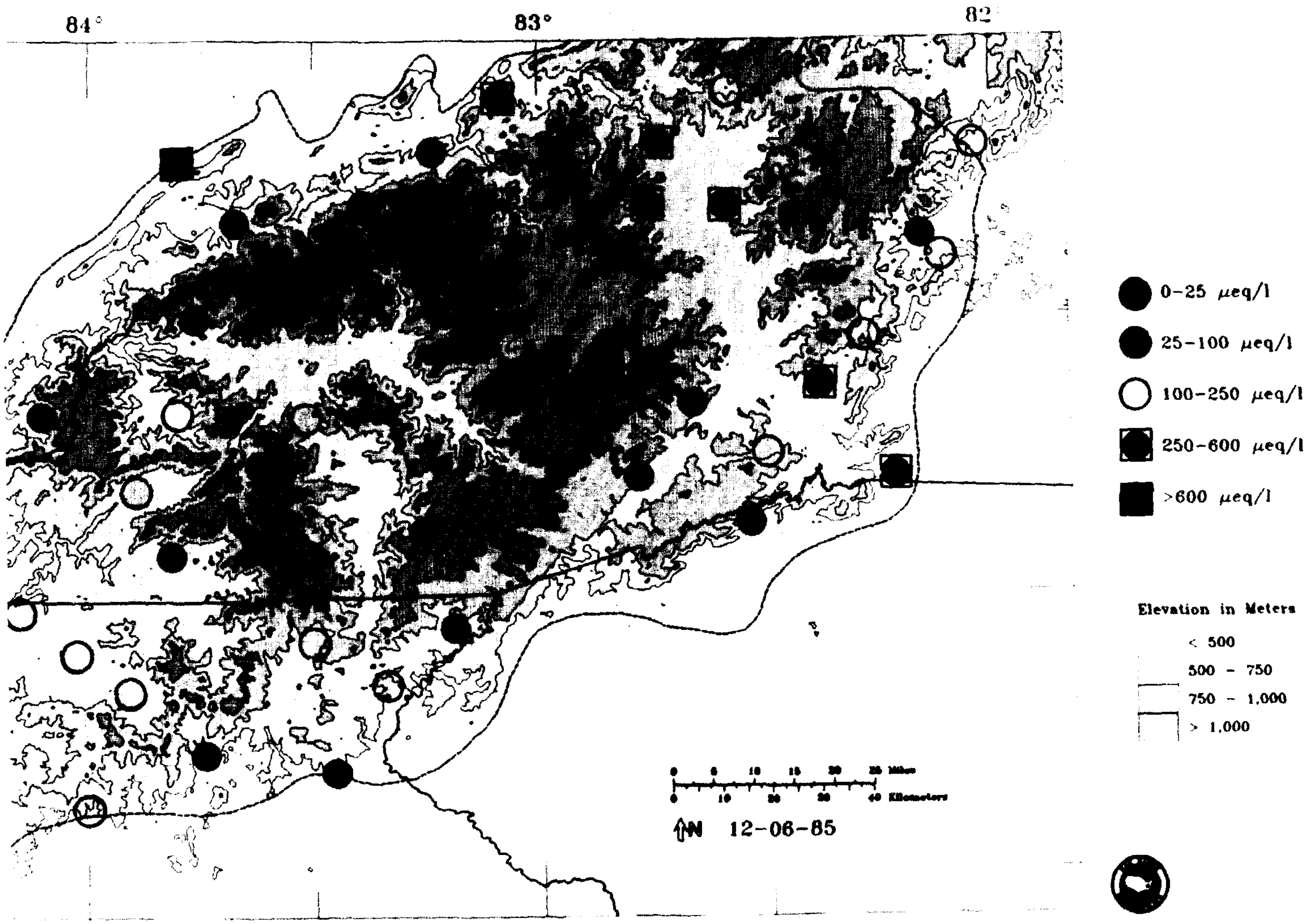

Fig. 1. National Stream Survey sample locations and measured ANC classes.

would model the local mean ANC (drift) at each stream node as a function of elevation. The mean ANC at each location would then be represented either as a function of surrounding elevations (ultimately a complex integrated watershed model) or as a function of the elevation at that location alone [see *Stein*, 1984; *Ahmed and DeMarsily*, 1987].

METHODS

Regional Survey Data

In the spring of 1985 a pilot study of the National Stream Survey was conducted in the SBRP [*Messer et al.*, 1986, 1988]. A target population was defined in the statistical design of the survey and can be summarized as the population of medium-sized stream reaches draining watersheds of around 10^2–10^4 ha. Streams to be included in the sample were selected by placing a grid over 1:250,000-scale U.S. Geological Survey (USGS) maps and identifying the first target reach encountered following the downhill gradient from each grid point [*Overton*, 1987]. The streams sampled were generally characterized as low-order reaches <1 m deep and <5 m wide during base flow conditions [*Messer et al.*, 1986]. Methods used in the pilot study and in the first phase of the NSS are described by *Messer et al.* [1986] and *Kaufmann et al.* [1988], respectively. For each of the reaches in the NSS sample, chemistry measurements were taken at the downstream node on three occasions. An average of the three ANC measurements sampled in the spring was referred to as the "index" chemistry in the NSS. This "index" chemistry was sampled in the spring because streams typically exhibit low ANC at that time and because sensitive life stages of biota are typically present [*Messer et al.*, 1986]. We have used spring index chemistry for lower nodes supplemented by available upstream measurements, providing a total of 75 sample locations (see Figure 1). Since the data used in this analysis derive from a synoptic survey designed to record a snapshot of stream chemistry in time, our results are also tied to the base flow conditions of the spring of 1985 and are not intended as predictions of future chemistry. However, base flow chemistry was selected for the index to provide a more stable characteristic over time and is relevant to regional assessment.

EPA Computerized Stream REACH Population

Ideally, ANC predictions would be produced for all target reaches in the SBRP. Our best approximation to the 1:250,000-scale target population of reaches is shown in Figure 2. The reservoirs and lakes shown on the map were excluded. These reach traces were obtained from 1:500,000-scale USGS maps but are not guaranteed to contain all reaches that appear on those maps. REACH files containing these traces and their attributes are maintained by the EPA and are available from the STORET retrieval system [*Olson et al.*, 1981]. We used the geographic information system ARC-INFO to obtain the locations for all nodes (intersections) from these reaches. Reach nodes falling on or outside of the boundary were excluded. The 1:500,000-scale REACH population consisted of 420 reaches and 416 reach nodes interior to the SBRP region boundary.

ELEVATION DATA

Computerized elevation data were available from digitized topographic maps at all points at which ANC predictions were desired. This abundance of elevation data is important, because the second variable (elevation) contributes to prediction of the main variable (ANC) only at locations where elevation is known and ANC is not.

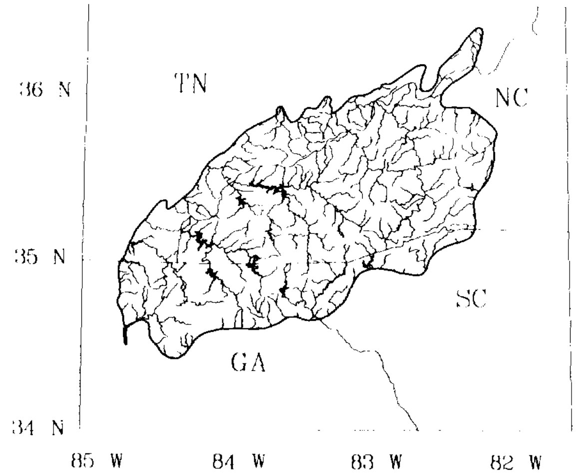

Fig. 2. REACH file reaches from 1:500,000-scale maps.

Elevations were obtained from a grid with 10-s intervals of latitude and longitude (about 30 m). At each EPA reach node, a distance-weighted average of the nearest elevations, reduced by a factor of 0.9649, was used. This factor was obtained by regressing the computerized elevations against those derived from 1:24,000-scale maps for NSS sampled streams (R^2 = 0.96). This correction counteracts a slight tendency to overestimate stream elevations because the grid point elevations are unlikely to occur exactly on the stream where elevation is at a minimum.

Kriging Methods

To illustrate the kriging approach used here, consider elevation as an example. If elevation comes from a random process, then the current topology is one realization of many possible topologies that could have developed on the Earth's surface. While the possible realized surfaces are different, ordinary kriging assumes that the statistical distribution function generating the topologies is characterized by an unknown constant mean and a correlation between locations that is determined by their proximity. Statistical distributions characterized by two parameters, a mean and a variance, are familiar in nonspatial statistics. Observations taken from different locations are usually assumed to be independent (zero covariance). In the spatial statistical approach taken here, the covariance between locations is not assumed to be zero but is assumed to be defined by a decreasing function of distance. In short, we assume that the sample points come from a multivariate normal distribution with a variance-covariance (*V-C*) matrix generated by an admissible covariance function (see *Armstrong and Jabin* [1981] for a discussion of admissible functions). More complete statistical treatments of kriging methods and variations in the assumptions required can be found in the works by *Matern* [1986] and *Delhomme* [1978].

Cokriging estimation requires the identification of an appropriate spatial covariance function for each variable: one for $\log_e$(ANC) and another for elevation. In addition, a cross-variogram function or cross-covariance function is required for each pair of variables. This cross covariance describes the covariance between $\log_e$(ANC) at one stream node and elevation at another node as a function of the distance between them. Spherical distances were used in our analysis, mainly to adjust for the difference between a degree in latitude versus longitude. The covariance functions that we considered require three parameters: (1) the range, or distance over which pairs of stream are spatially correlated; (2) the nugget, or small-scale variation; and (3) the sill, or large-scale variation. The covariance functions for the two variables and the cross covariance were constrained to share a common range and model form. This constraint combined with limits on the parameter values for the cross-covariance model and admissible functions for the three individual models ensures that the joint $\log_e$(ANC)-elevation model will be admissible [*Hoeksema et al.*, 1989].

We employed a variogram estimation procedure that defines the covariance function and/or variogram for each variable using maximum-likelihood (ML) estimation [*Kitanidis*, 1983, 1986]. The parameters obtained using a ML procedure constitute the most-likely values of the true parameters for the process, given the values observed in the sample, under the assumption that the covariance function chosen is correct and that the sample comes from a Gaussian process. A complete description of the technique used for ML estimation is given by *Kitanidis and Lane* [1984]. The program used here to conduct ML estimation of parameters and the cokriging analysis was developed by R. J. Hoeksema [see *Hoeksema et al.*, 1989].

Kriging Assumptions and Validation

Cokriging assumes that the vector of sample measurements comes from a jointly stationary process [*Stein*, 1984]. It is not possible to ascertain whether the stationarity assumption of cokriging is met from a single realization [*Myers*, 1989]. However, several properties of a realization are commonly used to reject the intrinsic hypothesis including (1) anisotropy, (2) the lack of a definite sill in the experimental variogram, and (3) a parabolic shape in the semivariogram near the origin [*Neuman and Jacobson*, 1984; *McBratney and Webster*, 1986].

We chose to model the joint spatial relationship between $\log_e$ (ANC) and elevation as a stochastic cokriging relationship, rather than a partially deterministic relationship involving elevation as an external drift for several reasons. First, the rejection of stationarity based on one realization with 75 points would be quite arbitrary and would require equally strong alternative assumptions including the selection of drift functions without any physical basis and the acceptance of drift parameters estimated from a limited sample size. Second, anisotropy is the only feature of the above three that might be attributed to this realization, and this appearance is caused to some extent by the considerable sample-size differences among direction classes due to the elongated shape of the SBRP region in the NE-SW direction (see Figure 3). In this case, we decided to involve elevation as a joint-stationary field and to err on the side of conservative cokriging variances rather than attempt the estimation of an unknown external drift based on elevation. It is hoped that the use of local cokriging, involving only closer neighbors in prediction, will protect against the effects of a slowly varying mean.

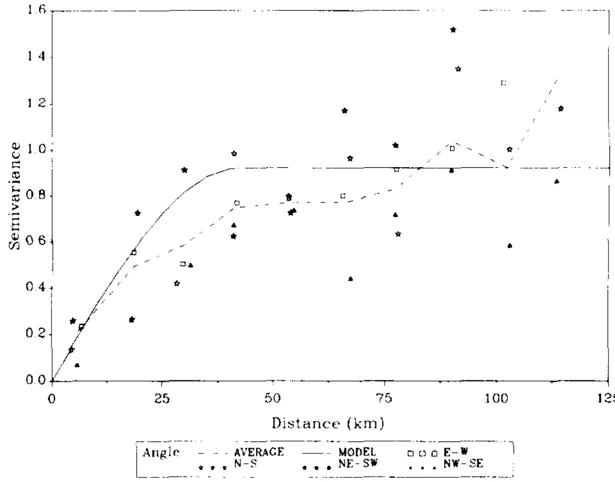

Fig. 3. Directional, average, and model semivariograms for $\log_e$ (ANC).

We make the additional assumption that the random processes involved in this cokriging model are Gaussian. This assumption is important for several reasons: (1) it enables us to use ML parameter estimation, (2) it allows cokriging variances to be used in constructing confidence bounds on the cokriged estimates, (3) it allows us to produce regional estimates by using conditional simulation, and (4) it permits testing the goodness of fit of a proposed Gaussian distribution under the hypothesis of second-order stationarity. In the goodness of fit test our goal is to find a combination of a data transformation and a covariance function dependent on distance such that the transformed data vector could derive from a multivariate normal distribution having both a constant mean and *V-C* matrix obtained from the proposed function. Our methods for testing the proposed hypothesis are presented below, including data transformation and a test for joint normality. Rejection of the test can result from any one of the following problems: (1) the process is not second-order stationary, (2) the underlying process is not Gaussian, or (3) the model and parameter values proposed are incorrect. Cross validation is presented as an alternative for comparing the cokriging variance estimates with the observed errors.

Lognormal Kriging

The advantages that are obtained when the assumption of joint normality is valid were outlined in the previous section. The frequency histogram of ANC values among sampled streams suggests that it would be difficult to justify the assumption of normality without first applying a log transformation to the stream ANC data. Practice has shown that the nonlinear estimator obtained in this way is generally better than the estimator obtained by kriging the untransformed data [*Journel and Huijbregts*, 1978; *Rendu*, 1979]. The estimate of ANC was calculated at each kriged location as $\exp [Z + \frac{1}{2} \operatorname{var} (Z)]$, where Z is the $\log_e$ (ANC) estimate and var (Z) is the kriging variance. We determined that this estimator was not significantly biased by comparison with ANC measurements in cross validation (mean error = -8.86, $p = 0.7231$). The choice of zero as the displacement in the log-transformation of ANC data precludes us from estimating any nonpositive ANC values, but no acidic systems were encountered in the NSS sample.

Joint Normality

Joint normality is influenced both by prior transformation of the sample vector and by the selection of covariance function. Our procedure for testing the goodness of fit of our data to a normal distribution was applied to the log-transformed sample vector, $\mathbf{z}$. Our null hypothesis is that $\mathbf{z}$ is normally distributed, with constant mean vector $\boldsymbol{\mu}$ and *V-C* matrix $\boldsymbol{\Sigma}$ defined according to the proposed covariance function of distance,

$$\mathbf{z} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \tag{1}$$

In order to test whether (1) holds, we first remove the mean vector $\boldsymbol{\mu}$ by premultiplying matrix $\mathbf{P}$, where $\mathbf{P} = \mathbf{I} - n^{-1}(\mathbf{11}')$ for sample size n. According to our hypothesis,

$$\mathbf{Pz} \sim N(\mathbf{O}, \mathbf{P\Sigma P}') \tag{2}$$

Eigenvalue decomposition of $\mathbf{P\Sigma P}' = \mathbf{EME}'$ yields an $(n-1)$ by n matrix $\mathbf{E}$ of eigenvectors and an $(n-1)$ square diagonal matrix of eigenvalues, $\mathbf{M}$. The $\mathbf{E}$ matrix can be used to make the sample vector independent as $\mathbf{E'Pz}$ has *V-C* matrix $\mathbf{E}'(\mathbf{P\Sigma P}')\mathbf{E} = \mathbf{E}'(\mathbf{EME}')\mathbf{E} = \mathbf{M}$. The final step is to premultiply by $\mathbf{M}^{-1/2}$, a diagonal $(n-1)$ square matrix with $m_i^{-1/2}$ on the diagonal, for each eigenvalue m_i. We assume here that $\boldsymbol{\Sigma}$ is positive definite.

In summary, if our hypothesis holds, then $\mathbf{y} = \mathbf{M}^{-1/2}\mathbf{E'Pz}$ is $N(\mathbf{O}, \mathbf{I})$, and standard univariate tests of normality can be applied. A test of the two-sided Kolmogorov-Smirnov statistic evaluates the likelihood of the observed maximum absolute deviation between the empirical cumulative density function (cdf) of vector $\mathbf{y}$ and the standard normal cdf, under the null hypothesis of joint normality [*Gibbons*, 1971].

Cross Validation of the Cokriging Model

Cross validation was used to help us to choose among the alternative covariance models with parameters selected by the ML procedure. In cross validation, sampled points are removed, one at a time, and estimated by kriging (or cokriging). If the covariance model is correct, then the kriging variance should be a good estimator of the squared difference between each measured value in the sample and its kriged estimate. The standardized difference for the ith sample point is defined as $y_i = [(z_k - z)/\sigma]_i$. If all kriging assumptions are met, then this quantity should come from a standardized joint-normal distribution.

Several statistics are commonly formed from these individual standardized differences y_i, based on the assumption that they are independent [*Hoeksema et al.*, 1989; *Samper and Neuman*, 1989]. In fact they are not independent and these statistics should be treated as crude indices. The two such statistics that we compare are the mean square error (MSE) obtained by squaring the difference between estimated and sampled values and the average kriging variance (AKV). Agreement between the MSE and AKV indicates that the kriging variance is estimated well, and a low MSE indicates that the estimated $\log_e$ (ANC) is accurate. These criteria can be used to compare different covariance models with particular emphasis on the agreement between the AKV and MSE.

Estimation and the Screening Effect

For each location where cokriged predictions are desired, a linear system of equations is solved based on two constraints: (1) the estimate is unbiased and (2) the cokriging variance associated with the estimate is minimized. Two formulations for the cokriging system are described by *Myers* [1982] and *Hoeksema and Kitanidis* [1984, 1985].

The cokriging estimation was conducted using the two nearest neighboring reach nodes from each of eight sectors surrounding the location of interest. This technique of using a small subset of available data in estimating each point is more stable from a numerical standpoint and also selects those points most highly valued in the interpolation. According to *Burgess and Webster* [1980, p. 320], "... near points carry more weight than distant points, points that occur in clusters carry less weight than lone points, and points lying between the point to be interpolated and more distant points screen the distant points so that the latter have less weight than they would otherwise."

Regional Resource Estimates—Conditional Simulation

In the NSS, one of the primary goals was to estimate regional distributions of stream chemistry. The same types of spatial information used in cokriging to make local predictions can be used to generate estimates of regional distributions. In this study, we are interested in obtaining population estimates for a finite population of stream nodes located within the SBRP region. Some quantities, such as the average ANC of the population, can be estimated directly by averaging cokriged estimates over the region of interest. Other types of regional estimates (those involving threshold values) can be produced by using conditional simulation. In this study, we are interested in comparing the regional population estimates obtained using spatial information with the original NSS estimates.

In the NSS, regional estimates were made of the numbers and proportions of stream resources with ANC values below selected reference values. Together, these estimates form a cumulative frequency curve for ANC. In the NSS, regional population estimates were constructed for the target population of stream reaches by applying weights to reflect the probability of inclusion in the survey sample. Variance estimates for these Horowitz-Thompson estimates involve joint inclusion probabilities and were used to produce confidence intervals [*Overton*, 1987].

The basic sample unit in the NSS survey was the stream reach. However, population estimates were reported for both upper and lower node populations associated with these reaches. When the entire population of reaches is enumerated, this reach-based population definition counts individual reach nodes twice when they are shared by converging (diverging) reaches: once for each reach that it is associated with as a lower (upper) node. Note also that numerous reach nodes are represented in both the upper and lower node populations.

Spatial regional estimates of ANC were obtained by using conditional simulation (CS) under the cokriging model selected earlier. For regional estimates involving threshold values, simply counting the proportions of reaches with cokriged ANC predictions below a selected reference value yields a biased estimator due to the smoothed nature of the estimator relative to the original surface. CS can be used to generate realizations that represent the full variability of the field [*Journel and Huijbregts*, 1978]. Spatial population estimates for ANC reference values and prediction intervals were obtained from these simulations.

The CS were generated by factoring the full cokriging *V-C* matrix associated with the cokriged estimates of each of the 416 nodes (local cokriging was not used). A collection of 500 pseudorealizations of $\log_e$ (ANC) following the spatial law of the cokriging model and conditioned on the observed ANC and elevation values were generated by premultiplying random standard normal deviates by the factored *V-C* matrix. For each simulation the number of reach nodes falling below each specified threshold value of ANC was counted and expressed as a proportion of the population size. In the counting procedure, each node was weighted by the number of reaches associated with it as an upper (or lower) node. The distribution median is used as the regional estimate and other quantiles provide distribution-free prediction limits.

Comparison of NSS Target and EPA REACH Populations

In the comparison of these population estimates the map scales of reach populations are different. The NSS reaches represent a finer scale of resolution than the REACH file population. The estimated number of NSS target reaches is 2031 and the number of REACH file 1:500,000-scale reaches is 420. Only stream nodes interior to the SBRP boundary were included in the REACH population, leaving 416 reach nodes. Using the reach-based definition from the previous section, we obtained populations of 382 upper and 324 lower nodes.

RESULTS

Modeling Spatial Covariance

We selected a spherical variogram model with a range of 42 km. This combination gave the best results in cross validation. The ML parameters imply that the correlation between $\log_e$ (ANC) and elevation at zero distance is -0.601, compared with the correlation of -0.508 estimated from the sample.

The following parameters were obtained by ML for $\log_e$ (ANC): nugget = 0.0 and sill = 0.92. For elevation the ML parameter estimates were nugget = 0.005 and sill = 0.04. The cross-variogram parameter estimates were nugget = 0.0 and sill = -0.227. The semivariogram model chosen for $\log_e$ (ANC) is shown in Figure 3.

We tested $\log_e$ (ANC) as data vector $\mathbf{z}$, with Σ defined by the spherical model and the ML estimation parameter choices listed earlier. The maximum Kolmogorov-Smirnov deviation from normal was $D = 0.055$. The probability of a larger deviation under the null hypothesis with a sample size of 75 is very high: $\Pr\{D(75) > 0.055\} = 0.976$. This test supports the assumption that (1) is reasonable for $\log_e$. (ANC). The same test was conducted for elevation with its covariance model. The maximum deviation from normal for elevation was $D = 0.081$. The probability of a larger deviation is 0.693. Small probabilities should cause concern over the validity of the assumption expressed in (1).

Cross validation was performed for both the kriging model for ANC without elevation and the cokriging model in which elevation was included. The estimated and measured NSS values of $\log_e$ (ANC) are compared in Figure 4. When elevation was not used in the prediction, the MSE was 0.389 and the AKV was 0.402. Adding elevation reduced the MSE by 27% to 0.286, which corresponds to an average cokriging variance of 0.297. The model parameters obtained by ML estimation did better in cross validation than other values chosen based on visual inspection of the experimental semi-

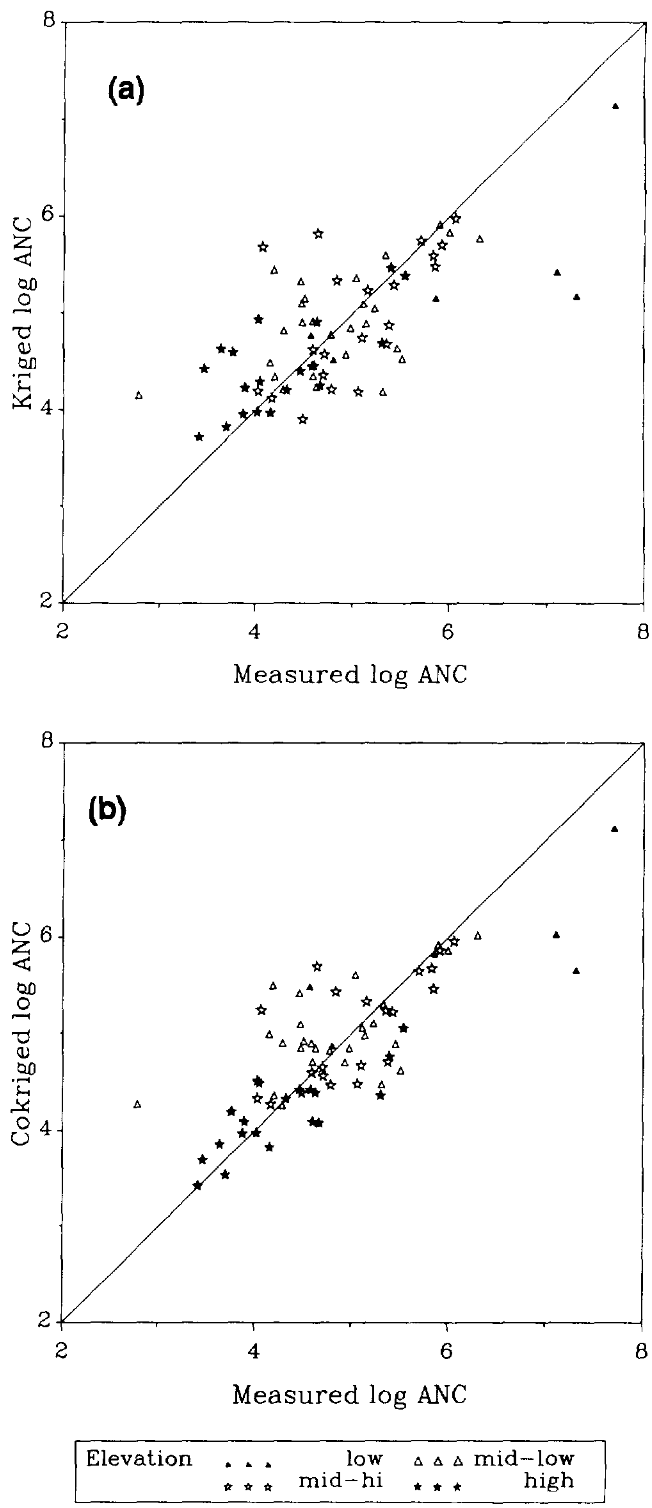

Fig. 4. Comparison of measured $\log_e$ (ANC) with (*a*) kriged and (*b*) cokriged estimates produced by cross validation, presented by elevation class.

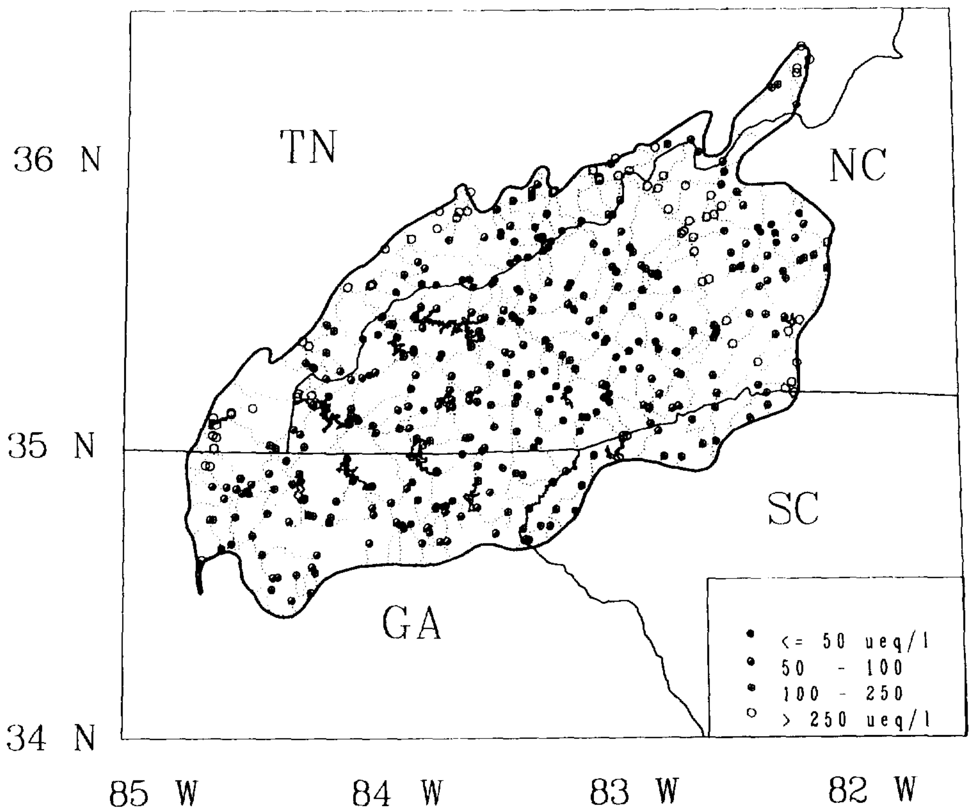

Fig. 5. ANC (μeq/L) estimates for REACH nodes obtained by cokriging.

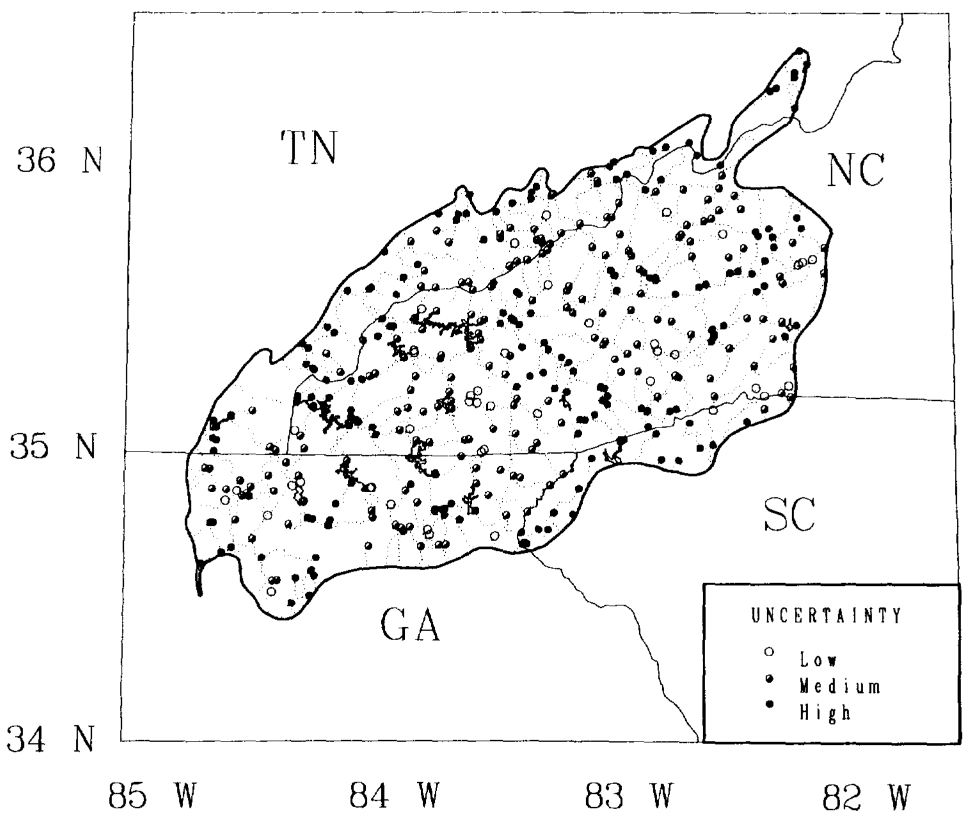

Fig. 6. Cokriging estimation variances in the Southern Blue Ridge Province.

variograms. We were also unable to formulate anisotropic models that performed better in cross validation than the isotropic models presented here.

Cross validation also provides a measure of the improvement in estimation obtained by kriging over using the regional mean. We used the cross-validation data to estimate the percent of variation in measured ANC explained by kriging (cokriging). We defined a coefficient of determination (R^2) as 1. − SSE/SST, where we defined SSE as the sum of squared differences between the measured ANC and kriged (or cokriged) estimate of ANC and SST as the sum of squared deviations from the overall mean of the NSS sample. ANC estimates were improved by 63.4% with kriging and by 70.4% with cokriging.

Estimates of Stream ANC

The cokriged ANC predictions for nodes of the EPA REACH population are shown in Figure 5. The ANC predictions follow the topography fairly closely (compare Figure 1). High buffering capacity is predicted by cokriging for reach nodes in the French Broad River valley (note the band of ANC >250 μeq/L in the northeast) and for reach nodes near the Tennessee River (ANC in the 100- to 250-μeq/L range). Cokriging predictions for reach nodes on the northern edge of the province boundary are generally lower in elevation with higher ANC estimates, while those on higher-elevation ridges fall below 50 μeq/L in predicted ANC. The reaches predicted to have the lowest buffering capacities occur in the three areas of Figure 5: (1) along the main ridge of the Great Smoky Mountains on the border between North Carolina and Tennessee, (2) in the Blue Ridge Mountains of southwest North Carolina, and (3) in the Black Mountains in the eastern portion of the SBRP.

Effect of Elevation in Reducing Uncertainty

The variances associated with kriging predictions are greatly reduced in the cokriging analysis from the kriging variances without elevation. Figure 6 is a map of cokriging variances with regions of low (≤0.2), medium (0.2–0.4) and high (>0.4) uncertainty. A map of cokriging variances reveals that the uncertainty is greatest in areas most distant from the NSS sample data locations and in areas with neighboring sample locations in only one direction. According to this map, the predictions of low ANC in the Great Smoky Mountains are more certain than the low ANC predictions near Mount Mitchell in the east and those farther south. Estimates of high ANC along the northern boundary and ANC estimates out on the northeastern tail are relatively uncertain. These kriging variances can be used to present only those regions for which an acceptable level of confidence is associated with the predictions.

Regional Elevation Estimates

We expected that the NSS target population derived from more detailed maps would include lower-order reaches characterized by higher elevations and lower ANC than reaches in the EPA REACH population. These expectations were not met by our results. The EPA 1:500,000-scale REACH population includes more high-elevation nodes than are found in the the NSS target population (see Figure 7). The high-elevation nodes are generally upper nodes, and about

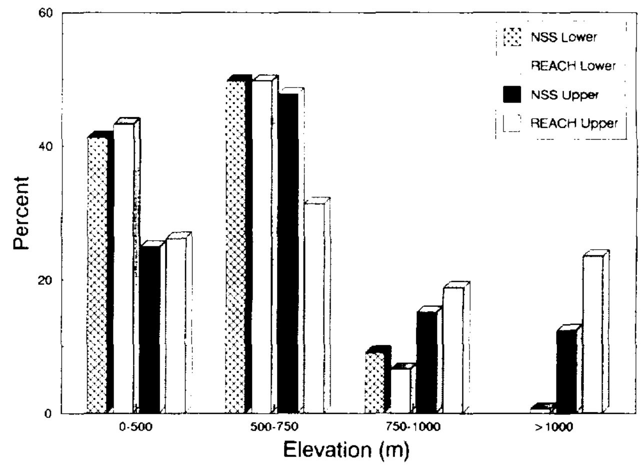

Fig. 7. Comparison of elevation for the NSS target 1:250,000 and the 1:500,000 REACH populations of stream reaches (upper and lower nodes).

half are headwater reaches. The same pattern is evident when just the headwater populations are compared and when all reaches are included.

Regional ANC Estimates

The cumulative proportion of lower and upper nodes predicted to have ANC levels below the reference values on the x axis are shown in Figures 8a and 8b. The NSS 1:250,000-scale population estimates can be contrasted with estimates obtained by CS for EPA 1:500,000-scale reaches. To be consistent with the NSS approach, we produced separate regional estimates for upper and lower nodes in the REACH population.

The variability in the distribution of spatial estimates is much smaller than for the nonspatial population estimates. This suggests, at first glance, that statements about the regional status of these streams can be made with greater certainty using the spatial estimates. The comparison is complicated by the fact that quantiles summarize the entire distribution of CS estimates, while confidence limits are available to surround the nonspatial Horowitz-Thompson estimates.

In the lower-node population, 4.6% of the reaches were predicted by CS to have ANC ≤50 μeq/L at their lower nodes. This is very close to the NSS estimate of 4.7%. Fewer than 5% of the 500 simulated lower-node populations predicted more than 6.8% with ANC below 50 μeq/L, suggesting that there is unlikely to be a very large proportion of reaches with low ANC values at their lower nodes. The CS distribution matches the NSS distribution well until around 100 μeq/L. At this point the NSS estimates a large fraction of the population having ANC between 80 and 150 μeq/L, and the CS estimates a more even distribution.

In the upper-node population the CS estimated 24% with ANC values below 50 μeq/L, compared with the NSS estimate of 6.2%. The CS estimated a larger percentage of upper nodes with ANC ≤ 100 μeq/L, but seems to follow the NSS distribution fairly closely for higher values up to 550 μeq/L.

Both cdf comparisons have similar features. In general,

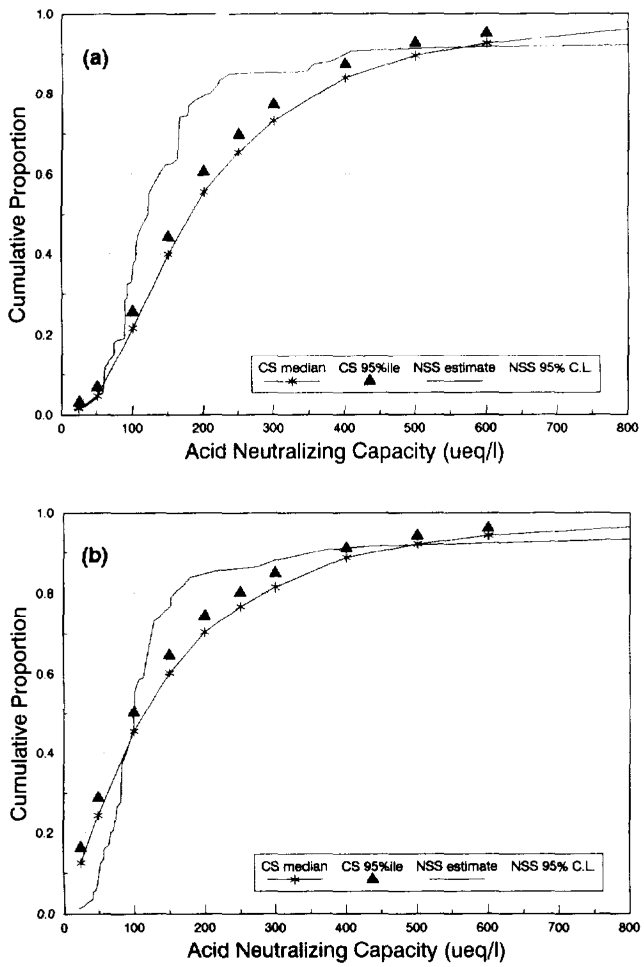

Fig. 8. Comparison of regional ANC distributions for (*a*) lower and (*b*) upper nodes of SBRP reaches estimated by spatial (CS) and nonspatial (NSS) methods.

the CS cdfs predict a relatively even distribution of ANC resulting in a smaller proportion of intermediate ANC values and a larger percentage of nodes with extreme values of ANC. In contrast, the NSS cdfs predict that the majority of reaches have ANC between 50 and 200 μeq/L. The evenness of the CS cdf may result in part from the fact that a local cokriging model was not used in producing the regional estimates, and development of a local CS algorithm may help to relax the constraining influence of the underlying assumptions.

DISCUSSION

Regional ANC Estimates

Two important differences were noted between the spatial population estimates of ANC and the NSS estimates. First, the estimates produced by CS suggest a larger proportion of low ANC stream nodes for the upper-node population. It is likely that the additional information about elevation plays an important role in the higher CS estimate. In the upper node population there is a substantially larger proportion of high elevation reach nodes than is represented in the NSS sample.

The regional estimates produced by CS appear to be much more precise than the NSS estimates. The uncertainty associated with the NSS estimates quantifies the uncertainty in extrapolating from the samples ANC values to the unsampled stream reaches using sample weights. The estimates obtained by conditional simulation with the cokriging model reduce this uncertainty by adding new sources of information, but at the cost of adding quite a few assumptions: (1) These spatial estimates provide new information about the locations of the unsampled reaches, but we have to assume that the population is correctly described by the digitized REACH files; (2) The spatial approach uses the ANC measurements at nearby sample reaches but requires an assumption of stationarity and normality for $\log_e$ (ANC); (3) New information about elevation is provided to the CS estimator, but assumptions about the spatial law of elevation are required; and (4) The CS variance estimates do not at present incorporate the uncertainty due to parameter estimation. While some of the reduction in uncertainty is "real," resulting from improved information, to some extent the reduction is exaggerated by unquantifiable assumptions. Further research is needed to incorporate as many of these sources of uncertainty as possible into the estimation variance, to develop methods requiring fewer assumptions (such as indicator cokriging), and to attempt field verification of the cokriged estimates.

Frequency of High-Elevation Sites

The cokriged CS estimates have information available to them about the locations of stream nodes in the population, the elevations at those nodes, and the ANC measurements from surrounding NSS sites. The estimated percentages of low ANC upper nodes differ from the NSS estimates to some extent because the NSS sample appears to underrepresent the frequency of high elevation sites for the upper node population. A larger percentage of upper nodes associated with high-elevation reaches occur in the REACH file population than in the extrapolated NSS target population.

An initial concern was that the difference in scale between the 1:500,000 REACH and the 1:250,000 target NSS population might cause this discrepancy in elevations. However, an analysis of detailed 1:100,000-scale digital line graphs also revealed a larger proportion of high-elevation upper nodes than estimated by the NSS, suggesting that differences in map scale are not responsible for the discrepancy. The frequency of high-elevation sites in the 1:500,000-scale REACH file population suggests that these high-elevation reaches represent a more significant fraction of the NSS target population than is indicated by the NSS population estimates.

CONCLUSIONS

Spatial statistical methods for obtaining local and regional estimates have been demonstrated for use in regional assessment of large-scale environmental problems. The cokriged regional classification of SBRP streams (Figure 5) shows the spatial distribution of potentially sensitive stream resources in much greater detail than the sample classification maps (Figure 1). The map of cokriged variance (Figure 6) indicates areas that would benefit most from additional sampling efforts and can be used in conjunction with Figure 5 to assess confidence levels in its predictions. The individual reach nodes identified in Figure 5 as potentially low-ANC sites belong to the NSS target populations and may be of interest in designing future studies. These reaches tend to be low-order streams occurring at the higher elevations of the SBRP.

The regional estimates that we obtained suggest that a larger percentage of stream reaches in the SBRP may be susceptible to acidification than previously estimated. The use of available elevation data permits the extremes of the ANC distribution to be estimated, despite the fact that they are rarely encountered in a limited survey sample. However, the estimated uncertainty of these estimates appears unrealistically small and points to the need for more robust methods and field verification. Together, the local and regional-scale estimates have provided us with the capability to summarize the status of stream resources in the SBRP for assessment purposes and to identify specific local subpopulations that are more susceptible to acidification.

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