The Role of Retrospective Weather Forecasts in Developing Daily Forecasts of Nutrient Loadings over the Southeast US

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Abstract

It is well-known in the hydrometeorology literature that developing real-time daily streamflow forecasts in a given season significantly depend on the skill of daily precipitation forecasts over the watershed. Similarly, it is widely known that streamflow is the most important predictor in estimating nutrient loadings and the associated concentration. The intent of this study is to bridge these two findings so that daily nutrient loadings and the associated concentration could be predicted using daily precipitation forecasts and previously observed streamflow as surrogates of antecedent land surface conditions. By selecting 18 relatively undeveloped basins in the Southeast US (SEUS), we evaluate the skill in predicting observed total nitrogen (TN) loadings in the Water Quality Network (WQN) by first developing the daily streamflow forecasts using the retrospective weather forecasts based on K-nearest neighbor (K-NN) resampling approach and then forcing the forecasted streamflow with a nutrient load estimation (LOADEST) model to obtain daily TN forecasts. Skill in developing forecasts of streamflow, TN loadings and the associated concentration were computed using rank correlation and RMSE, by comparing the respective forecast values with the WQN observations for the selected 18 Hydro-Climatic Data Network (HCDN) stations. The forecasted daily streamflow and TN loadings and their concentration have statistically significant skill in predicting the respective daily observations in the WQN database at all the 18 stations over the SEUS. Only two stations showed statistically insignificant relationship in predicting the observed nitrogen concentration. We also found that the skill in predicting the observed TN loadings increase with increase in drainage area which indicates that the large-scale precipitation reforecasts correlate better with precipitation and streamflow over large watersheds. To overcome the limited samplings of TN in the WQN data, we extended the analyses by developing retrospective daily streamflow forecasts over the period 1979-2012 using

reforecasts based on the K-NN resampling approach. Based on the coefficient of determination ($R^2_{Q-daily}$) of the daily streamflow forecasts, we computed the potential skill ($R^2_{TN-daily}$) in developing daily nutrient forecasts based on the R^2 of the LOADEST model for each station. The analyses showed that the forecasting skills of TN loadings are relatively better in winter and spring months while skills are inferior during summer months. Despite these limitations, there is potential in utilizing the daily streamflow forecasts derived from real-time weather forecasts for developing daily nutrient forecasts, which could be employed for various adaptive nutrient management strategies for ensuring better water quality.

1. Introduction

Anthropogenic interventions of biogeochemical cycles have resulted in increased nutrient loadings in streams over the past few decades (Galloway et al., 1995; Caraco and Cole, 1999). Continuous concerns about water quality degradation have resulted in the development of active water quality management programs such as total maximum daily load allocation (TMDL) as well as establishment of policy instruments related to water quality trading. Of particularly interest is the total nitrogen (TN) loadings whose contribution from the land surface to the North Atlantic Ocean, has increased from 5 to 20 folds in comparison to the pre-industrial/natural level (Howarth et al., 1996). Nitrate levels have tripled in major rivers over the northeastern US since 1900's while nitrate concentration doubled in the Mississippi River basin since 1965 (Turner and Rabalais, 1991; Howarth et al., 1996; Vitousek et al., 1997; Goolsby and Battaglin, 2001).

Excess nitrogen results in overproduction of phytoplanktons, which in turn causes anoxic conditions and eutrophication in lakes and coastal regions (Vitousek et al., 1997; Pinckney et al., 1999). Such eutrophication, due to natural and anthropogenic nitrogen sources, is an important water quality degradation issue, which ranges from small streams (Duff et al., 2008) to large water bodies such as Gulf of Mexico (e.g. Bricker et al., 1999; Alexander et al., 2000; Rabalais et al., 2002; Alexander and Smith, 2006). There have been several efforts to reduce nitrogen loadings to streams but such programs are often too costly. For example, North Carolina Department of Energy and Natural Resources (DENR) have spent several billion dollars in nutrient management of Falls Lake in the Neuse River to control total nitrogen loadings under permissible range (North Carolina DENR). But, availability of data on total nitrogen is limited with concentration being measured on a non-continuous basis. Studies have tried to overcome these limitations by using the long available records of streamflow, since both instream nutrient concentration and loadings primarily depend on streamflow variability (Borsuk et al., 2004, Paerl et al., 2006, Lin et al., 2007) and antecedent flow conditions (Vecchia, 2003, Alexander and Smith, 2006). Various nutrient simulation models have been developed to estimate loadings using semi-distributed hydrologic models (e.g., WASP, HSPF, SWAT, GWLF) or statistical models (e.g., LOADEST). Both these types of models are typically implemented under a simulation mode by using observed meteorological forcings to estimate nitrogen loadings. Similarly, considerable progress has been made in developing daily streamflow forecasts using statistical models, e.g. parametric models (Rajagopalan and Lall 1999; Anderson et al., 2002; Salas and Lee, 2010), and semi-distributed watershed models (e.g., Clark and Hay, 2004; Mcenery et al., 2005, Georgakakos et al., 2010). Developing daily streamflow forecasts over a large region using semi-distributed models require intensive spatial data (e.g. topography, land cover, soils) and computational resources, hence, we employed a semi-parametric approach in this study. In particular, we employed the K Nearest Neighbor (K-NN) semi-parametric scheme to develop daily streamflow forecasts contingent on updated climate forecasts since it can capture nonlinear relationships that are typically observed in daily streamflow data (Salas and Lee, 2010). The K-NN scheme has been widely used in hydrologic studies (Rajagopalan and Lall 1999; Prairie et al. 2006; Sharif and Burn 2006). Although daily streamflow forecasts could be developed with reasonable skill, there is a gap in linking those forecasts to develop daily nutrient loading forecasts. Furthermore, several studies have utilized antecedent streamflows as surrogates of initial catchment conditions (e.g. Chiew and McMohan, 2002; Piechota et al., 2001; Wang et al., 2009) including 3-day average streamflow conditions (Majumdar and Kumar, 1990; Srinivas and Srinivasan, 2000; Cigizoglu, 2003). In our analysis, the maximum auto-correlation between observed streamflow and the previous-day streamflow occurred with a lag of 3 days for the selected sites (figure not shown). Given that skillful forecasts of daily nutrient loadings could be utilized in improving in-stream water quality, we intend to investigate the potential in forecasting daily nutrient loadings conditional on daily precipitation forecasts and previously observed streamflow as surrogates of antecedent moisture conditions for 18 watersheds that are minimally affected by anthropogenic interventions over the Southeast US (SEUS).

The manuscript is organized as follows: Section 2 details the data sources for daily streamflow, observed daily total nitrogen samplings and retrospective daily precipitation forecasts that were utilized in the study. Following that, we describe the methodology behind the development of daily streamflow and nutrient loadings forecasts. Section 4 provides the results on the skill in predicting the observed nutrient loadings over the selected 18 watersheds. Finally, in Section 5, we summarize the salient findings and conclusions arising from the study.

2. Data Description

This section outlines the streamflow, Water Quality Network (WQN), retrospective weather forecasts associated with the development of total nitrogen forecasts over the SEUS.

2.1 HCDN Streamflow Database

Given the intent of the study is to associate daily nutrient loadings with daily precipitation forecasts, we focus our analysis on 18 undeveloped basins over the SEUS from the Hydro-Climatic Data Network (HCDN) database (Slack et al., 1993). Figure 1 shows the location of 18 HCDN stations and Table 1 provides the list of the 18 stations considered in this study along with their drainage areas. Daily streamflow records in the HCDN basins is purported to be relatively free of anthropogenic influences such as upstream storage and groundwater pumping and the accuracy ratings of these records are at least ‘good’ according to United States Geological Survey (USGS) standards. Since the streamflow data (Q) in the HCDN database is available only up to 1988, we extended records up to 2009 based on the USGS historical daily streamflow database.

2.2 Weather Forecasts Database

We employed retrospective weather forecasts from the National Oceanic and Atmospheric Administration (NOAA) to forecast daily streamflow at multiple sites in the SEUS (Hamill et al, 2004; Hamill et al., 2006). NOAA's Earth System Research Laboratory/Physical Science Division (ESRL/PSD) reforecast project provides daily precipitation forecasts from the Global Forecast System (GFS) model, which was formerly called the Medium-Range Forecast Model (MRF). The GFS forecasts model has 28 sigma (pressure) levels and a T62 spatial resolution (~200 km grid size), which represents physical processes to estimate atmospheric forcings such as winds, temperature, precipitation, geopotential heights at different pressure levels (Hamill et al., 2006). 15 ensemble forecasts are obtained by initializing different atmospheric states of the GFS model every day. The control run is initialized by the National Center for Environmental Prediction (NCEP)-National Center for Atmospheric Research (NCAR) reanalysis data (Kalnay et al., 1996) while the other 14 ensemble members use a set of seven bred pairs of initial conditions (Toth and Kalnay, 1997), which are re-centered each day on the reanalysis initial condition. In this study, we make use of daily precipitation reforecasts from the GFS model consists of 15 ensemble members, up to 15 days in advance, starting from 1979 to till date. We considered the ensemble mean of daily precipitation forecasts to forecast daily streamflow and daily total nitrogen loadings for the selected watersheds.

2.3 Water Quality Monitoring Network (WQN) Database

USGS provides national and regional descriptions of stream water quality conditions in Water Quality monitoring Network (WQN) across the nation (Alexander et al., 1998). The WQN database comprises of water quality data from the USGS monitoring networks for large watersheds (National Stream Quality Accounting Network, NASQAN) as well as watersheds that are minimally developed (Hydrologic Benchmark Network, HBN). We used the observed daily concentrations of Total Nitrogen (TN) for the 18 stations in the SEUS from the WQN database. By selecting watersheds from the HCDN database, we basically ensure that both the streamflow is minimally affected by anthropogenic influences. Bu, water quality data is influenced by the land use type. Based on the USGS National Land Use Classification Data (NLCD) data of 2001, we calculated the percentage area under agriculture and urban (Table 1) land use. From Table 1, we can see the distribution with seven, six and five watersheds having 20%-30%, 10%-20% and 0%-10% of area under agriculture respectively. On the other hand, the urban land use is less than 10% with the exception being station #3(23%). TN loadings for these stations are available over a period of 12-23 years with samplings being available on average 5 to 6 times per year (Table 1). For additional details about the WQN database, see Alexander et al. (1998). We next provide details on the methodologies behind the development of streamflow and total nitrogen loadings forecasts for the selected watersheds.

3. Streamflow and Total Nitrogen Forecasting Models

The overall schematic diagram of the daily streamflow and nutrients forecasting methodology is shown in Figure 2. Daily streamflow forecasts using weather forecasts have been pursued by many studies (Day, 1985; Wang et al., 2011; Yang et al., 2014), but efforts to use those streamflow forecasts to develop nutrient forecasts are very limited.

3.1 Daily Streamflow Forecasts

To develop daily streamflow forecasts, we first identified the grid points of large scale 1-day ahead forecasted precipitation (referred as FP, hereafter) that exhibit significant correlation with daily streamflow from the HCDN database (Table 2). The correlation was considered statistically significant when it was greater than *1.96/sqrt(n-3)*, where '*n*' denotes the number of days over 1979 to 2009 period. This helps us to identify the neighboring grid points that modulate the streamflow of a particular watershed.

Given that the selected large scale FP grids are inter-correlated with each other, Principal Component Analysis (PCA) was applied to select first few principal components which explained over 90% variability in the precipitation data. PCA, also known as empirical orthogonal function (EOF) analysis, transforms the correlated variables to orthogonal uncorrelated principal components (See details in Oh and Sankarasubramanian, 2013). The number of principal components varies from 2 to 5 among different sites (Table 2). These principal components (PCs) of 1-day ahead FP as well as daily streamflow over the previous three days, prior to the forecasting date, were selected as the predictor for the semi-parametric statistical model. For example, to forecast streamflow on a particular day WQN data was observed, say March 14 in a given year, predictors were the 1-day ahead FP issued on Mar 13 and the 1-day average daily streamflow from March 11 to March 13 in that year. Thus, the number of predictors varies from 3 to 6 (i.e., the number of selected PCs shown in Table 2 and one predictor for the 1-day average streamflow). The streamflow over the previous three days could be considered as a surrogate for antecedent soil moisture conditions. Then, the nearest neighbor resampling method was employed to predict daily streamflow for that particular day in which WQN was observed.

K – Nearest Neighbor (K-NN) resampling approach

After obtaining the predictors, PCs of the FP grids and 1-day average streamflow, we utilized the K - Nearest Neighbor (K-NN) resampling method proposed by Lall and Sharma (1996). Similar application of K-NN resampling approach was employed for developing monthly streamflow forecasts conditional on climatic predictors (Souza et al., 2003; Devineni et al., 2008). The K-NN approach resamples daily (or monthly data) from historical data to generate values that were observed in the past. Typically, the K nearest neighbors are identified between predicted time series and the historical series based on the Euclidean distance. Then a weighing function (e.g. Lall and Sharma, 1996) is generally assigned such that more weights are given to the nearest neighbors while less weights are given the farthest neighbors to estimate the predicted time series. Finally, multiple ensembles are generated to estimate the conditional mean of the time series.

In the K-NN scheme, we used the Mahalanobis distance instead of the Euclidean distance, since the selected predictors – PCs of the principal components and the streamflow over the past observations- could be correlated. Therefore, for forecasting the streamflow for a given day observed in the WQN data, all the neighbors were chosen based on the historical time series of 1-day ahead FP and previous 1-day average streamflow for that day over the period 1979 to 2009, leaving out the daily predictors and predictands over the entire forecasting year (i.e., 365 days). This implies that in order to forecast streamflow for a given day, 30 historical years are available (excluding the forecast year) for identifying similar conditions. Since this is a small sample size for identifying neighbors, we also considered daily streamflow over the three previous days, resulting in a total 120 neighbors, to develop streamflow forecasts for a given day. Mahalanobis distance for all these 120 neighbors were estimated using equation (1) (Mahalanobis, 1936):

$$D_{i,j} = \sqrt{(X_i - X_j)^T S^{-1} (X_i - X_j)} \qquad (1)$$

where X_i and $X_j = (X_1, X_2, \cdots, X_{120})$ are the multivariate vectors containing predictor variables at the conditioning time step i and j denote the rest of the time periods that are considered for identifying the neighbors with T representing the transpose operation and S^{-1} denoting the inverse of the predictor (X_j) covariance matrix. The matrix, $X_{\bullet} = \left[x_{1\bullet} \quad x_{2\bullet}\right]$ denotes the multivariate vector with $x_{1\bullet}$ and $x_{2\bullet}$ denoting the 1-day averaged streamflow before the forecasted day and the PCs of 1-day ahead FP. The first 50 nearest neighbors and their corresponding daily streamflow values were selected based on Mahalanobis distance, $D_{i,j}$, to develop ensemble of daily streamflow forecasts. These daily streamflow values from the 50 neighbors were used to draw 500 ensembles that represent the conditional distribution with the density/weight represented by each member, j, by the kernel in equation (2):

$$w_j = \frac{1/j}{\sum_{k=1}^{K} 1/k} \ , \ i = 1, 2, \cdots, K \tag{2}$$

where $K = 50$ (the number of neighbors), w_i represents the probability with which neighbor is resampled in constituting the 500-member ensemble. Finally, the forecasted streamflow for each day is calculated as the conditional mean of these 500 realizations obtained from the 50 neighbors. The ensemble mean of daily streamflow forecasts are specifically obtained for the days on which WQN data is available, so that the ensemble mean of daily streamflow forecasts could be used for developing forecasts of total nitrogen loadings, whose details are described in the next section.

3.2 Daily Nitrogen Loadings and Concentration Forecasts Development

Daily nitrogen loadings forecasts are developed by forcing the daily streamflow forecasts with the Load Estimation (LOADEST) program. The LOADEST model can be employed with the observed or predicted daily streamflow time series at any given site. Streamflow forecast developed using large-scale precipitation forecasts and previous 3-day average streamflow using the non-parametric model is forced with the LOADEST model to develop nutrient forecasts.

LOADEST is a statistical model that estimates daily loadings based on the observed daily streamflow and the centered time (*dtime*) of the year of the observation (Runkel et al., 2004).

$$\ln(L_j) = a0 + a1 \ln(Q_j) + a2 \ln Q_j^{\,2} + a3 \sin(2\pi dtime) + a4 \cos(2\pi dtime) + \hat{\varepsilon}_j \quad \ldots(3)$$

where L_j denotes the observed daily loadings from the WQN database with '*j*' denoting the day of observation, Q_j is the observed daily flow and *dtime* is the centered time which is a function of the observation's number of days (from January 1) in the calendar year, *a0-a4* denote the model coefficients and $\hat{\varepsilon}_j$ is the estimated residual for the model. The expression *dtime* is centered to avoid multi-collinearity and *dtime* also represents the seasonality in loadings pattern. For a detailed expression on *dtime*, see Cohn et al. (1992).

The LOADEST model allows the user to select the best-fitting regression model from eleven predefined regression models using the Akaike Information Criterion (AIC) (Akaike, 1981). Five regression models that include a linear time trend are not appropriate, since we are employing observed streamflow to estimate simulated loadings for HCDN watersheds. Therefore, the simulated nutrient loadings based on the remaining regression models (i.e., model forms: 1, 2, 4 and 6 as defined in Runkel et al., 2004) in the LOADEST program do not have any time trend. Equation (3) represents the model form 6. Model form 1 (2) considers only the first two (three) terms in the right hand side (RHS) of equation (3), whereas model form 3 considers all the terms except the third term in the RHS of equation (3). For further details on model forms, see Runkel et al. (2004). Table 3 shows the "goodness of fit" statistics (coefficient of determination (R^2) and AIC) in predicting the observed daily loadings in the WQN database (Table 1) and the coefficients of the best fitting regression model for total nitrogen for the selected18 stations.

From Table 3, we infer that R^2 ranges from 0.83-0.97 indicating good fit of the observed daily loadings over 18 stations. Using these parameters, we next estimate the forecasts of daily loadings using the ensemble mean of daily streamflow forecasts developed using the retrospective weather forecasts. Strictly speaking, these parameters should have been obtained by leaving out the observed WQN loadings on the day of the forecasting. Since we have more than 50 observations at each site (Table 1), the regression coefficients and model forms did not change substantially. Hence, we used the parameters of the regression coefficients given in Table 3 to estimate the forecasted total nitrogen loadings. These forecasted loadings are divided by the forecasted streamflow to estimate the forecasts of total nitrogen concentrations for the 18 selected watersheds. The forecasted daily streamflow and total nitrogen loadings and concentration are respectively compared with the observed streamflow and the observed WQN daily loadings based on Spearman rank correlation and Root Mean Square Error (RMSE) in predicting the observed information.

4. Results and Analysis

In this section, we present skill in predicting variability (rank correlation) and accuracy (RMSE) of observed streamflow and WQN loadings using the forecasted daily streamflow obtained using the K-NN approach.

4.1 Skill in Forecasting Daily Streamflow

We first summarize the performance of the daily streamflow forecasts for only those days when TN loadings are measured (Figure 4a). Based on that, we infer that all the stations show statistically significant correlations with 8 sites showing correlations greater than 0.8 (Figure 3a). Similarly, RMSE (in cfs per unit area) is lesser than 1 for all states except stations #11, 17 and 18 (Figure 3b). These errors primarily occur due to the inability of the model to predict high values as indicated by very high residuals. For instance, RMSE for station #17 drops from 3.56 to 0.55 by excluding only one extreme observation recorded on 2/10/1981 (not shown here). The RMSE for station #11 (#18) are adjusted to 0.73 (0.29) by dropping one (two) high flow value(s). Although this conditional bias is not observed at all the stations, we infer that the daily streamflow forecast model has poor skill in predicting high flow values. We defer this issue for further discussion at the end of this section. Given this evaluation in predicting observed streamflow on days with WQN data, we next evaluate the performance of daily nitrogen loadings and concentration forecasts for the 18 stations.

4.2 Skill in Forecasting Total Nitrogen Loadings and Concentration

Using the ensemble mean of the daily forecasted streamflows as a predictor in the LOADEST model, we estimate the forecasted TN loadings for those days in which measurements are available in the WQN database. Figure 4a (4b) shows rank correlation (RMSE) between forecasted daily loadings and observed loadings for the 18 stations. Daily loadings of TN forecasts exhibit statistically significant relationship between observation and forecasts at all the stations with correlation coefficients being greater than 0.8 in nine stations. We also infer the correlation is higher in coastal regions as opposed to the inland watersheds. Similar to the skill of daily streamflow forecasts, loadings forecasts produce high RMSE in some stations despite their ability to predict the observed variability. This failure in forecasting TN loadings is primarily due to the inability in estimating high flow events as discussed in Section 4.1.

Further extending our analysis, we estimated TN concentration from the LOADEST model utilizing the forecasted streamflow and loadings and then compared the forecasted TN concentration with the observed concentrations available in the WQN database (Figure 5). Though the forecasted concentration is smaller compared to correlation reported for streamflow and loadings, the correlation is statistically significant at all stations except stations #6 and #18. Given that concentration is the ratio of loadings to the streamflow, the error in predicting both loadings and streamflow result in reduced skill. We are not reporting the RMSE since the trend is similar to Figures 4 and 5.

4.3 Factors affecting the skill in forecasting TN loadings

In order to understand what factors control the skill in forecasting the TN loadings utilizing the weather forecasts, we plotted the rank correlation against basin area (Figure 6). Rank correlation in forecasting streamflow (Figure 6a) and TN loadings (Figure 6b) are statistically significant for all the stations and the skill increases as the drainage area increases, which is consistent with previous findings (Bloeschl and Sivapalan, 2013). This is primarily due to the fact that retrospective weather forecasts being available over large spatial scales, the developed streamflow and TN loadings forecasts modulate better with the observed streamflow and WQN loadings.

To gain further understanding on how the developed model estimate the observed streamflow and nutrients, we present the performance of daily streamflow and TN forecasts for the sites that have the best and worst skill under each case (Figure 7). For quantifying the performance of streamflow, we considered the continuous daily streamflow records available from USGS instead of comparing the performance on the days with WQN data. From streamflow forecasts for the site with best skill (Figure 7a), we understand that overall performance is good, but the K-NN resampling approach based daily streamflow forecasts consistently underestimate high flow events. This underestimation/error in streamflow forecasts partially arises from the errors in the precipitation forecasts also. We discuss this issue in detail in the next section. From Figure 7b, the site performs poorly in forecasting flows above 8000 cfs. It is important to note that for the same site we observed significant correlation in predicting both the streamflow and the loadings on those days with WQN data being present. Thus, evaluating the performance of K-NN resampling model over the entire time series of observed records provide a more confirmatory evaluation of the model. The primary reason the K-NN resampling model performs poorly at site 3 (Rocky River near Norwood, NC) is due to the limited correlation between the observed precipitation and the forecasted precipitation during the summer months (figure not shown). Thus, the error resulting from K-NN resampling arises from both errors in the precipitation forecasts and in estimating the initial conditions as well as from the model itself. Even if one uses physically-based distributed models (e.g., Sacramento model), the skill of streamflow forecasts is heavily dependent on the skill of precipitation forecasts as well as the season of forecasting.

Figure 7c shows the performance of the TN loadings forecasts obtained using the streamflow forecasts with the LOADEST model. Even here, the same issue is highlighted with the limited ability of the forecasts in predicting the nutrients on days with high flows resulting in underestimated TN loadings. But, the model estimates the variability of the observed nutrients very well. Figure 7d shows the performance of TN loadings for a station with the worst skill. The skill of the streamflow forecasts resulting from the K-NN resampling approach in predicting the observed daily streamflow recorded at USGS stations is marginal with an average daily correlation of 0.6. Given that the R^2 of the LOADEST model is 0.912 for the selected station (Table 3), the poor performance primarily results from the inability of the streamflow forecasts which partly arises from the resampling model as well as from the skill of the precipitation forecasts. Thus, to develop nutrient forecasts, it is important that the skill of daily precipitation and streamflow forecasts should be good and also the load estimation model should have very high skill in predicting the observed nutrients. Given that these basins are virgin, it could be argued the predominant source of nutrient loadings arise from the nonpoint sources whose primary transport is the streamflow. Thus, for developing a broader understanding of what could be achieved in forecasting daily nutrients in virgin basins, one could look at the skill in predicting daily streamflow forecasts using the retrospective weather forecasts for the selected 18 stations. We summarize this information under the discussion in the next section by summarizing the skill of daily streamflow forecasts under each month for the selected 18 stations.

4.4 Discussion

The intent of this study is to develop daily forecasts of total nitrogen (TN) loadings and its concentration in 18 HCDN watersheds that are minimally impacted by anthropogenic influences over the southeastern US. Given that these watersheds experience virgin flow, our hypothesis is that most of the nutrient transport at daily time scales could be explained based on observed streamflow. For this purpose, we related the observed daily streamflow and loadings using the LOADEST model (Table 3), which showed significant skill in predicting the daily variability in TN loadings purely based on observed streamflow. Given that the predominant driver of streamflow in watersheds under rainfall-runoff regime is precipitation, we utilized the retrospective 1-day ahead precipitation forecasts from the reforecasts database of Hamill et al., (2004) and daily streamflow over previous three days (as a surrogate for soil moisture storage) for developing daily streamflow forecasts on the days with recorded WQN observations. The forecasted ensemble average of the streamflow obtained using the K-NN resampling model was used within the LOADEST model to estimate the forecasted daily TN loadings and the concentrations. We observed the correlation between observed TN loadings and the forecasted TN loadings being significant in almost all the stations. But, the forecasted concentration showed reduced skill, since it accounted for the errors in both loadings and streamflow. Though one could improve the streamflow forecasts developed using the K-NN resampling approach by considering physically distributed hydrologic models and by explicitly considering additional input variables (e.g., temperature forecasts, humidity), we certainly captured the first-order information on the daily streamflow variability by utilizing the retrospective precipitation forecasts and employed that for assessing the potential in developing nutrient forecasts. Another advantage with the streamflow forecasts using K-NN approach is in specifying the conditional distribution of flows. Thus, one could use the conditional distribution of streamflows with the LOADEST model to develop the conditional distribution of loadings, which could be used to estimate the probability of violating the concentration at the daily time scale.

It is important to note that all the skill reported in Figures 3-6 consider the ability to predicting those days when the WQN observations are available. The primary difficulty in assessing the potential for developing nutrient forecasts at daily time scale is the discontinuous nutrient samplings recorded in the WQN database. Oh and Sankarasubramanian (2012) addressed this issue by computing the coefficient of determination (R^2) of the winter TN loadings forecasts as a product of the R^2 in forecasting the seasonal streamflow and the R^2 of the LOADEST model for the winter season. Similarly, we express the skill of TN forecasts (equation 4) at daily time scale as a product of the R^2 of streamflow (Q) forecasts developed from the K-NN approach for each day in the calendar year and the R^2 of the LOADEST model reported in Table 3.

$$R^2_{TN-daily} = R^2_{(LOADEST)} * R^2_{Q-daily} \qquad \ldots(4)$$

$R^2_{Q-daily}$ is computed between the observed daily streamflow over the period 1979-2010 and the computed ensemble mean of the streamflow forecast from the K-NN resampling approach. Since the skill of daily streamflow forecasts differ substantially depending on the season, we plot the $R^2_{TN-daily}$ as a box-plot for each month (Figure 8). Basically, Figure 8 pools the daily correlation, $R^2_{TN-daily}$, for a given month across the 18 stations. For instance, in January, we expect 31*18 daily correlations and the box-plot simply summarizes the skill in predicting daily TN for that month over the Southeast US. About 75% of the $R^2_{TN-daily}$ at daily level are statistically significant level over the period January to May and also from November and December (Figure 8). Daily TN forecasts show relatively better skills in predicting observed TN variability during winter and spring. On the other hand, the skill of $R^2_{TN-daily}$ is poor during the summer and fall seasons. It has been well-known that retrospective precipitation forecasts have lower skill during the warm-season (Hamill et al., 2004). One of the possible reasons of relatively poor skill during summer and fall is that weather phenomena during these seasons depend greatly on local scale processes while large-scale models do not have the ability to capture it (Hamill et al., 2006). Thus, the poor skill of $R^2_{TN-daily}$ primarily arises from the skill in forecasting precipitation during the summer and fall seasons. Additionally, the role of temperature during the summer season is also much higher with enhanced evapotranspiration. However, considering temperature as additional predictor did not result in substantial increase in the $R^2_{Q-daily}$ for the summer season. Perhaps, if one considers a physically-based hydrologic model, the skill in predicting daily streamflow could improve during the summer season. We plan to investigate this as a future work in assessing the potential for developing nutrient forecasts with streamflow forecasts being derived from a physically-based distributed hydrologic model. Thus, the potential skill ($R^2_{TN-daily}$) in predicting daily nutrients is statistically significant for the winter and spring season in almost all the stations. One could utilize this to develop adaptive nutrient management strategies for controlling the point sources (e.g., waste water treatment plants) so that the downstream TN concentration does not exceed the desired/ EPA standards.

Given that consideration of both forecasted precipitation and 3-day average streamflow prior to the forecasting day exhibit significant skill in predicting the observed TN loadings from the WQN database, we investigated the role of each predictor in contributing to the overall skill reported in Figures 3-5. This analyses will also provide information on the role of basin storage, 3-day average streamflow, in contributing to the forecast skill. For this purpose, we developed the streamflow forecasts using only one predictor and then used that streamflow forecast to estimate the TN loadings. Figure 9 quantifies the role of each predictor, 3-day average streamflow prior to forecasting day (Q) and 1-day ahead precipitation forecasts (FP), in contributing to the skill, correlation and RMSE, in forecasting TN loadings for all the 18 sites. It is important to note that the correlation and RMSE were obtained by forecasting for the actual day for which the samples are available in a given site in the WQN database. Figure 9 clearly indicates that the combination of both 3-day average streamflow and 1-day ahead precipitation forecasts as predictors result in improved correlation and reduced RMSE in estimating daily TN loadings at all the sites. Comparing the skill obtained using only one predictor, 3-day average streamflow or forecasted precipitation, we infer that for most of the watersheds, the skill obtained using 3-day average streamflow (prior to the forecasting day) alone as a predictor provides better skill in comparison to the skill obtained using forecasted precipitation alone as a predictor with the exception being stations 6, 8 and 18. On an average, in most of the basins, 3-day average streamflow prior to the forecasts alone can explain around 25% (average correlation across all the sites is 0.52) of the variability in the observed nutrients. Several studies have shown that antecedent moisture/flow conditions also play a critical role in influencing the nutrient loadings from the watershed (Vecchia 2003, Alexander and Smith 2006). This analyses further confirms the critical role of basin storage, both streamflow and nutrients, in influencing the forecast skill. On the other hand, forecasted precipitation alone, can explain on average 20% (average correlation across all the sites is 0.45) of the variability in the observed TN loadings in the WQN database. Thus, including both of them as a predictors in the proposed modeling framework results in overall improvement.

We also investigated how the type of land use influence the skill in forecasting TN loadings. Figure 10 shows the scatter plot between the forecast skill, correlation coefficient between the observed TN loadings and the forecasted TN loadings, and the percentage area under agriculture for each watershed. This indicates basins with higher percentage of agricultural land exhibits higher skill in forecasting the TN loadings. Basin with increased agricultural activity could potentially experience increased fertilization application, which could increase the streamflow-induced transport. This indicates the role of basin nutrient storage in influencing the forecast skill. Similar analyses on urban land use did not reveal any relationship with the skill. Thus, analyses from Figures 9 and 10 show that both antecedent moisture conditions and in-basin nutrient storage influence the forecast skill for the selected 18 stations over the SEUS.

5. Summary and Conclusions

We developed a semi-parametric statistical model, which utilizes 1-day ahead precipitation forecasts from the reforecasts from the NOAA GFS climate model (Hamill et al., 2004) and daily streamflow over the previous three days as predictors, to develop daily streamflow forecasts, which in turn was used to implement a load estimation model, LOADEST, for estimating daily nutrients. For each day, conditioned on previous day's streamflow and 1-day ahead forecasted precipitation, 50 nearest neighbors over a three-day window were selected based on the Mahalanobis distance and then observed daily streamflow corresponding to those 50 neighbors were resampled to constitute 500 ensemble members to develop a daily streamflow forecast. It is important to note that to develop a forecast for a given day in a year, the entire year's predictors and predictand were left out for identifying the 50 nearest neighbors. Finally, the conditional mean of these daily streamflow ensemble was forced in the LOADEST model to obtain daily forecasts of TN loadings and concentration for days with recorded WQN observations. Skill in developing forecasts of streamflow, TN loadings and the associated concentration were computed using rank correlation and RMSE, by comparing the respective forecast values with the WQN observations for the selected 18 HCDN stations. The forecasted daily streamflow and TN loadings and their concentration exhibit statistically significant skill in predicting the respective daily observations in the WQN database at all the 18 stations over the SEUS.

The study also found that the skill in predicting the observed TN loadings is higher for large watersheds indicating the large-scale precipitation forecasts from the reforecast database better correlate with precipitation and streamflow over large watersheds. Analyses also showed that compared to the forecast precipitation, the 3-day average streamflow prior to the forecasting period played a dominant role in contributing to the skill of the forecast. We also observed the skill in forecasting TN loadings is higher for basins having higher percentage of the area under agriculture. These findings confirm that basin storage, both streamflow and nutrients, play a critical role in influencing the skill of the forecast. Further, to overcome the limited samplings of TN in the WQN data, we extended the analyses by developing retrospective daily streamflow forecasts over the period 1979-2012 using reforecasts based on the K-NN resampling approach. Based on the coefficient of determination ($R^2_{Q-daily}$) of the daily streamflow forecasts, we computed the potential skill ($R^2_{TN-daily}$) in developing daily nutrient forecasts based on the R^2 of the LOADEST model for each station. The analyses showed that the forecasting skills of TN loadings are relatively better in winter and spring months while skills are inferior during summer months. These findings are consistent with other studies (Devineni and Sankarasubramanian, 2010; Sinha and Sankarasubramanan, 2013) which show that large-scale precipitation forecasts derive their skill from ENSO climatic modes in the SEUS. One possible reason for this poor skill in summer is due to the dominance of local-scale processes during the summer season. Other possible reasons could be due to the limitations in the methodology. We resampled neighbors to develop daily streamflow ensemble, which of course will not have members beyond the maximum observation over the selected 50 neighbors. Further, air temperature can play a dominant role during the summer and fall seasons, resulting in enhanced evapotranspiration and reduced baseflow from the watershed. Despite these limitations, there is potential in utilizing the daily streamflow forecasts for developing daily nutrient forecasts, which could be employed for various adaptive nutrient management strategies for ensuring better water quality.

Though the watersheds considered under this study have experienced moderate agricultural activity, extending the above modeling framework for basins experiencing significant urbanization will require additional information. For instance, as the basin gets urbanized, it is natural to expect the point TN loadings from waste water treatment (WWT) plants to influence the downstream loadings and concentration. Under such situation, it would be useful to consider the discharges from the WWT plants as predictors in developing the model. One could also use the TN forecast to control point loadings so that the downstream TN concentration is within the prescribed standard. For basins experiencing significant non-point pollution from agriculture, one could use information from remote sensing satellites that quantify the chlorophyll concentration could be also be considered as nutrient storage in the river reach and water bodies (Jones et al., 2005). Thus, adequate monitoring of changes in basin land use and nutrient conditions could provide additional information in developing a TN forecasting model for watersheds experiencing significant human interference.

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Table 1: Baseline information for the 18 selected stations. Percentage land use area under urban and agriculture are calculated based on the 2001 USGS NLCD data. Values in the parentheses in the last column show the total number of daily total nitrogen loadings and concentration samplings available for each station.

Station Index	**Station Number**	**Station Name**	**Drainage Area (km^2)**	**% Area under Agriculture**	**% Area under Urban**	**Number of Years (# of daily Obs.)**
1	**2047000**	Nottoway river near Sebrell, VA	3732.17	16.9	5.0	17 (95)
2	**2083500**	Tar river at Tarboro, NC.	5653.94	28.9	8.0	22 (152)
3	**2126000**	Rocky river near Norwood, NC	3553.46	28.7	22.8	14 (65)
4	**2176500**	Coosawhatchie river near Hampton, SC	525.77	23.9	6.8	13 (100)
5	**2202500**	Ogeechee river near Eden, GA	6863.47	23.5	5.0	20 (141)
6	**2212600**	Falling creek near Juliette, GA	187.00	0.6	2.4	14 (56)
7	**2228000**	Satilla river at Atkinson, GA	7226.07	20.4	7.6	20 (123)
8	**2231000**	St. Marys river near Macclenny, FL	1812.99	3.8	5.9	14 (108)
9	**2321500**	Santa Fe river at Worthington springs, FL	1489.24	12.3	6.4	21 (82)
10	**2324000**	Steinhatchee river near Cross city, FL	906.50	0.8	4.8	19 (92)
11	**2327100**	Sopchoppy river near Sopchoppy, FL	264.18	0.0	1.0	22 (125)
12	**2329000**	Ochlockonee river near Havana, FL	2952.59	28.6	6.9	22 (133)
13	**2358000**	Apalachicola river at Chattahoochee, FL	44547.79	22.5	9.8	23 (152)
14	**2366500**	Choctawhatchee river near Bruce, FL	11354.51	19.6	5.6	21 (119)
15	**2368000**	Yellow river at Milligan, FL	1616.15	17.6	6.5	21 (123)
16	**2375500**	Escambia river near Century, FL	9885.98	12.5	4.8	22 (145)
17	**2479155**	Cypress creek near Janice, MS	136.23	0	0.9	16 (54)
18	**2489500**	Pearl river near Bogalusa, LA	17023.99	15.2	6.8	12 (57)

Table 2: Station ID, number of selected PCs, and cumulative Eigen values for large scale precipitation grids from the NOAA's GFS model, which provide 1-day ahead precipitation forecasts (Grid numbers are shown in Figure 1)

Station ID	Selected Grids (total # of selected grids)	# of Selected PCs	Cumulative Eigen value of selected PCs
1	5, 7, 12, 19-21 (6)	4	0.962
2	5, 7, 12 (3)	2	0.905
3	4-5, 11-13, 18-20 (8)	4	0.948
4	11-13, 18-20, 27 (7)	3	0.909
5	17-18, 24-27 (6)	3	0.922
6	9-12, 16-19, 23-26 (12)	4	0.903
7	24-26, 31-33 (6)	3	0.918
8	17-19, 24-26, 31-33 (9)	4	0.918
9	17-19, 24-26, 31-33 (9)	4	0.918
10	16-19, 23-26, 30-33 (12)	5	0.921
11	16-18, 23-25, 30-32 (9)	4	0.930
12	16, 30-32 (4)	3	0.975
13	23-25, 30-32 (6)	3	0.934
14	18, 22-25, 30-32 (8)	4	0.938
15	18, 22, 24 (3)	2	0.912
16	22, 29-31 (4)	3	0.977
17	15-17, 22-24, 29-31 (9)	4	0.929
18	17, 22-24, 30-31 (6)	3	0.932

Table 3: Performance of LOADEST model in predicting the observed TN loadings from the WQN database. Models with linear time components (Model No: 3,5, 7-9) are not considered.

Station Index	**R^2 (Daily)**	**AIC (Daily)**	**Model No**	**Coefficients of selected LOADEST model**				
				a0	**a1**	**a2**	**a3**	**a4**
1	0.948	0.892	4	6.768	1.114	-0.283	-0.069	
2	0.966	-0.131	4	8.122	0.980	0.108	-0.018	
3	0.966	0.496	4	8.863	1.066	-0.195	0.090	
4	0.956	0.905	6	4.446	1.013	0.026	0.238	-0.036
5	0.916	0.837	4	7.721	1.069	-0.084	-0.317	
6	0.853	2.094	1	2.647	1.095			
7	0.968	0.518	6	7.521	1.005	-0.025	-0.083	0.103
8	0.963	0.250	6	6.428	1.088	-0.075	-0.027	0.187
9	0.986	-0.219	6	5.690	1.086	-0.037	-0.078	0.059
10	0.979	0.279	6	5.549	1.241	-0.069	-0.096	0.071
11	0.979	0.516	6	4.351	1.139	-0.043	0.187	0.007
12	0.923	0.585	1	7.341	0.846			
13	0.902	0.193	4	10.563	0.981	0.074	0.165	
14	0.835	0.423	4	9.077	0.931	-0.145	-0.042	
15	0.834	1.085	6	7.238	1.123	-0.131	-0.004	0.176
16	0.873	0.758	4	8.868	1.039	0.147	0.032	
17	0.912	1.233	4	4.555	1.188	0.206	0.328	
18	0.899	0.853	1	10.193	1.047			

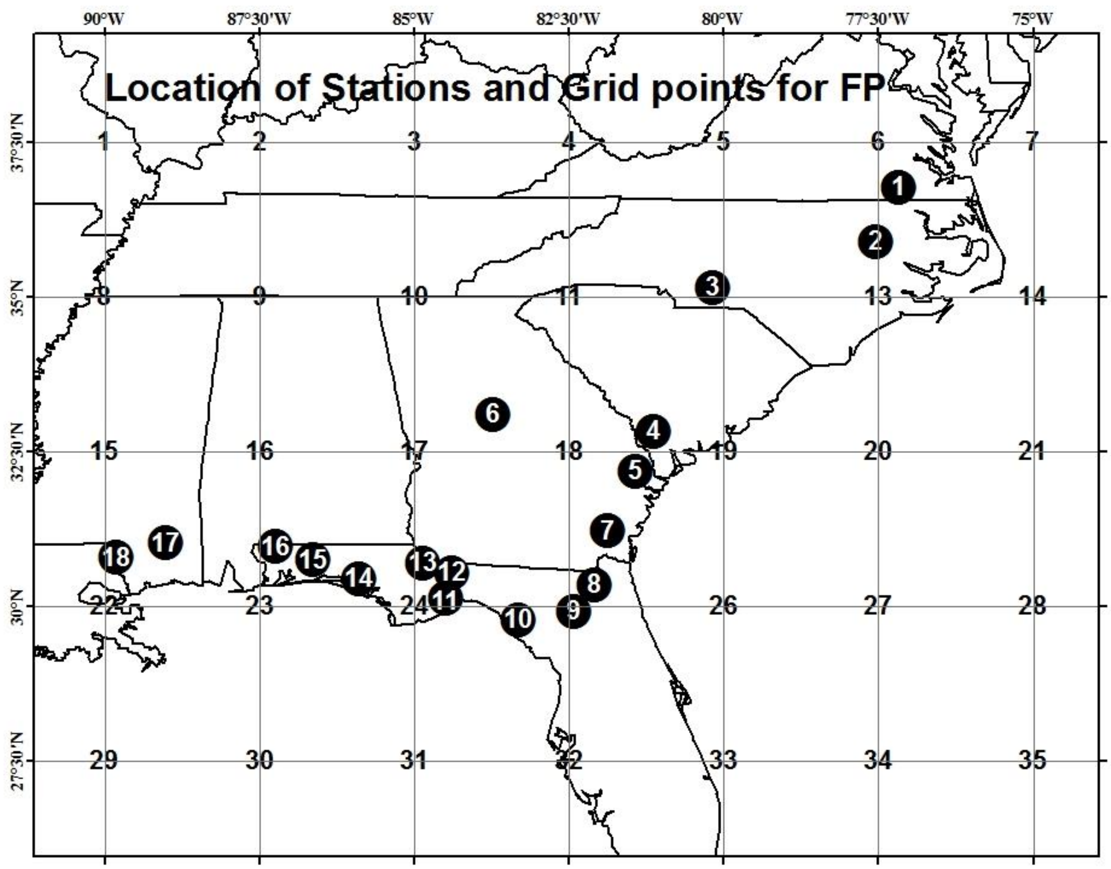

Figure 1. Locations of 18 water quality monitoring stations and grids of forecasted precipitation from NOAA's reforecast model.

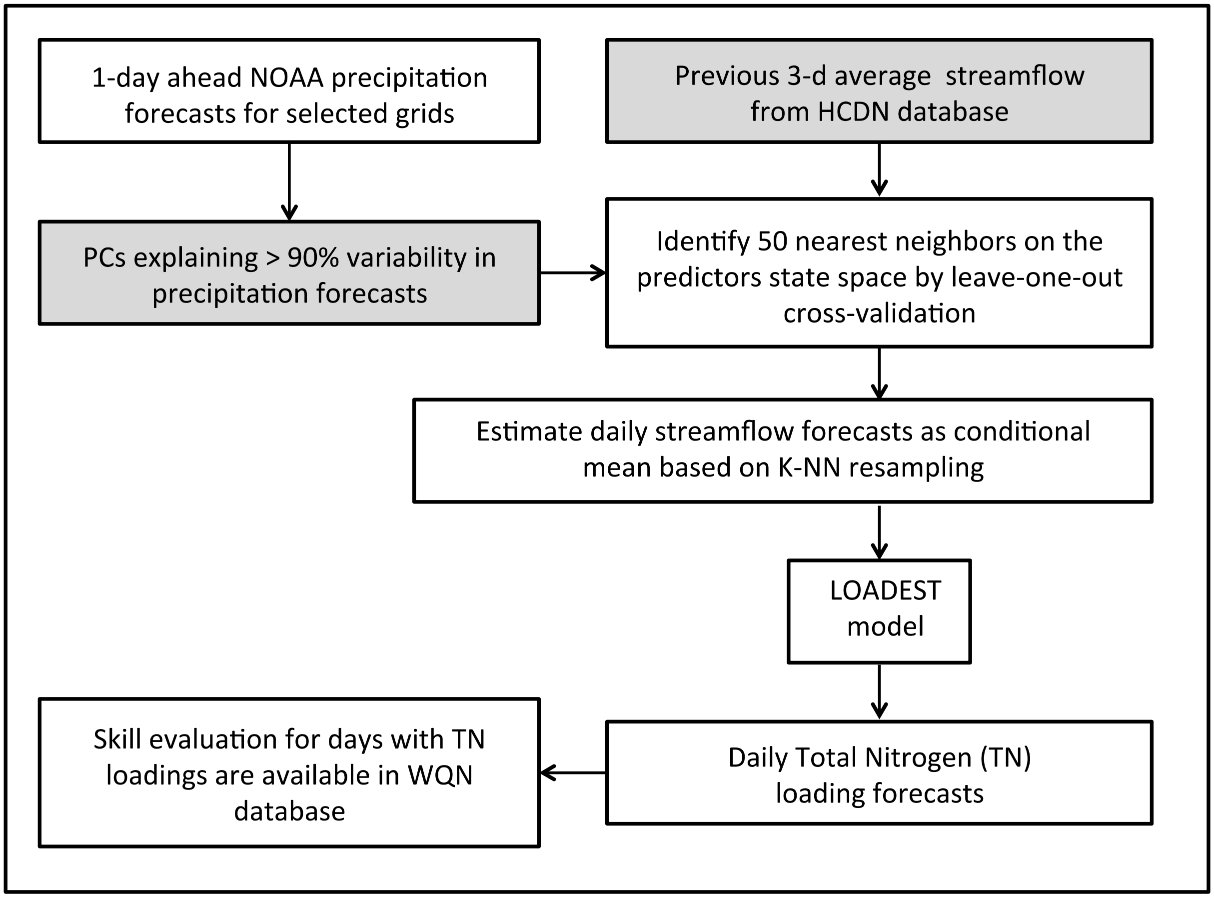

Figure 2: Schematic diagram illustrating the overall approach to forecast daily streamflow and total nitrogen loadings conditioned on the predictors (gray boxes), daily weather forecasts and daily average streamflow values for previous 3 days, based on Kernel-Nearest Neighbor (K-NN) resampling approach.

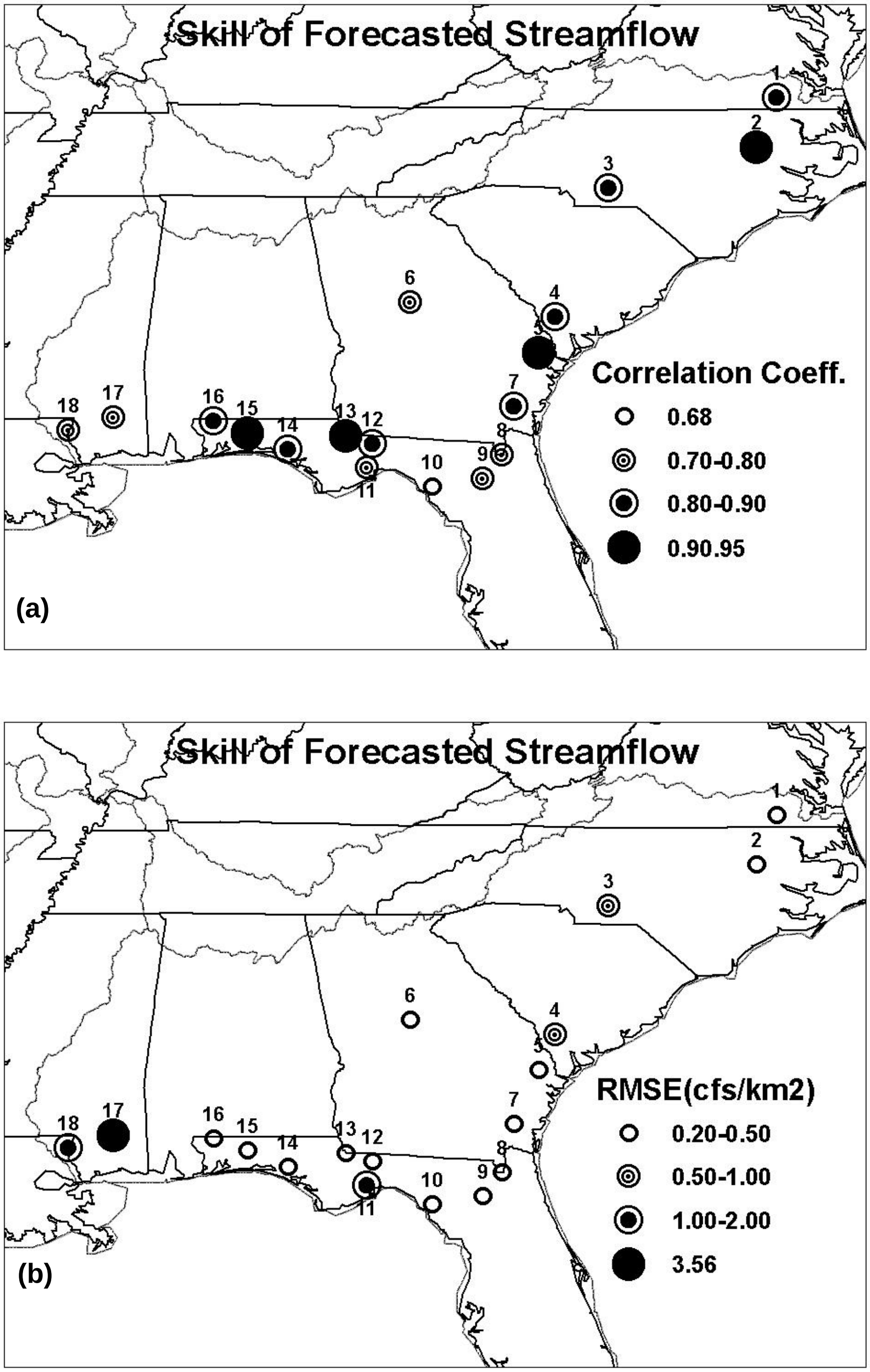

Figure 3: a) Rank correlation and b) RMSE (cfs per unit area) between observed daily streamflow and forecasted daily streamflow for those days with TN loadings being available in the WQN database.

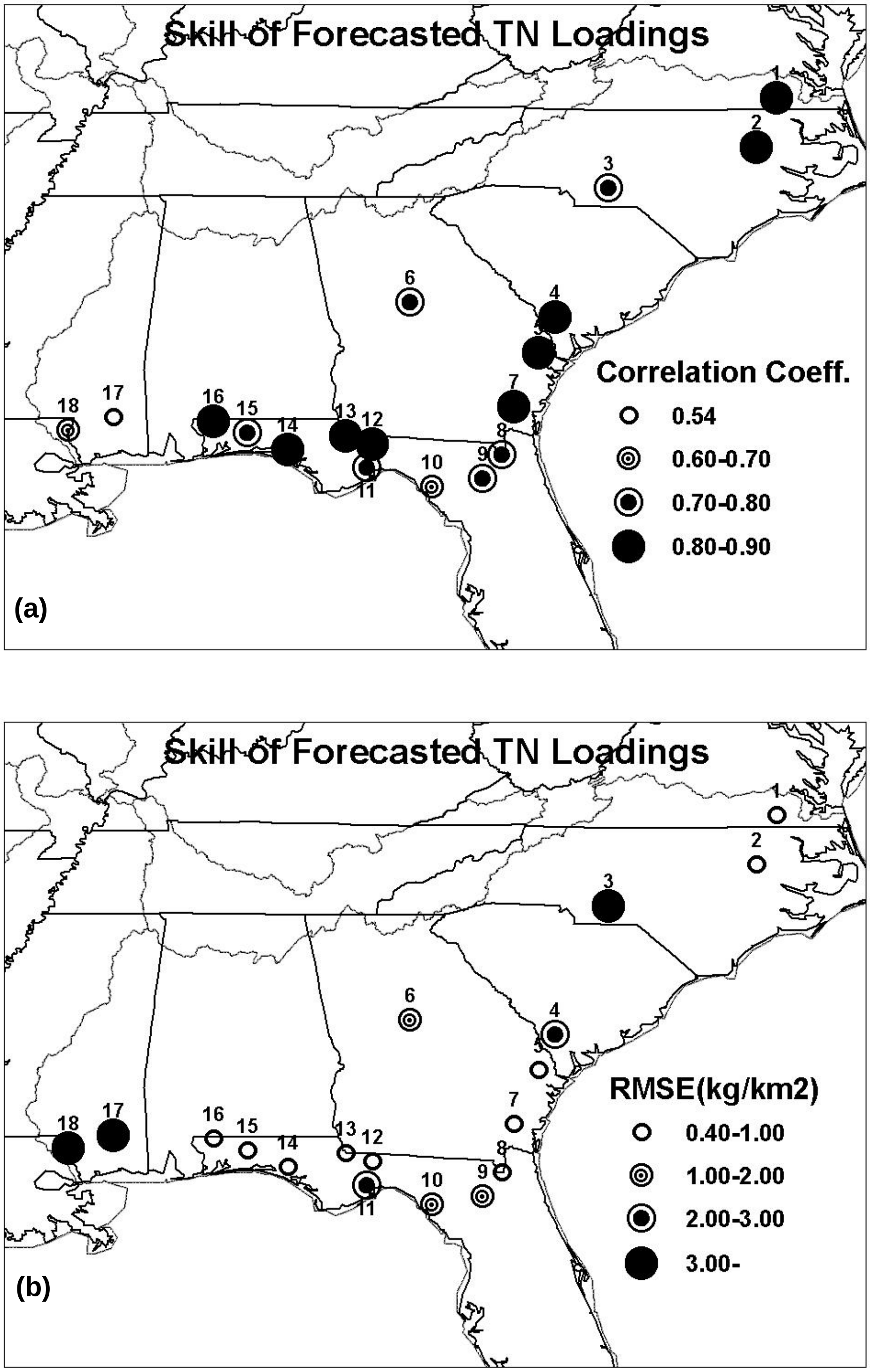

Figure 4: a) Rank correlation and b) RMSE between observed TN loadings and forecasted TN loadings for those days with TN loadings being available in the WQN database.

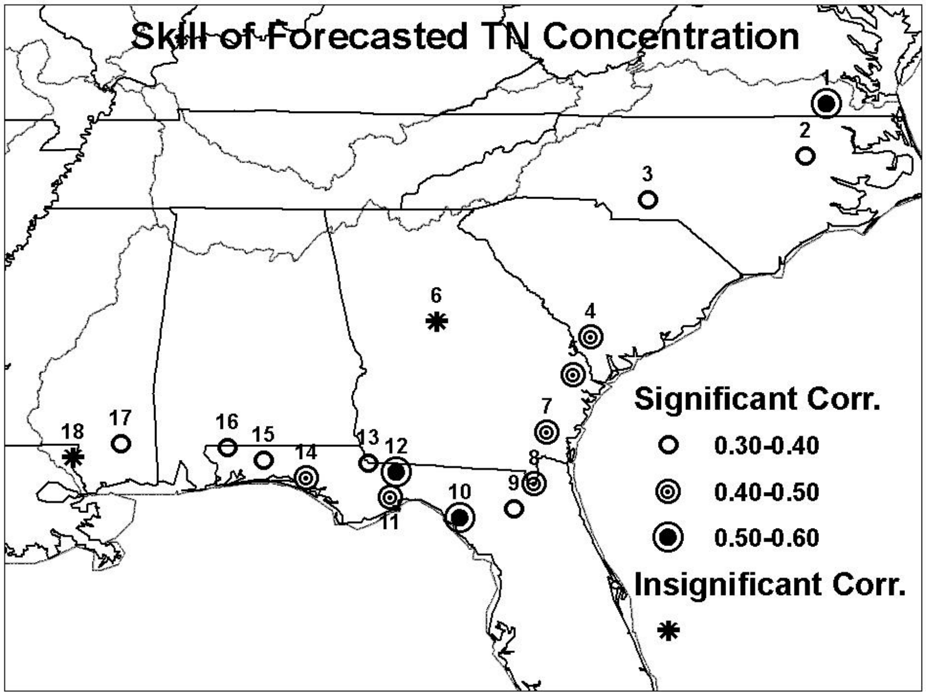

Figure 5: Correlation between observed TN concentration and forecasted TN concentration for those days with TN loadings being available in the WQN database.

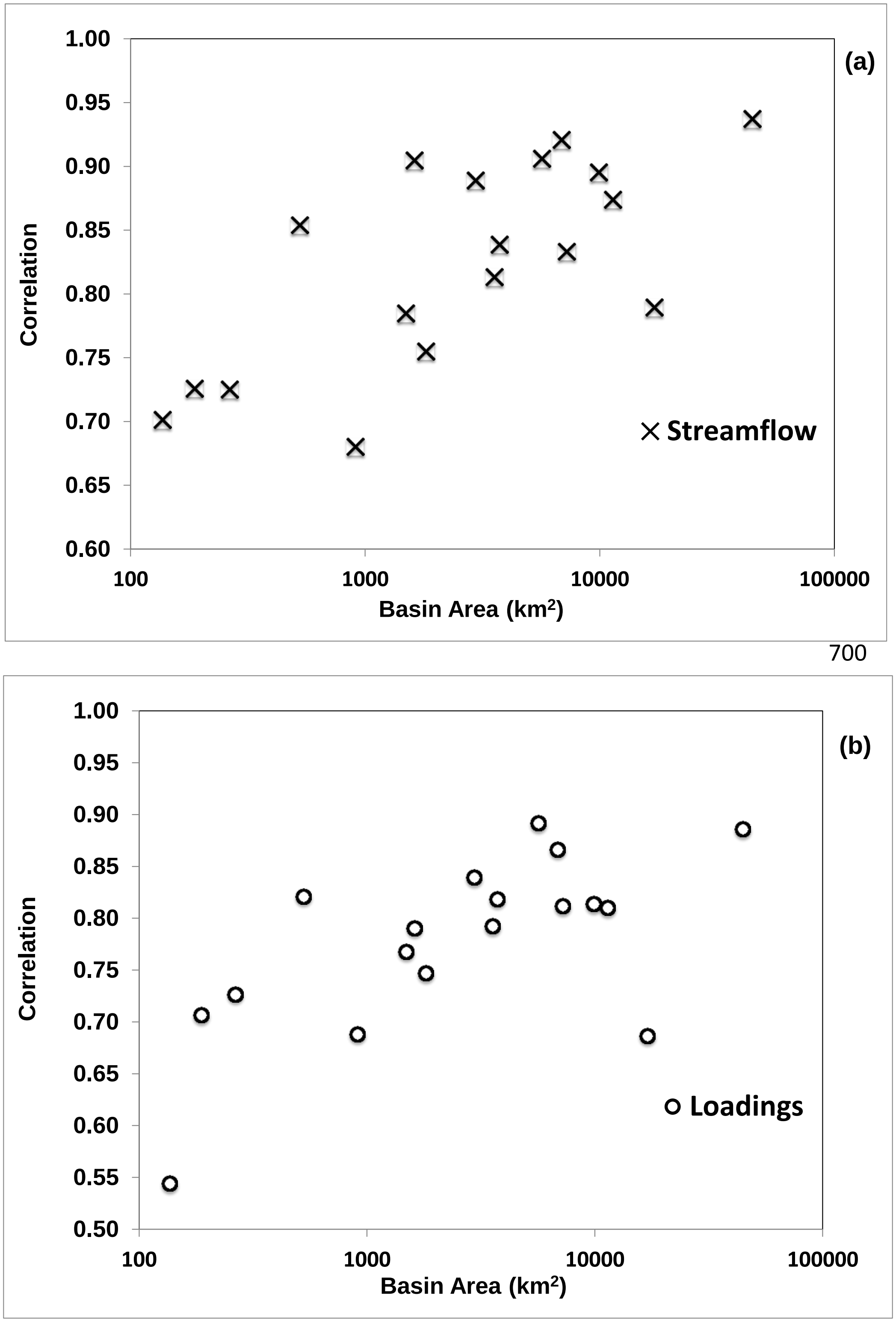

Figure 6: Role of basin scale, drainage area, in forecasting observed (a) streamflow and (b) TN loadings provided in the WQN database for the 18 stations.

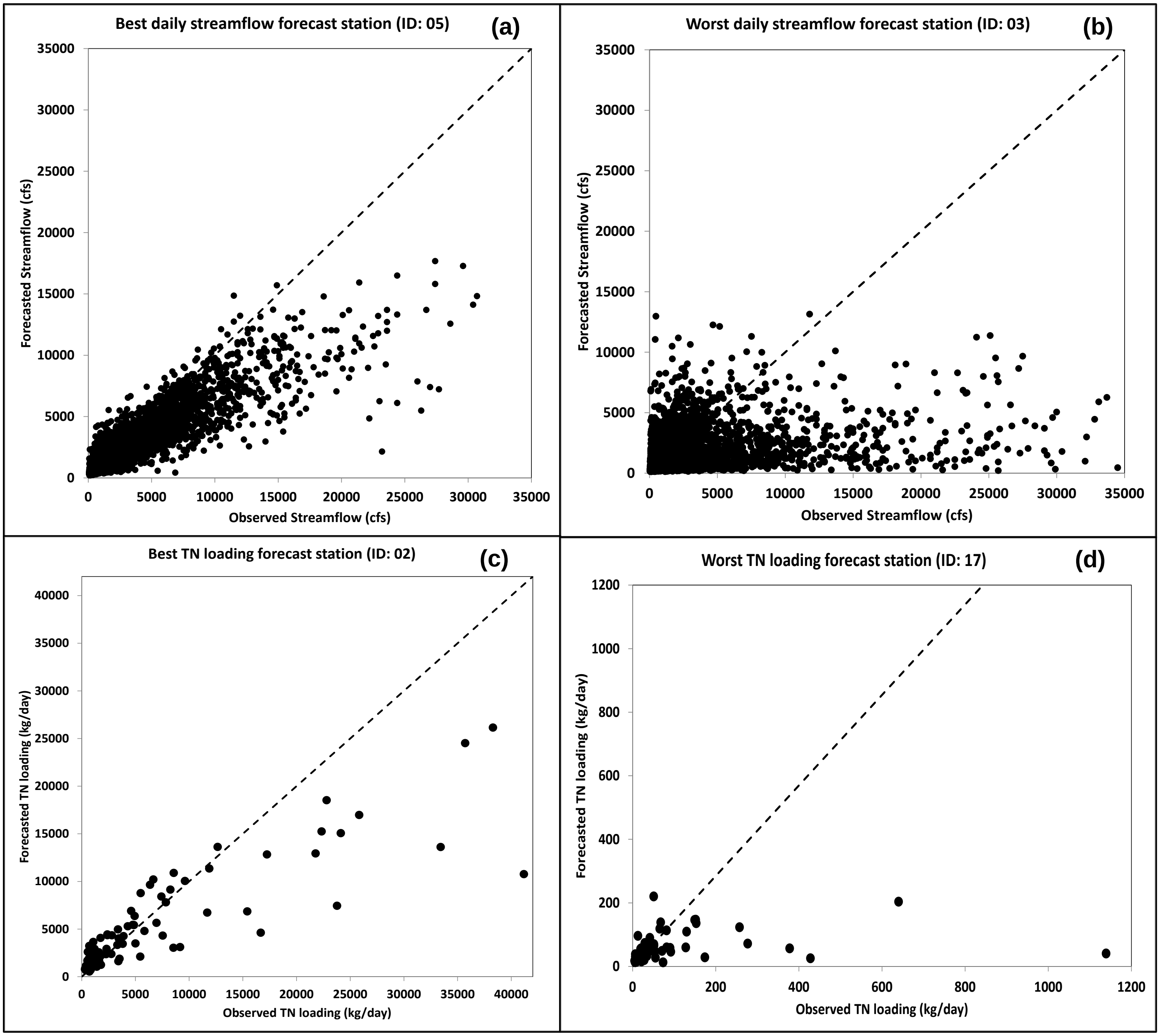

Figure 7: Comparison of observations and forecasts of streamflow (a and b) and TN loadings (c and d) for the stations with best (Streamflow: Ogeechee river near Eden, GA, TN: Tar river at Tarboro, NC) and worst forecasting skill (Streamflow: Rocky river near Norwood, NC, TN: Cypress creek near Janice, MS).

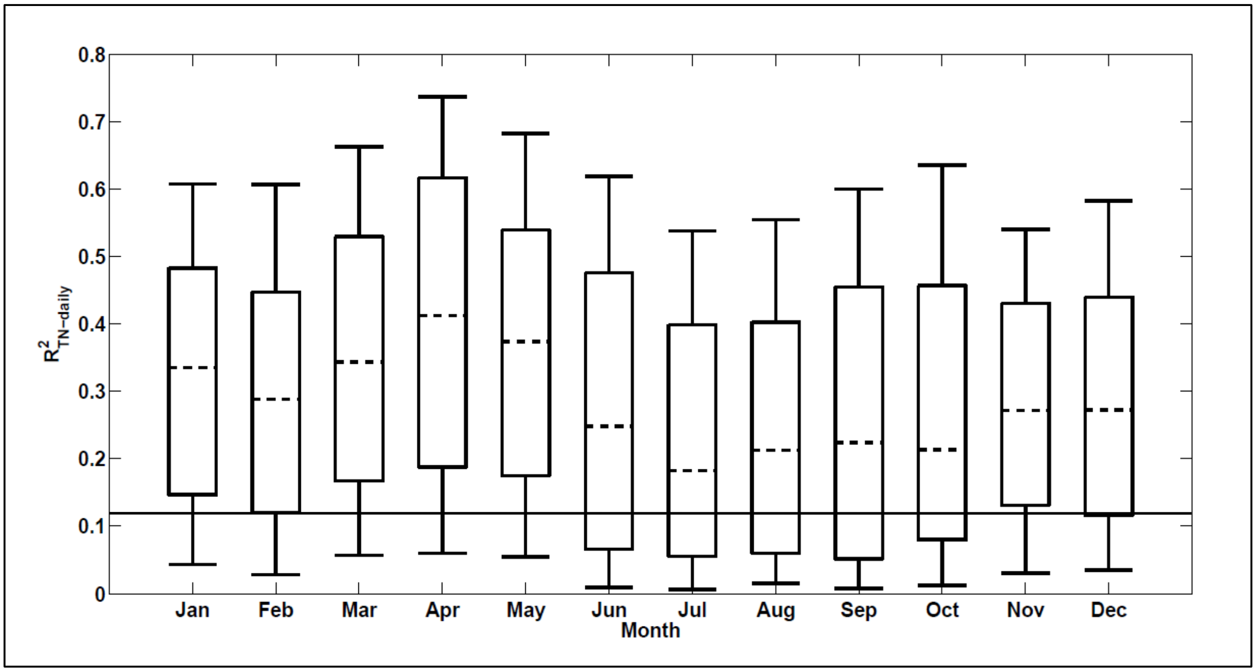

Figure 8: Box plot showing rank correlations between observed daily streamflow and forecasted streamflow aggregated over each month from 1979 to 2009 period. Each plot includes 558 correlations (18 stations × 31years). The solid line represents the statistically significant (95%) R^2 corresponding to the null hypothesis that R^2 being equal to zero.

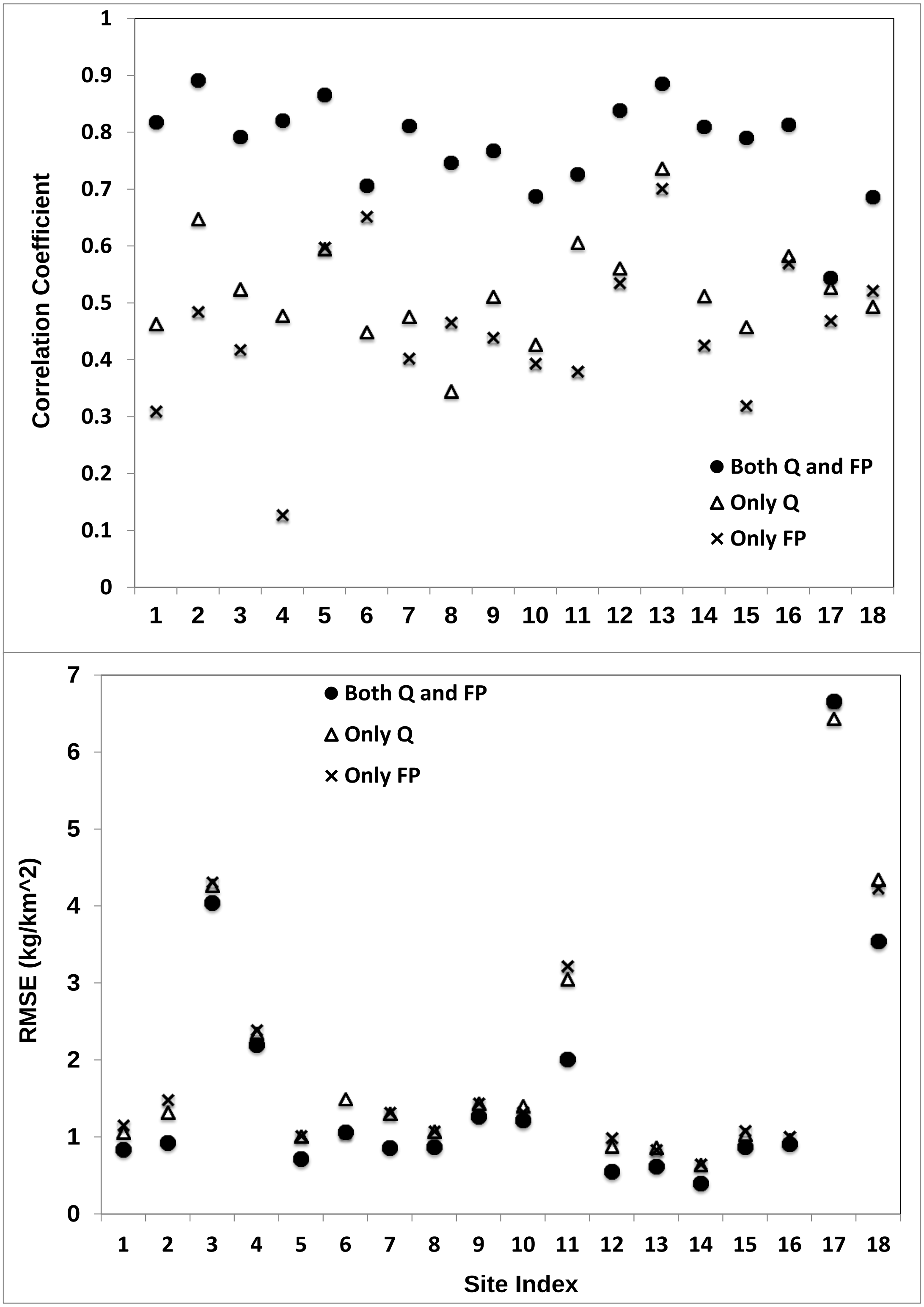

Figure 9: The role of different predictors, 3-day average daily streamflow prior to forecasting day (Q) and 1-day ahead precipitation forecasts (FP), in forecasting the observed TN loadings is expressed as (a) correlation coefficient and (b) RMSE between the observed TN and the forecasted TN loadings for the 18 selected sites.

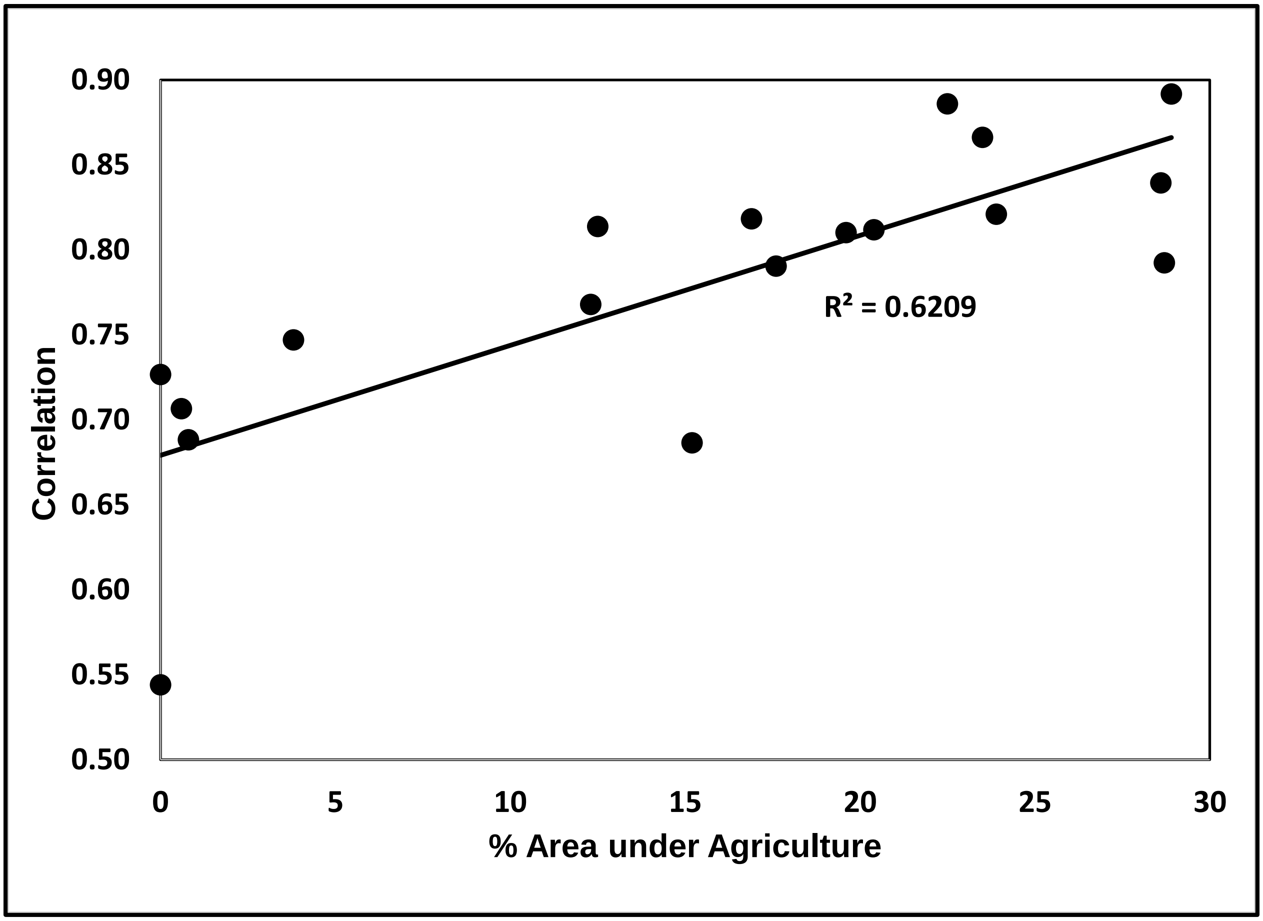

Figure 10: Role of the type of land use, percentage area under agriculture, in influencing the forecast skill which is expressed as the correlation coefficient between the observed TN loadings and the forecasted TN loadings for the 18 selected watersheds.