Comparison of Regional Stream ANC Predictions for the George Washington National Forest Using Spatial and Non-Spatial Regression Modeling

Final Report

T.C. McDonnell and T.J. Sullivan

E&S Environmental Chemistry, Inc.
P.O. Box 609
Corvallis, OR 97339

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ABSTRACT

First approximations of predicted stream water acid neutralizing capacity (ANC) have been developed for streams throughout the southern Appalachian Mountains (SAM) region. They have contributed to the development of an Ecosystem Management Decision Support (EMDS) modeling system that is currently being used by the US Forest Service (FS) to address concerns related to biological effects associated with stream acidification caused by air pollution. Accurate maps of predicted stream water acid-base chemistry are essential to managers who must identify acid-sensitive streams and potentially affected biota, and create resource protection strategies.

Streams differ from terrestrial systems in that they channel flows of materials through corridors in the landscape. Thus, stream conditions are often spatially autocorrelated because the stream condition at a particular point can be influenced by conditions that occur upstream or downstream, and observations may not be independent. Spatial stream network (SSN) models that address spatial autocorrelation are now available, and their use is growing.

Non-spatial regression techniques relied on by Povak et al. (2013) for generating ANC predictions for the SAM region as part of the EMDS effort did not consider spatial relationships among measurement locations. It was assumed that the observed values were independent; that is, the value at one site was not related to or influenced by the value at any other site. This assumption is typically violated when modeling aspects of stream chemistry because the nature of flowing water in a stream network connects observations with one another.

Spatial modeling techniques that can be applied to stream networks were not generally available when these regional ANC estimates were generated for EMDS. However, recently published statistical modeling techniques that can account for the spatial connectivity that exists among stream observations are now available. The analyses reported here use these new

statistical methods to develop a new set of regional predictions of stream ANC in the SAM that offer improvements over those previously developed. In addition to the potential for generating more accurate ANC estimates, the new spatial modeling techniques are also able to generate error estimates associated with each prediction point. Uncertainty in predicted ANC is expected to be low in areas of high density of observed data and higher at locations further from the measurement sites.

We re-calculated the regional predictions of stream ANC for the George Washington National Forest (GWNF) that were previously developed by Povak et al. (2013). We also developed a full spatial coverage of the standard error of the ANC predictions (this is not shown). Results reported here were developed from a spatial stream network model that incorporated autocorrelation functions derived from both network-connected and Euclidean (i.e. “ordinary” distance measured by a straight line) distance measures.

Results of these analyses showed that the distribution of ANC prediction results from the RF model was more constrained, whereas the distribution of SSN model predictions included a number of more extreme ANC values. For example, the SSN models generally predicted lower ANC at values below 35 µeq/L as compared with RF. In particular, the James River and Lee Ranger Districts (RDs) of the GWNF generally showed lower predictions of ANC by the SSN model. Overall, differences between the two approaches were modest. However, the generally lower predictions of ANC by the SSN model suggested somewhat greater acid sensitivity than did the predictions, using RF, which did not account for spatial autocorrelation.

INTRODUCTION

Atmospheric sulfur (S) deposition, originating largely from emissions from coal-fired electrical power generation and other industrial sources, has resulted in decreased stream acid neutralizing capacity (ANC) and pH across broad areas of the southeastern United States (U.S. EPA 2008). Stream acidification has been linked with reduced fitness and richness of aquatic species and changes to benthic communities. Regional estimates of stream ANC provide forest resource managers with valuable information for developing management strategies to protect and restore sensitive stream ecosystems.

When monitoring stream water acid-base status, ANC is often chosen over other metrics, such as pH, due to its relative insensitivity to changes in concentrations of CO_2, aluminum reactions, and the presence of organic acids (Neal et al. 1999). ANC is widely used in studies of regional critical loads (CLs; Henriksen et al. 1995, Duan et al. 2000, U.S. Environmental Protection Agency 2009, Clark et al. 2012). The CL is a quantitative estimate of the level of sustained S deposition above which harmful ecosystem effects are likely (Nilsson and Grennfelt 1988). Various ANC thresholds are associated with biological effects (U.S. EPA 2009). Negative effects on macroinvertebrate and fish species richness have been associated with ANC concentrations between ~50 and 100 μeq/L (Cosby et al. 2006, Sullivan et al. 2007), and more substantial effects are observed at lower levels (Cosby et al. 2006, Sullivan et al. 2007, U.S. EPA 2009).

Stream water ANC is used to identify acid-sensitive stream reaches (McDonnell et al. 2013). A spatial ANC coverage can be used to inform decisions about where best to mitigate acidification of aquatic habitats. ANC modeling and CL are used in a decision support modeling framework to guide resource management and policy decisions focused on the southern Appalachian Mountains (SAM) region regarding S emissions (Reynolds et al. 2012).

The SAM region has a long history of atmospheric S deposition and contains threatened aquatic resources. The region exhibits complex land use patterns superimposed on steep climatic and topographic gradients. The diverse environmental settings make this region well suited to regional ANC estimation.

First approximations of stream water ANC across the region have been developed for streams throughout the SAM region, including those contained within the George Washington, Jefferson, Monongahela, Cherokee, Pisgah, Nantahala, Chattahoochee, and Sumter national forests (Povak et al. 2013). These results have contributed to the development of an Ecosystem Management Decision Support (EMDS) system that is currently being used by the US Forest Service (FS) to address concerns related to biological effects associated with stream acidification caused by air pollution.

Accurate maps of predicted stream water acid-base chemistry are essential to managers who must identify acid-sensitive streams and potentially affected biota, and create resource protection strategies. Povak et al. (2013) developed correlative models to predict the ANC of streams across the SAM region. Models were developed using stream water chemistry data from 933 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 a variety of non-spatial regression models. Predictor variables represented key aspects of the contributing geology, soils, climate, topography, and acidic deposition. To reduce model error rates, Povak et al. (2013) employed a hurdle model to screen out well-buffered sites and predict continuous ANC for the remainder of the stream network. Models predicted acid-sensitive streams mainly in forested watersheds with small contributing areas, siliceous lithologies, cool and moist environments, low clay content soils, and moderate or higher dry sulfur deposition.

Biogeochemical and climatic influences on ANC involve many interactions among environmental and climatic processes that together influence the ultimate susceptibility of a stream to the acidifying effects of S deposition. Known processes include (1) soil mineral base cation weathering and associated cation exchange reactions; (2) long-term rate of S and base cation deposition; (3) plant nutrient base cation uptake and removal via harvest; and (4) adsorption/desorption of S on soil ion exchange sites (Turner et al. 1990, Henriksen and Posch 2001). Modeling the susceptibility of aquatic systems to acidic deposition at a regional scale requires an understanding of these processes, access to adequately resolved data layers that accurately portray the complexity of environmental conditions, and reliable statistical modeling.

METHODS

Streams differ from terrestrial systems in that they channel flows of materials through corridors in the landscape. Properties of stream systems include branching structure, longitudinal connectivity, and occasional abrupt changes at tributary junctions (Peterson and Ver Hoef 2010, Isaak et al. 2014). Spatial stream network (SSN) models that address spatial autocorrelation have been in development over recent years and are now available (Ver Hoef et al. 2006, Peterson and Ver Hoef 2010, Isaak et al. 2014, Peterson and Ver Hoef 2014, Ver Hoef et al. 2014).

Stream networks in the national forests can be extensive, and direct measurement of water quality condition is typically too difficult and expensive to collect everywhere. Tools such as regression models can predict conditions at locations that have not been sampled. A spatial regression model based on covariance structure for stream networks can be used to extrapolate water quality data. This type of approach can account for spatial autocorrelation among stream sites and allows model application to databases that have clustered and autocorrelated measurement locations (Isaak et al. 2014). An SSN model can make such predictions and use information from the autocovariance function to improve predictive accuracy near measurement locations (Isaak et al. 2014). This is done through a two-step process that entails a linear regression prediction followed by an adjustment for autocorrelation.

Now that suitable statistical prediction methods exist to incorporate spatial autocorrelation within stream networks, the assumption of independence among observations associated with non-spatial regression modeling no longer needs to be violated. Rather, this dependence among observations is leveraged to improve predictions at sampled and unsampled locations. As a consequence, prediction accuracy can be improved. These tools can also improve understanding of spatial patterns in stream chemistry (McGuire et al. 2014). Comparisons between spatial and non-spatial regression models for predicting stream temperature were made by Isaak et al. (2014). Their results showed nearly twice as much variance explained by the spatial model and a reduction in root mean squared error (RMSE) of almost one-half. The analyses reported here use these new statistical methods to develop refined regional estimates of stream ANC that offer improvements over those previously developed for EMDS.

In addition to the potential for generating more accurate ANC predictions, the new spatial modeling techniques are also able to generate error estimates associated with each prediction point. Uncertainty in predicted ANC is expected to be low in areas of high observed data density and higher at locations further from the measurement sites.

We re-calculated the regional predictions of stream ANC for the GWNF that were previously developed for EMDS (Povak et al. 2013). We also developed a full spatial coverage of the standard error of the ANC predictions. These results are provided as a regional database.

Spatial Tools for the Analysis of River Systems (STARS; version 2.0.0) were implemented to develop the spatial data and attributes required for SSN modeling. The R package SSN (version 1.1.3) was used to develop the spatial model and predictions for comparison with the Random Forest (RF) model employed by Povak et al. (2013). The SSN model developed in this study was derived from the same set of ANC response and predictor variable data as was used to develop the continuous RF model. In addition to these landscape predictors, the SSN model incorporated spatial autocorrelation among observed ANC values derived from flow-connected (i.e. tail-up autocorrelation function) and Euclidean distance measures. Results reported here focused mostly on those derived from flow-connected distances to isolate the effect of a single network distance measure to represent spatial autocorrelation. However, the development of mixed models to account for multiple types of spatial relationships is possible. Results are also reported for an SSN model that incorporated spatial autocorrelation derived from both flow-connected and Euclidean distance measures.

RESULTS

Model Comparison

Spatial autocorrelation in the regional ANC data was evident based on flow-connected distances up to approximately 5 km (Figure 1). Spatial autocorrelation did not appear to be present beyond about 5 km (or about 3 miles). Based on the cross validation technique currently available in the SSN package (leave-one-out cross validation [LOOCV]), the RMSE of the tail-up SSN model was 54.1 μeq/L with an r^2 of 0.48. Although not directly comparable, these results are similar to those derived from 10-fold cross validation (10-fold CV) of the RF model based on 10 predictor variables (cf., Figure 5 of Povak et al. [2013]). It is noted that 10-fold CV is considered to provide a more thorough analysis of model robustness.

The GWNF is used here as an illustrative example for comparing predicted ANC results from the two models. It is comprised of five RDs (Figure 2). Mapped results of RF and SSN predictions of ANC are shown in Figures 3 and 4. Relative to the observed ANC values used to build the model (Figure 5a), the distribution of ANC predictions from the RF model is more constrained (Figure 5b) whereas the SSN model predicts a distribution that includes a number of more extreme values of ANC (Figure 5c). For example, the SSN model generally predicted lower ANC below 35 μeq/L as compared with RF (Figure 6). It is hypothesized that this difference between models is most likely caused by the averaging function that was used by the RF model to report a final prediction from among the 1,000 individual regression trees built from random selections of the data (cf. Povak et al. 2013). This is important because the FS requires information regarding locations of the most acid-sensitive watersheds for management decision-making.

Absolute differences between SSN and RF ANC predictions were calculated as $ANC_{SSN} - ANC_{RF}$. The vast majority (4,908 out of 4,913; 99.9%) of the differences between prediction methods ranged from -98 to +98 μeq/L. Five sites showed differences in predicted ANC to be outside of this range, with SSN predictions greater than RF by 100, 101, 107, 150, and 411 μeq/L. These five sites were removed prior to data analysis.

There was no clear spatial pattern in the differences between results from the two statistical methods (Figure 7), and the distribution of the difference in predicted ANC was approximately normal, centered on zero difference (Figure 8). We found generally similar results for stream sites located within and outside wilderness areas (Figure 9).

Differences between SSN and RF predictions were stratified by RD (Figure 10 and Figure 11). The James River and Lee RDs generally showed lower predicted ANC from the SSN model as compared with RF. Overall, differences between the two approaches were modest. Absolute difference results were also stratified by the three most important predictor variables for predicting continuous ANC with RF (cf., Table 1; Figures 12-14). Measures of regional variation in temperature (Figure 13) and precipitation (Figure 14) did not explain the differences in ANC predictions. Greater percentages of siliceous lithology tended to be associated with lower SSN model ANC predictions as compared with RF (Figure 12). However, this relationship did not hold for watersheds underlain by the highest percentages of siliceous lithology.

Table 1. Predictor variables included in the RF model to predict ANC. (Adapted from Povak et al. 2013)

Model Variables	Short Name	Relative Importance
Percent siliceous lithology	LITH_SIL	18.64
Mean penultimate maximum days without precipitation while $\geq 10\ ^{o}C$	NPDAYMAX	11.98
Mean number of GS days above $32.2\ ^{o}C$	AB90GROW	11.51

Model Confirmation

Observed spring season water quality data sampled from streams on the GWNF from 1992 to 2000 were selected for model confirmation. Data were initially screened to remove sites having sulfate and chloride concentrations greater than 300 μeq/L and 100 μeq/L, respectively. These screenings were selected to minimize the inclusion of watersheds having substantial influence from geologic S and road salt. A set of 92 candidate sites with observed ANC were evaluated for use as confirmation sites. Candidate sites were excluded from the dataset if the site was co-located on the same stream reach as an observed ANC site that was used for model building or if the location of the site on the stream network was ambiguous given the site coordinates and locations of nearby tributaries. An additional 5 sites were removed from the confirmation set because they occurred on streams considered by the RF model to exhibit relatively high (> 300 μeq/L) ANC. The final dataset included 54 sites for model confirmation. Results were generally similar between SSN (r^2 = 0.27; RMSE = 68 μeq/L) and RF (r^2 = 0.25; RMSE = 71 μeq/L; Figure 15). The SSN model showed slight improvement over RF at low (< 50 μeq/L) ANC.

Mixed Model Results

Although observations of stream chemistry are expected to be spatially autocorrelated according to a tail-up function derived from flow connected distances, consideration of Euclidean distance measures is also appropriate and may contribute to predictive accuracy. This is because stream sites may, in some cases, be located in close proximity, and yet not be flow-connected. Such adjacent streams may share common characteristics, such as lithology, soil chemistry, vegetation, topography, or climate that control acid sensitivity and impact spatial autocorrelation. The SSN model that included both flow-connected and Euclidean distance measures ($SSN_{up,eu}$) showed modest improvement in RMSE (49.9) as compared with the SSN model with spatial autocorrelation shown previously that had been based only on flow-connected distances (RMSE = 54.1; r^2 was unchanged).

The $SSN_{up,eu}$ model predicted nearly twice the number of stream segments with ANC < 0 μeq/L as compared with the non-Euclidean SSN model (96 vs. 50) and an additional 131 stream reaches with ANC between 0 and 50 μeq/L (Figure 16). Results compared similarly with RF, although more sites showed lower predicted ANC based on $SSN_{up,eu}$ model results (Figure 17).

CONCLUSIONS

Regional ANC predictions across the GWNF using a spatially explicit SSN model offer some improvements over the non-spatial RF approach that had been previously available for EMDS modeling. The distribution of ANC predictions was somewhat less constrained using SSN. As a consequence, the SSN model predicted more sites having low (< 35 μeq/L) values of ANC. Overall differences between the two modeling approaches were generally modest. However, the lower estimates of ANC generated by SSN may be important in view of the need by federal land managers to manage the most acid-sensitive watersheds in the national forests.

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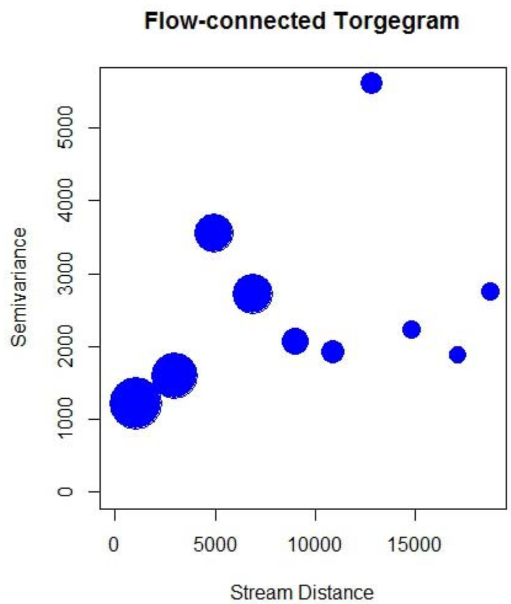


Figure 1.	Torgegram for stream ANC developed from measured water chemistry data at 933 sites located in multiple stream networks within the southern Appalachian Mountains. Dot sizes are proportional to the number of paired distances used to derive the semivariance within each bin. The semivariance expresses the degree of relationship between points on a surface. As points are compared to increasingly distant points, the semivariance increases. This variable is used in regionalized variable theory in place of autocorrelations.

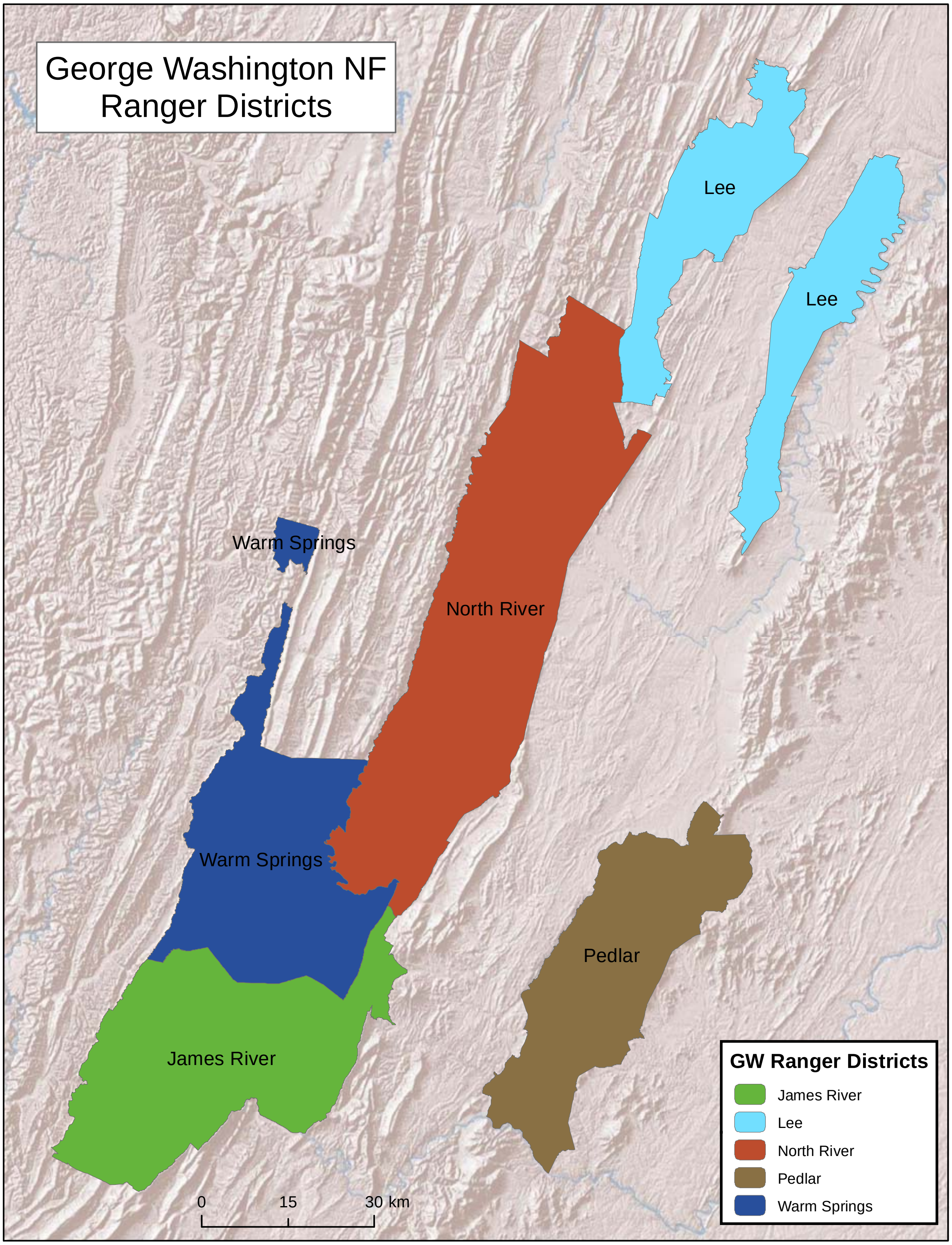


Figure 2. Ranger districts located within the George Washington National Forest.

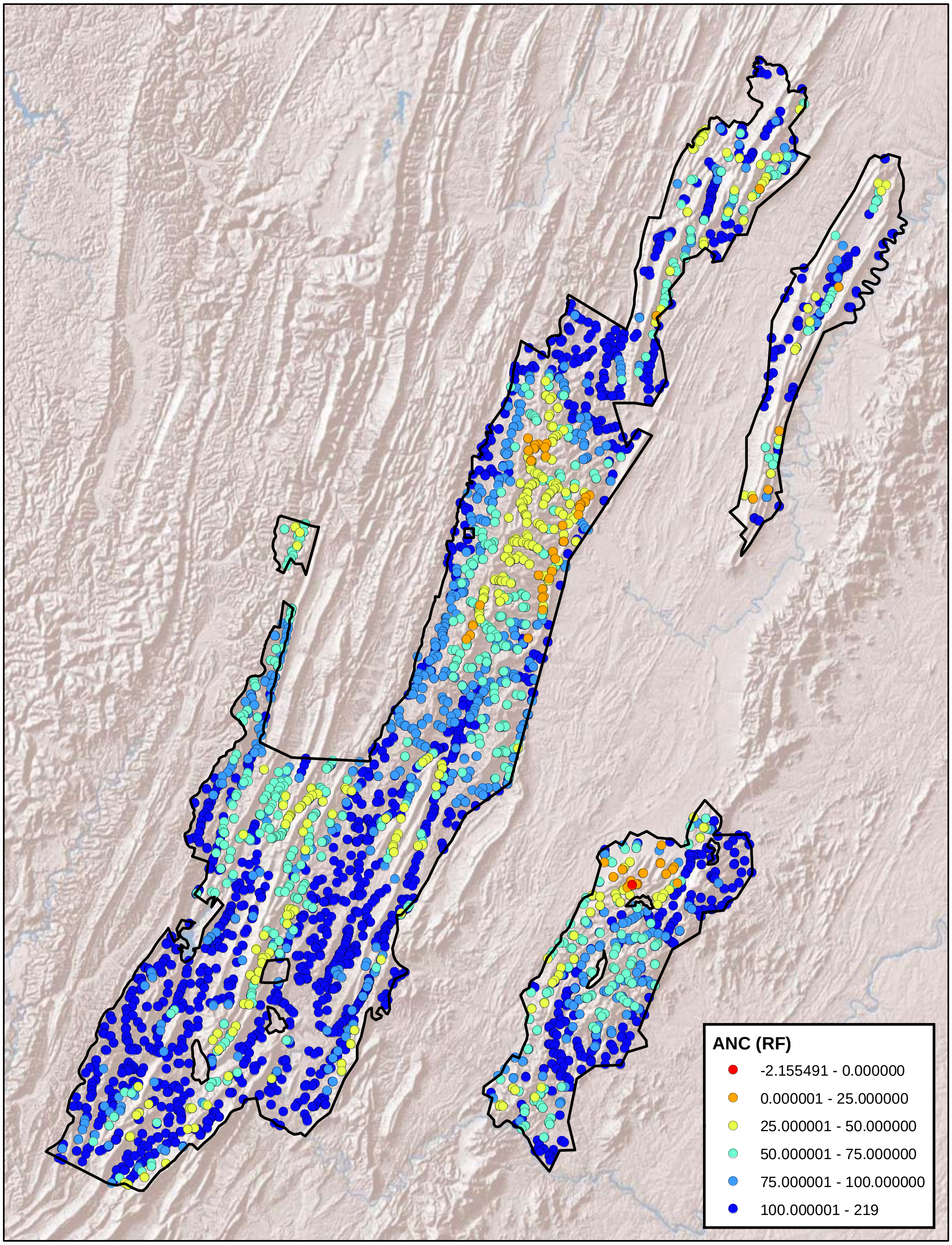


Figure 3. Classes of ANC predictions based on random forest (RF) predictions (Povak et al. 2013).

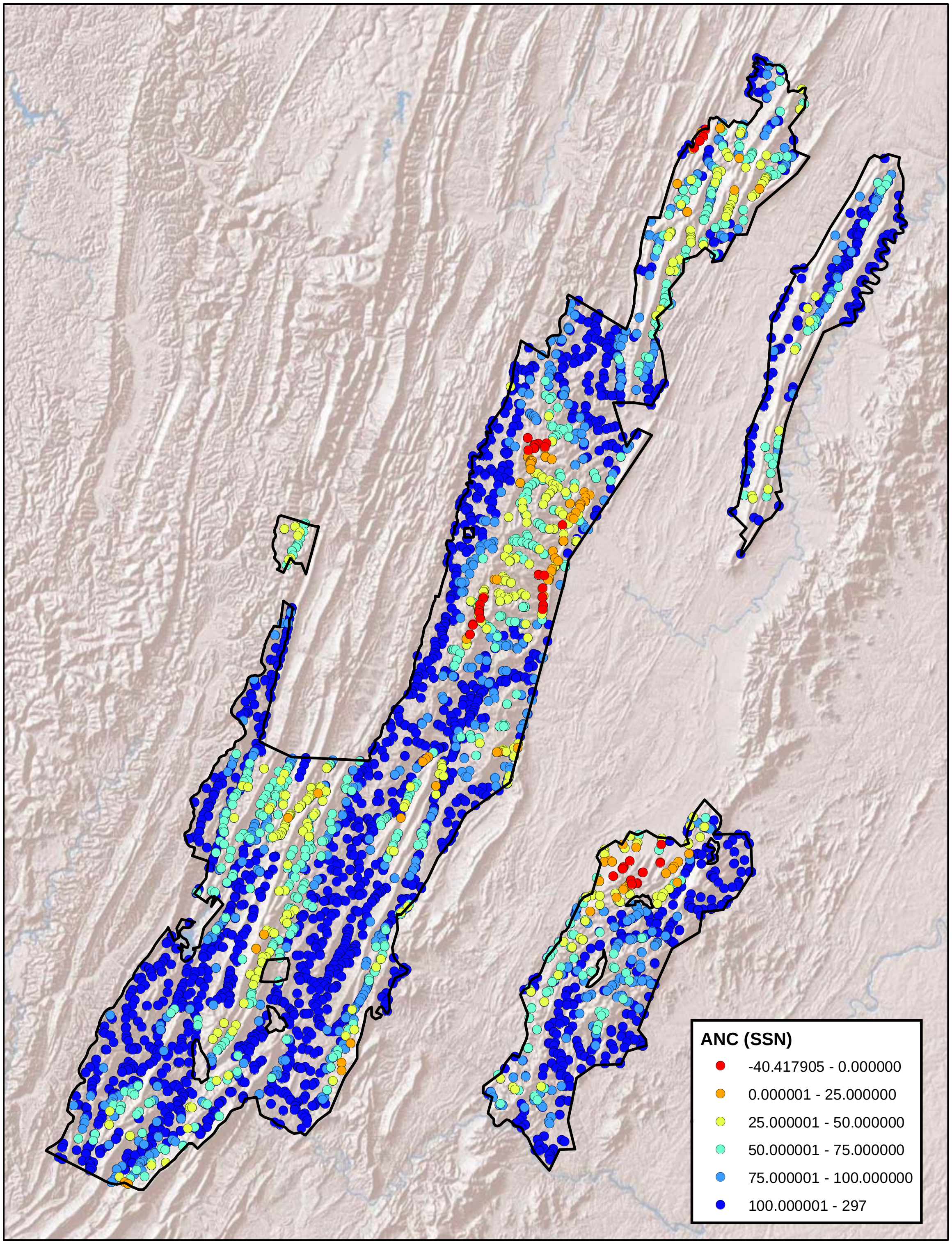


Figure 4. Classes of ANC predictions based on spatial stream network (SSN) model predictions.

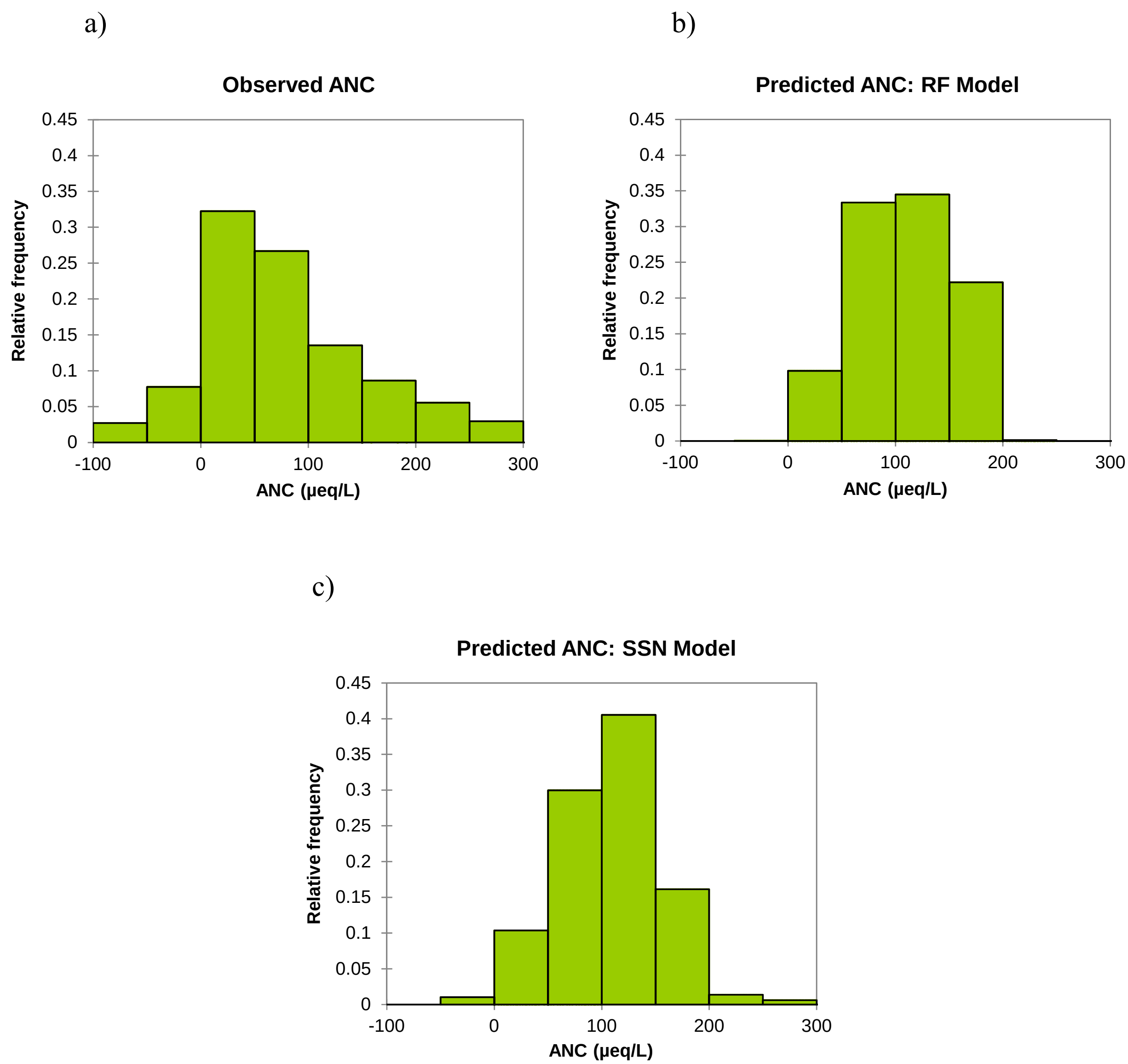


Figure 5. Relative frequency of ANC measured values a) and predictions generated by b) the RF model, and c) the SSN model.

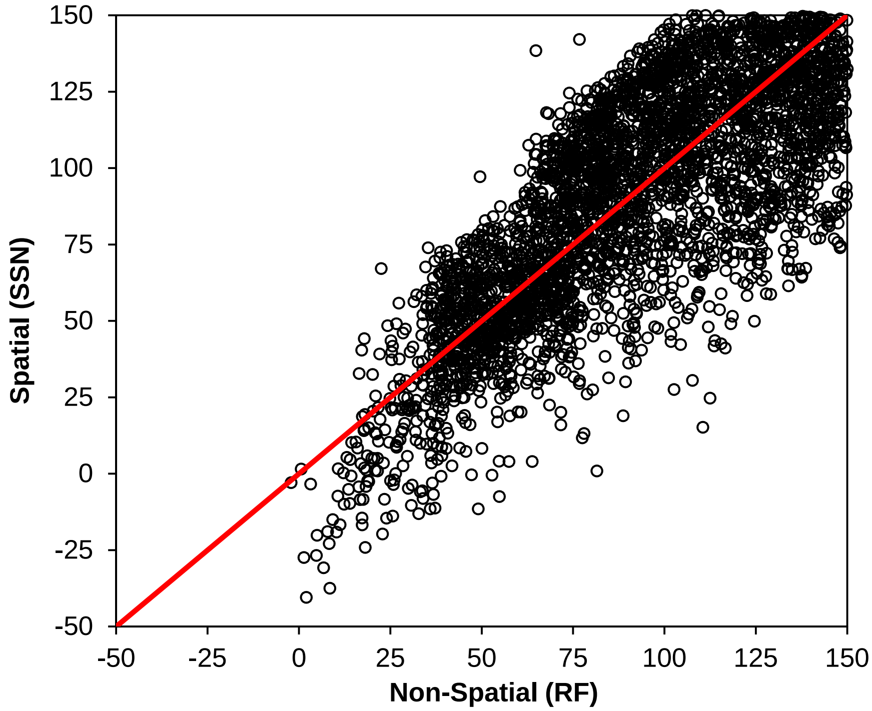


Figure 6. Predictions of stream ANC using the SSN spatial versus the RF non-spatial model. A 1:1 line is added for reference.

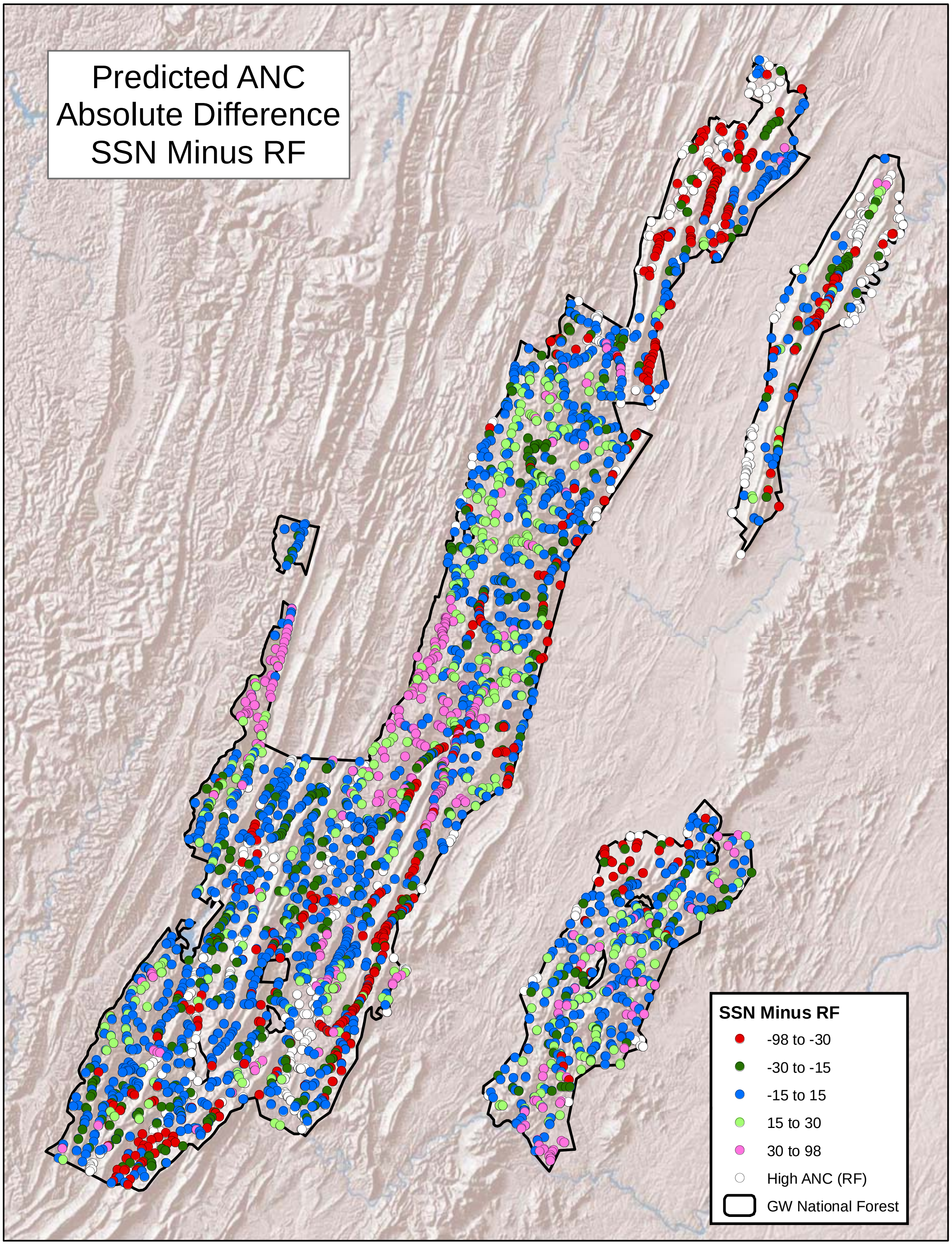


Figure 7. Absolute difference between SSN and RF ANC predictions.

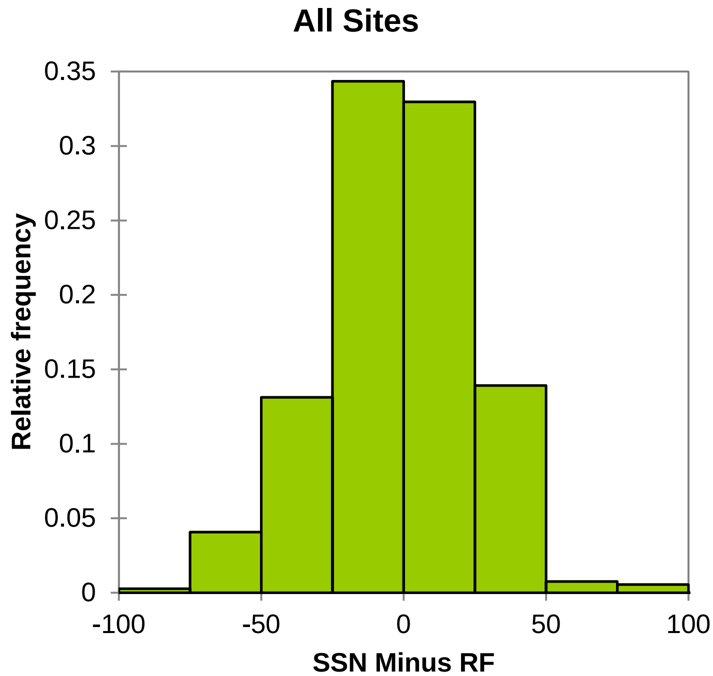


Figure 8. Distribution of absolute difference in ANC prediction between SSN and RF models.

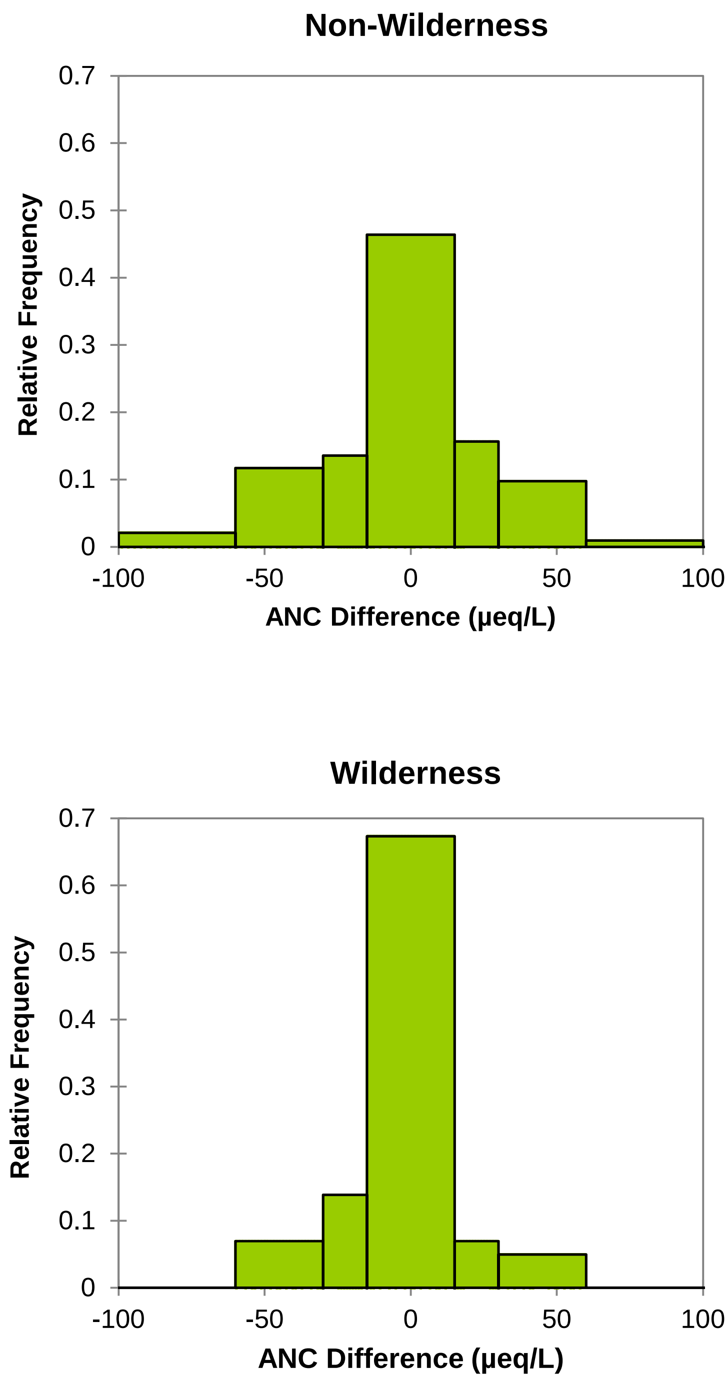
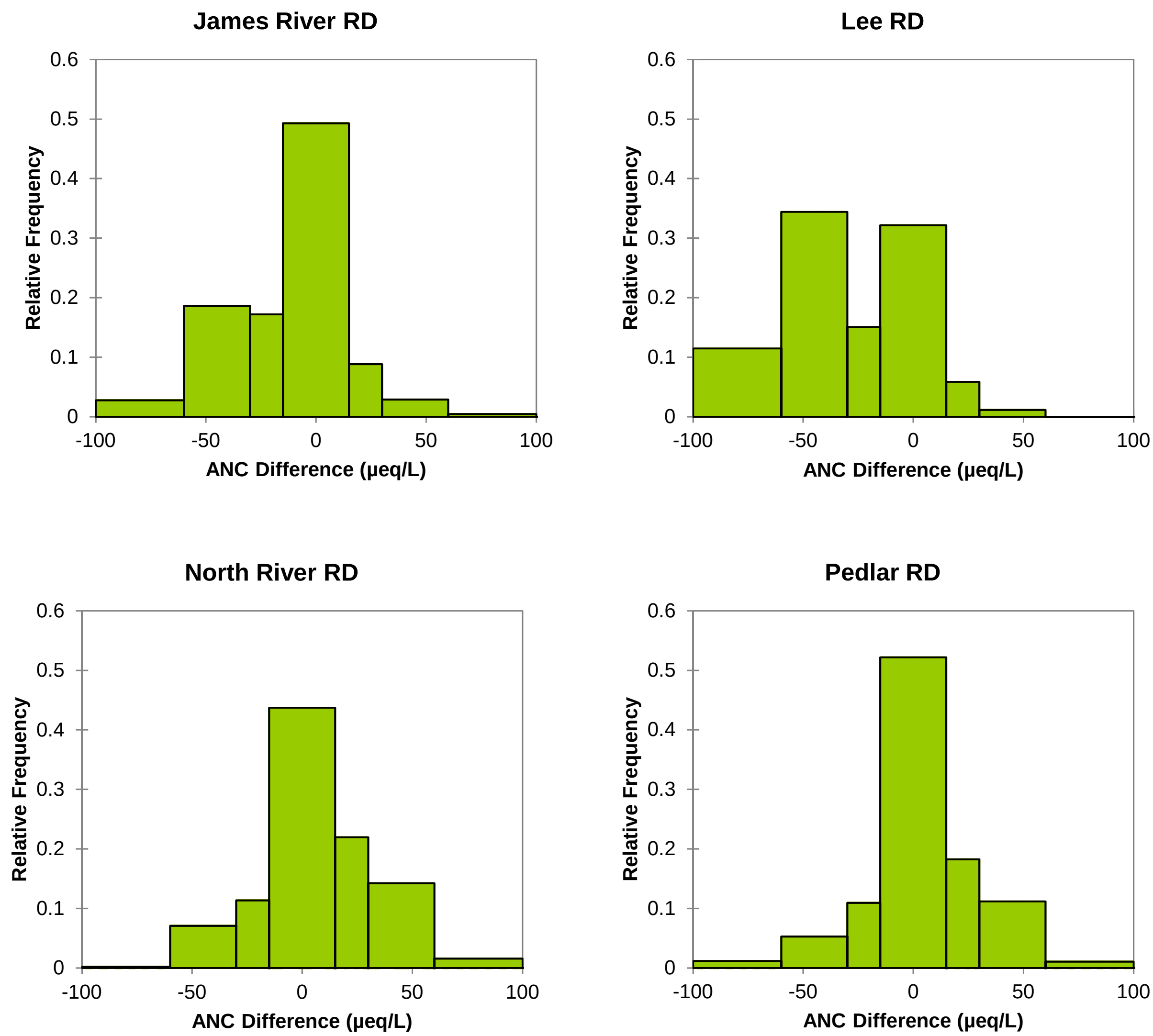


Figure 9. Distribution of absolute differences in ANC prediction with the SSN model between wilderness and non-wilderness sites.



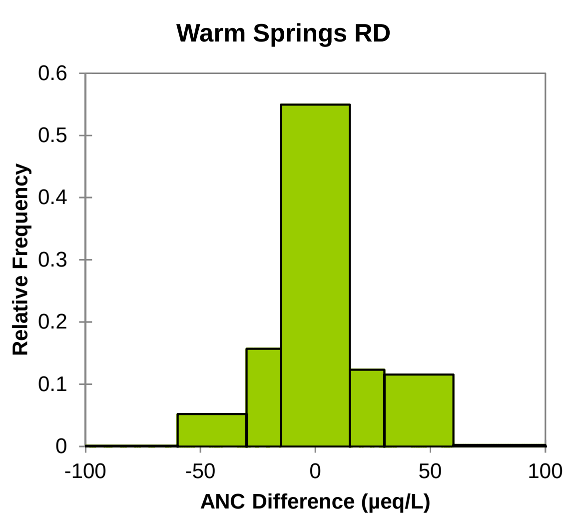


Figure 10. Distribution of absolute difference in ANC prediction among ranger districts of the George Washington National Forest.

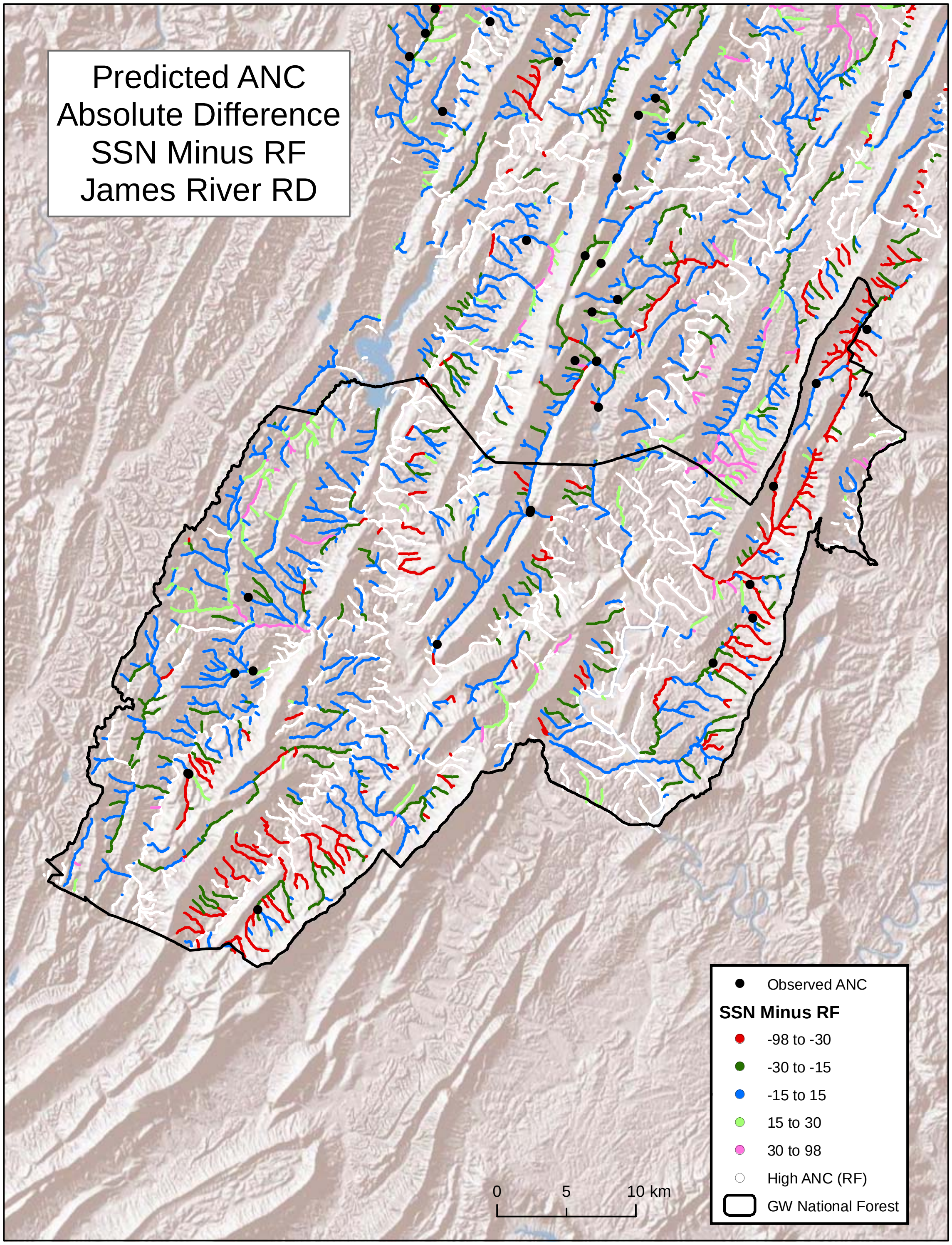
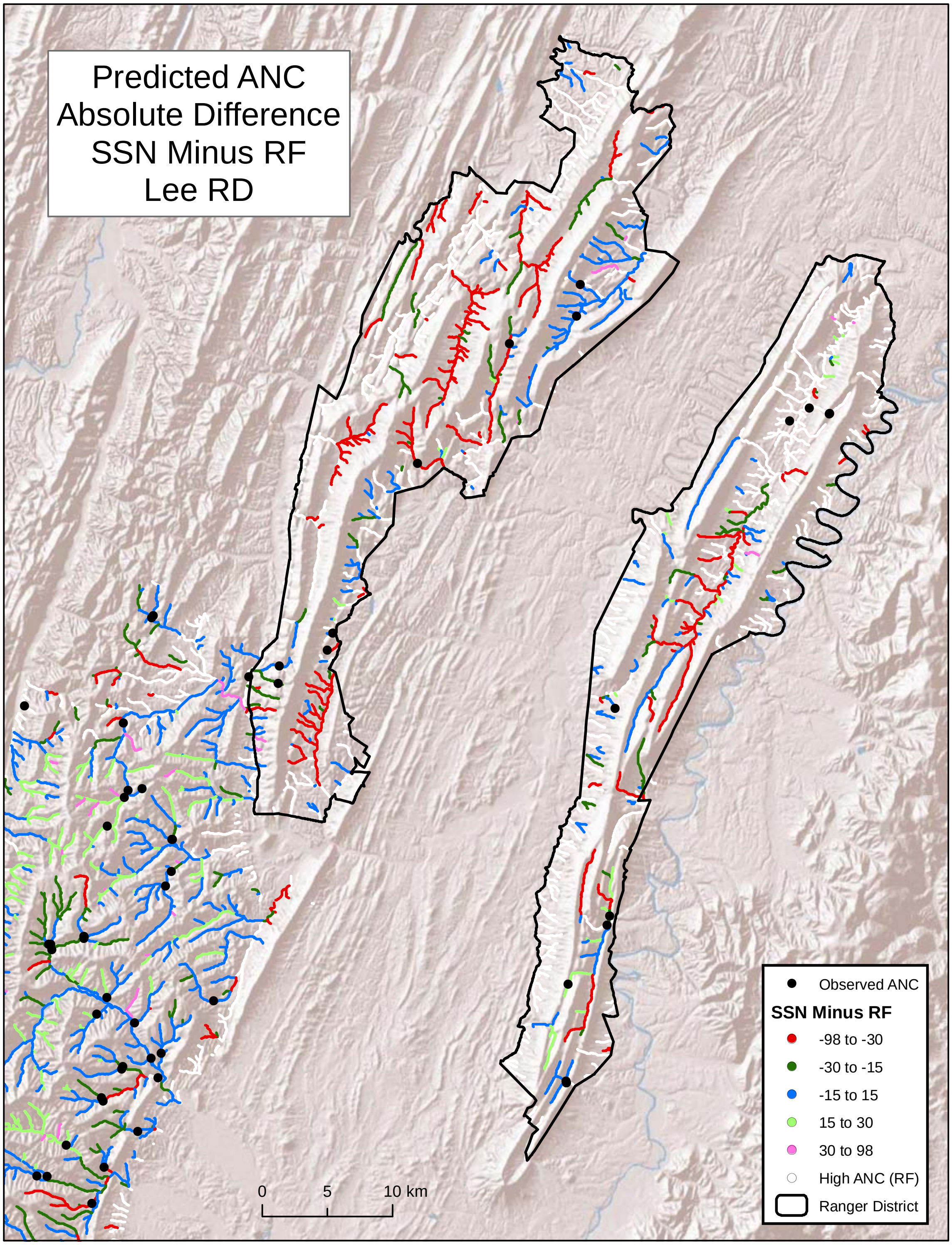


Figure 11. Predicted absolute difference in stream ANC (μeq/L) expressed as SSN minus RF model results for a) James River RD, b) Lee RD, c) North River RD, d) Pedlar RD, and e) Warm Springs RD.



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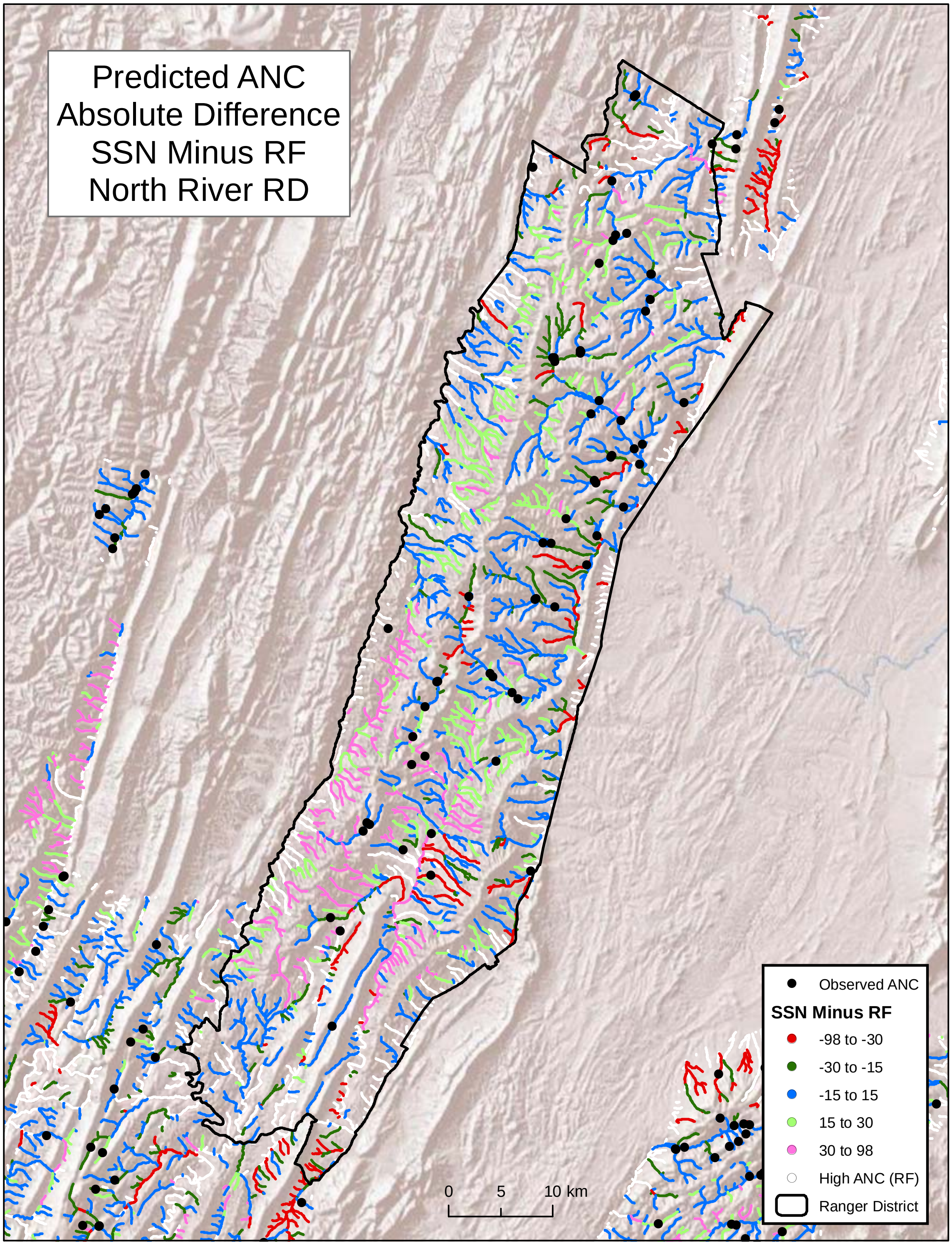

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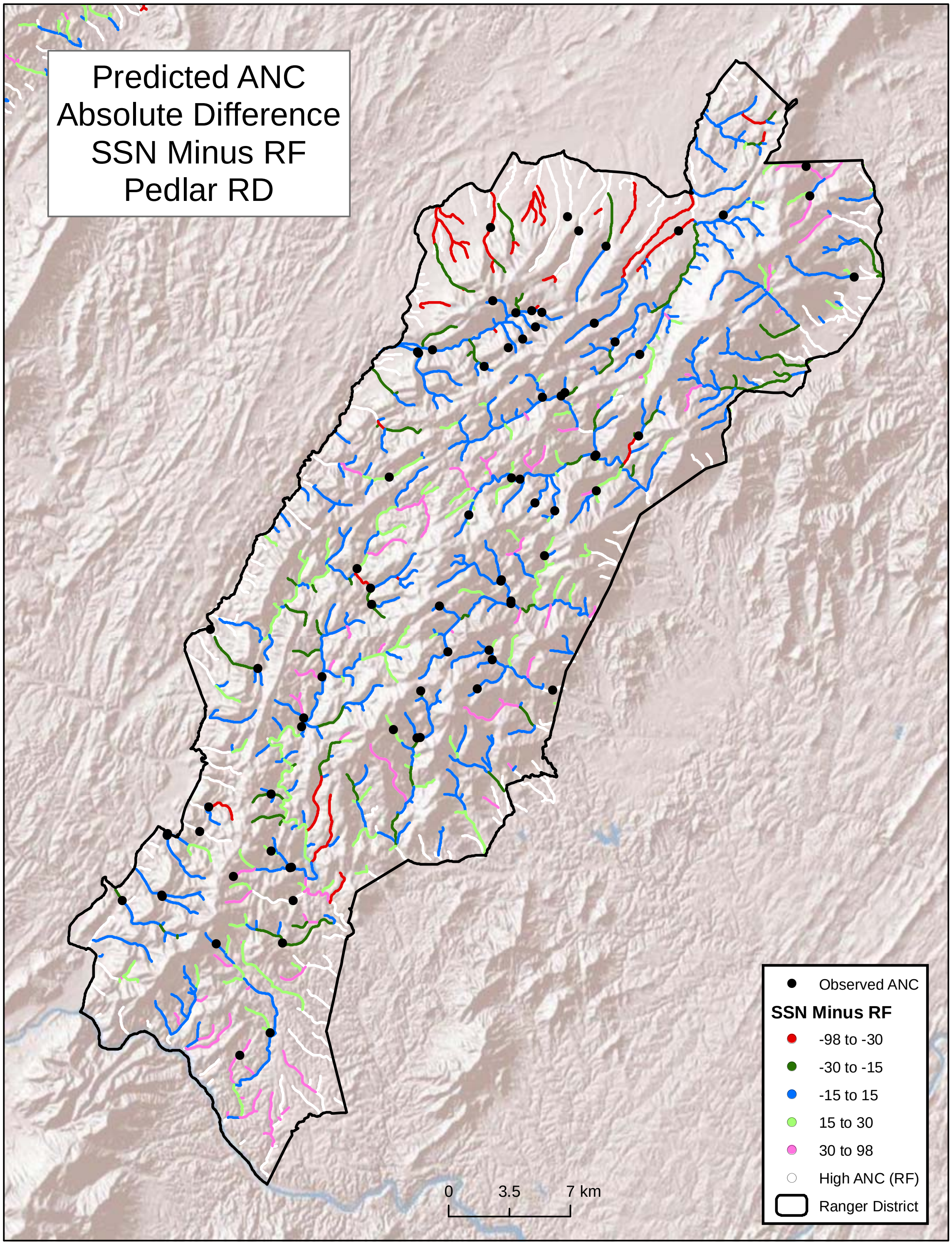

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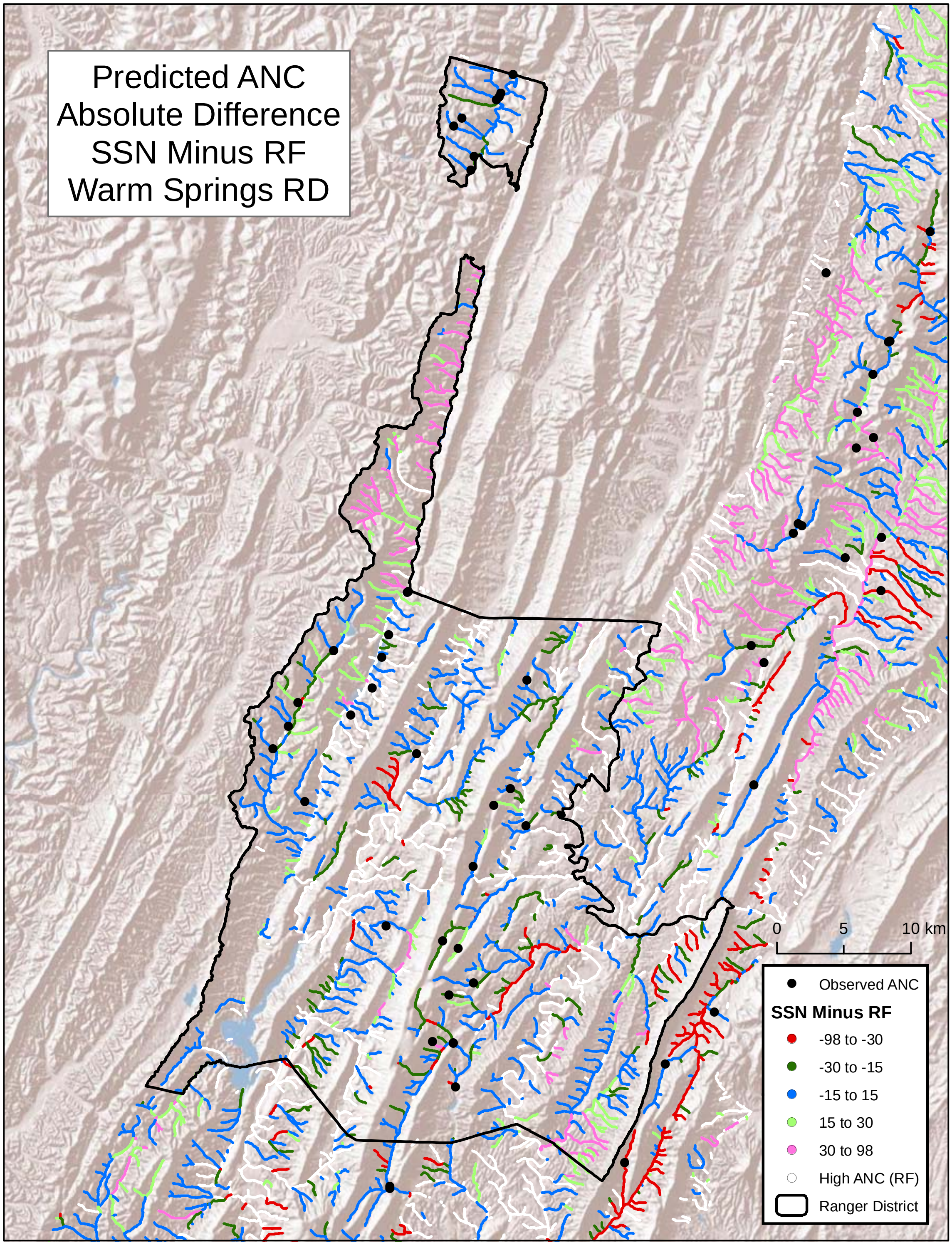

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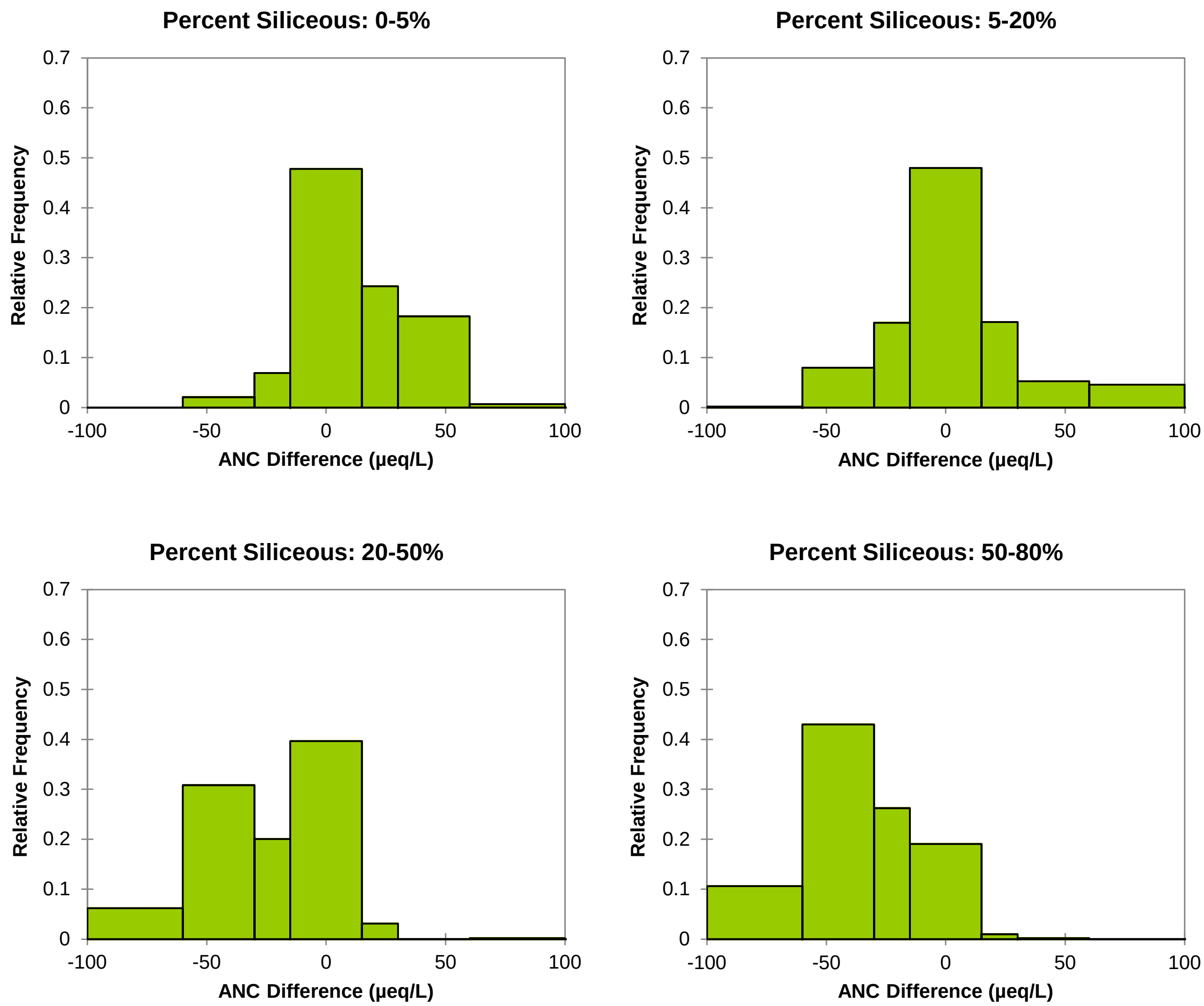


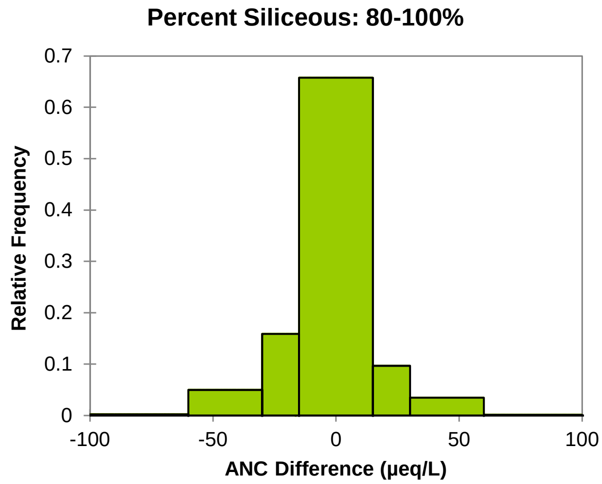


Figure 12. Distribution of absolute difference in ANC prediction among classes of percent siliceous lithology. Results are expressed as SSN minus RF model results.

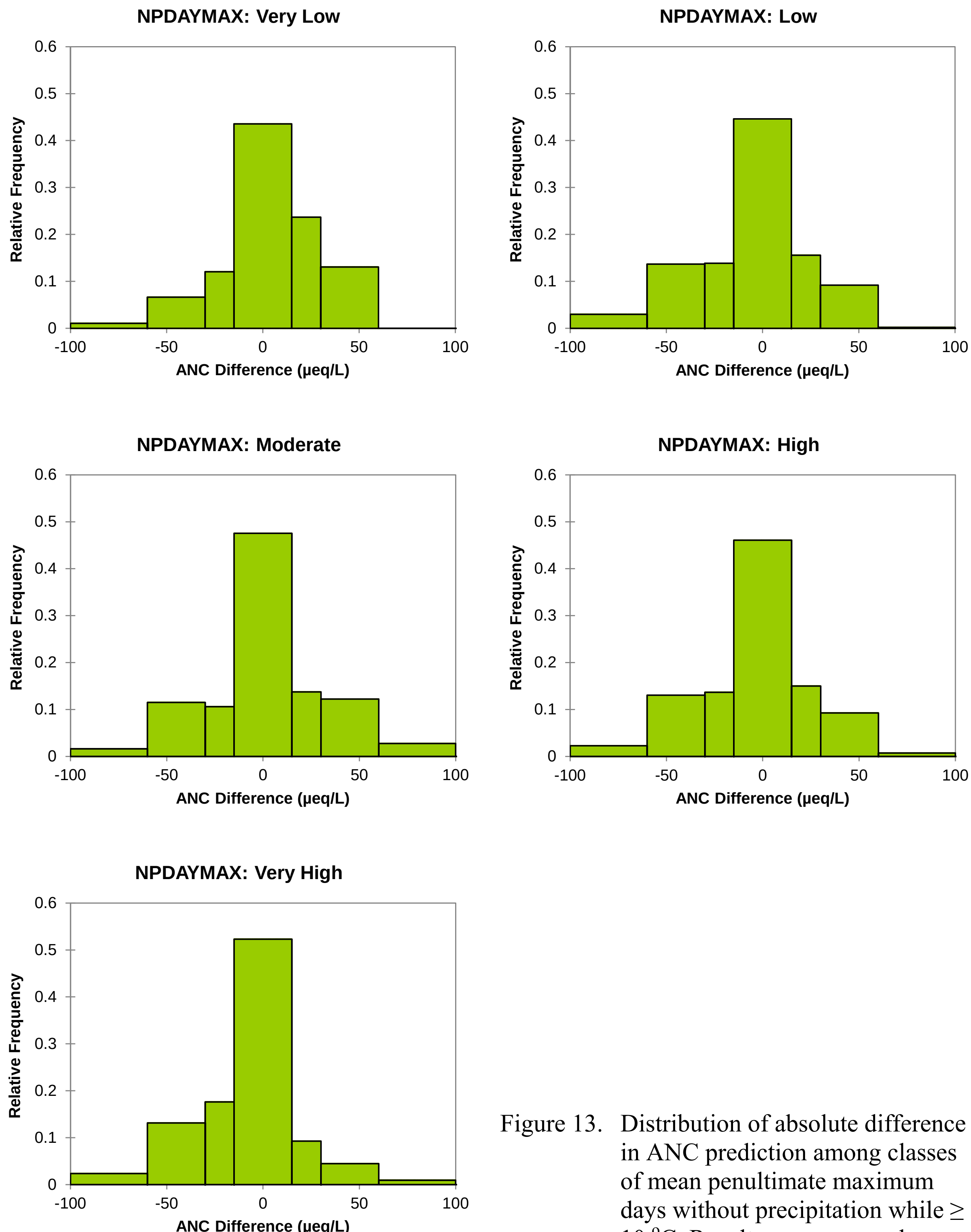


Figure 13. Distribution of absolute difference in ANC prediction among classes of mean penultimate maximum days without precipitation while ≥ 10 °C. Results are expressed as SSN minus RF model results.

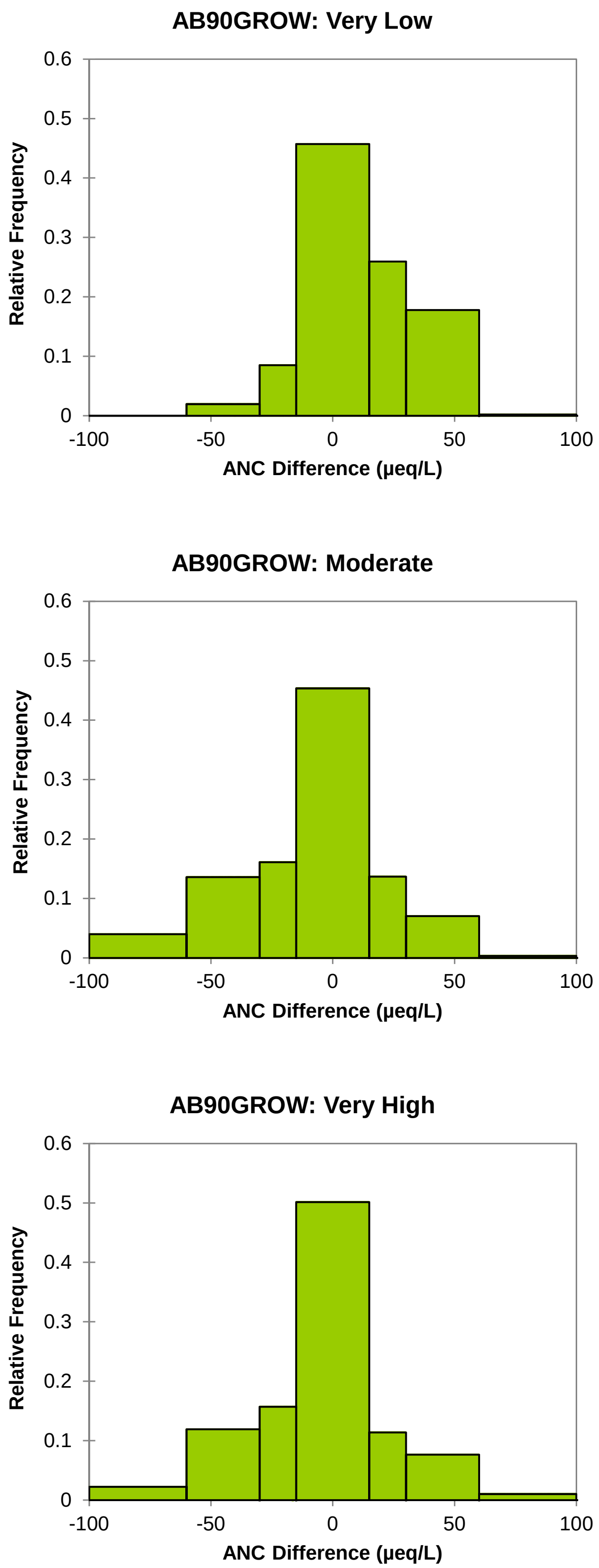
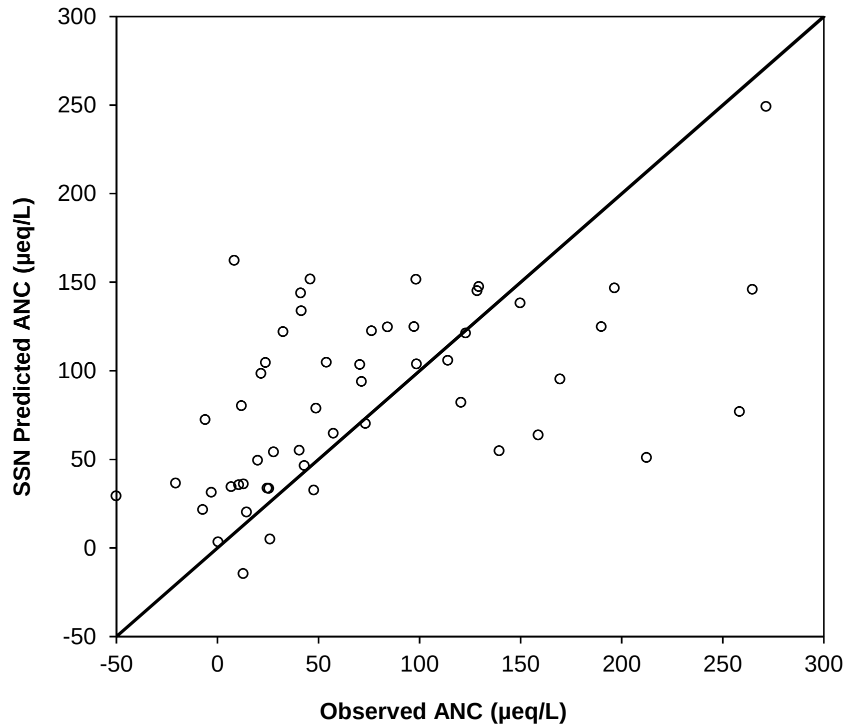


Figure 14. Distribution of absolute difference in ANC prediction among mean number of days above 32.2 ^{o}C. Results are expressed as SSN minus RF model results.

a)



b)

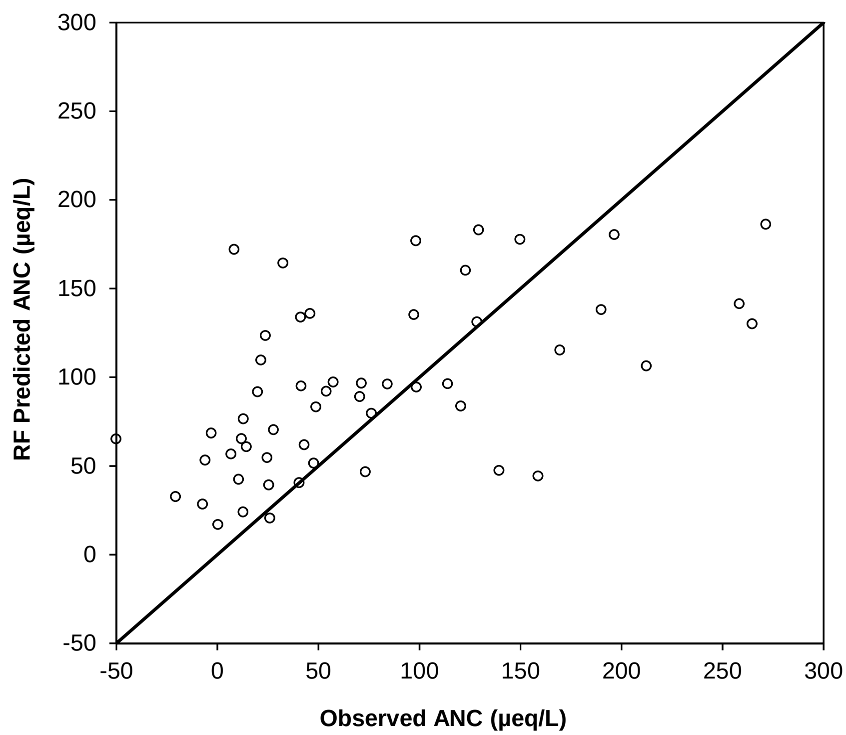


Figure 15. Confirmation results for the a) SSN model and b) RF model at 54 observed ANC sites.

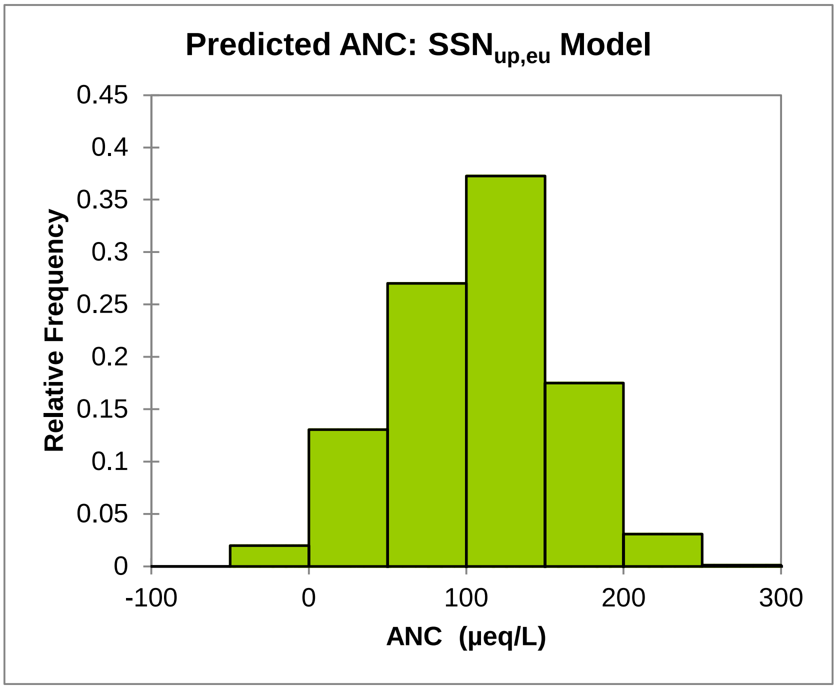


Figure 16. Frequency distribution of predicted ANC using an SSN model that included both flow-connected and Euclidean distance measures to represent spatial autocorrelation.

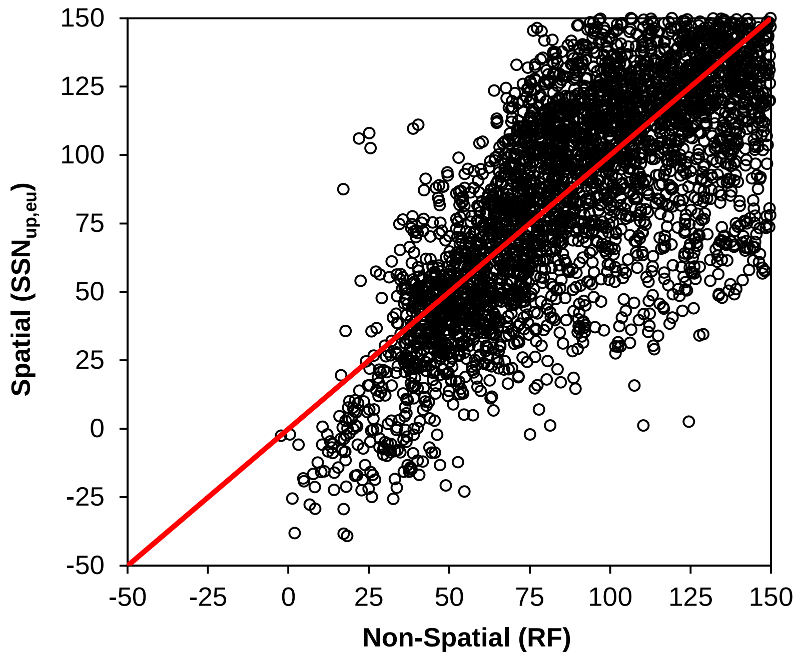


Figure 17. Predictions of stream ANC using the RF non-spatial versus the $SSN_{up,eu}$ spatial model. A 1:1 line is added for reference.