ABSTRACT

CHAZAL, NATALIE. Past and Future Coastal Water Quality: Trend Testing and Predictive Modeling Using Regulatory Shellfish Sanitation Data. (Under the direction of Dr. Natalie Nelson).

Water quality monitoring is essential for maintaining the health and safety of coastal communities. In states where shellfish are harvested for human consumption, Shellfish Sanitation programs implement long-term water quality monitoring strategies motivated by fishery specific water quality hazards. Fecal coliforms (FC) are specific indicators of potential pathogens in the water and can be concentrated in the tissues of bivalve shellfish. Regulatory agencies have been testing the waters for FCs since the early 1900s. While this data is generally used for day-to-day management, this thesis examined the application of these water quality datasets for both historical trend testing and short-term forecasting purposes.

In the first study, we (1) analyzed spatiotemporal trends from multidecadal FC concentration observations collected by a shellfish sanitation program, (2) identified possible management and environmental drivers of FC trends, and (3) assessed the feasibility of using these monitoring data to infer long-term water quality dynamics. We evaluated trends in FC concentrations for a 20-year period (1999-2021) using data collected from spatially fixed sampling sites (n = 466) in North Carolina. Mann-Kendall trend testing along with the analysis of rates of change (Sen slope) were used to determine the degree and significance of trends in FC levels in relation to changes in environmental covariates. Trends were evaluated on full coast and smaller estuarine scales. While trends varied from site to site, findings indicated that shellfish sanitation data can be used for long-term water quality inference under certain management conditions. Further, corresponding salinity trends could be used to measure the extent of management-driven bias in FC observations collected in a particular area.

In the second study, we (1) trained regression-based Random Forest models to predict FC concentrations using regulatory FC observations, (2) updated these models with forecasted rainfall inputs, and (3) identified key drivers of FC dynamics. We trained and tested Random Forest regression models for each of 5 major management areas along Florida's coast to predict mean FC concentrations across sampling stations with similar watershed characteristics. Potential predictors included rainfall, wind speed and direction, length of

natural and modified waterways, land use and land cover, soil drainage, tidal stage, air temperature, river stage, and season. Using hold out testing data, our model performed with R2 values varied from 0.36 to 0.72 between the 5 management areas. Using variable importance scores, antecedent precipitation values were among the most important predictors. When the models were updated with the forecasted rainfall values, wind components became increasingly important to predicting FC concentrations on Florida's coast. Ultimately, these forecasts will enable resource managers and shellfish growers to plan ahead and maximize their resources as this industry expands.

Combined, these two studies revealed how regulatory shellfish sanitation data can be leveraged for long-term water quality trend testing and short-term FC forecasting. Drivers of long and short term changes in FC concentrations were also revealed. The modeling performed in this thesis can be used by coastal water resource managers and shellfish farmers to optimize decision making processes that support coastal communities.

Past and Future Coastal Water Quality: Trend Testing and Predictive Modeling Using Regulatory Shellfish Sanitation Data

by
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DEDICATION

This thesis is dedicated to North Carolina's coast: the vibrant and protective marshes, the windswept live oaks, the refreshing cold wind on the dark winter beaches, and the estuaries that provide the perfect theater to experience the rhythm of ecologies. These habitats create my home. Also to all of my family, friends, and dearest animals that live in this beautiful ecosystem and beyond.

BIOGRAPHY

Natalie Chazal grew up in Morehead City, North Carolina. Throughout high school she had volunteered at the Cape Lookout National Seashore helping to manage the wild horse herd on Shackleford Banks. As an avid animal lover, she pursued bachelors degrees in Animal Science and Zoology with a minor in Statistics at North Carolina State University. She joined the Biosystems Analytics Lab in the fall of 2021 as a Masters student under Dr. Natalie Nelson. Natalie's Master's research focuses on using regulatory data from shellfish sanitation programs to analyze historic trends and make water quality predictions in estuarine waters.

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INTRODUCTION

1.1 Background

Water quality impairments due to fecal bacterial pollution can often become public safety hazards, such as by contaminating shellfish. Bivalve shellfish are filter feeders that filter particles in the water column (Jørgensen 1990). This effectively means that any matter that could contain potential pathogens can become concentrated in their meat and present a public health risk when consumed (Newell and Jordan 1983; Wittman and Flick 1995). Shellfish fisheries are of particular importance, as they are highly sensitive to water quality standards. As the world's population grows, shellfish aquaculture is becoming one of the most sustainable and cost effective sources of food (Theuerkauf et al. 2019; Botta et al. 2020; FAO; Azra et al. 2021). Given the economic impact of the growing shellfish aquaculture industry (Wijsman et al. 2019; FAO; Azra et al. 2021; Petrolia et al. 2022), improvement in water quality monitoring, development of effective management tools, and projects that reduce fecal bacteria in aquatic systems must be made a priority.

Shellfish sanitation programs aim to mitigate human exposure to pathogens by prohibiting shellfish harvesting in potentially contaminated waterways. Fecal indicator bacteria (FIB) concentrations are used as proxies of the concentrations of human-disease causing pathogens from fecal matter in the water. A common group of FIB that is utilized by shellfish sanitation programs are fecal coliforms (FC) (Chung et al., 1998)(Chung et al. 1998). FC sources are generally associated with human land development and animal excrement. This includes nonpoint source contributors such as livestock production and agricultural operations, large populations of waterfowl and other wildlife, and the extent of impervious surfaces within a watershed (Mallin et al. 2000). Point sources include wastewater treatment plants, industrial point sources, and septic tank failures.

While point sources supply FC into the waterways through often human-controlled events, nonpoint source inputs are dependent on transport factors like heavy rainfall events and higher river stages to move the terrestrial sources of FC into the waterways. Accordingly, rainfall is most commonly considered the major driver of FC loads in coastal waters via runoff (Jeng et al. 2005; Coulliette et al. 2009; NSSP 2019). However, this relationship is not uniform for all waterways along the coast. The sensitivity of an area to nonpoint source FC loading is dependent on a combination of biogeochemical, hydrographical, and meteorological factors unique to that area (Crowther et al. 2001; Chigbu et al. 2005; Campos et al. 2013). For example, Coulliette et al. (2009) found that there were both non-linear and linear relationships between different FIBs and rainfall in the Newport River Estuary, NC using a hydrological model that incorporates both antecedent rainfall levels and distance away from shore (Coulliette et al. 2009). In this study, Coulliette et al. (2009) suggest these differential relationships can be explained by tidal influences that change the salinity gradient within the estuary which, in turn, affects the survivability of FIB (Coulliette et al. 2009).

Another major transport mechanism within these coastal waters is wind-driven erosion (Chigbu et al. 2004; Ufnar et al. 2006; Lewis et al. 2013; NSSP 2019). Wind causes turbulence in the water column which resuspend sediments that FIB are associated with (Kay et al. 2005; Feng et al. 2016). In a study dedicated to characterizing FC sources and transport in the Mississippi Sound, Ufnar et al. (2006) found that elevated FC concentrations were correlated with significant changes in wind speed and direction (Ufnar et al. 2006). They suggest this relationship is due to sediment disturbance by larger wave action during higher wind activity which would explain the elevated FCs during times of little to no rainfall in this system (Ufnar et al. 2006).

After their transport from sources into the waterways, some identified factors that affect the survivability of FCs in estuarine environments include salinity, FIB species-specific stressors, and water temperature. FCs are bacteria that live and grow in the gastrointestinal tracts of animals. When they are excreted through feces and enter the environment, the FCs are no longer in the conditions to which they are generally adapted. These organisms change their metabolic activity rapidly in response to this stress and depending on the species, this can extend or shorten the length of time they can sustain themselves in a marine environment (Munro et al. 1989; Troussellier et al. 1998). Salinity is one of the major effectors of survivability because of the osmoregulatory shock that the bacteria can tolerate (Munro et al. 1989; Troussellier et al. 1998). A negative relationship between FIB survival and water temperature has been shown (Faust 1976; Howell et al. 1996; Chigbu et al. 2004). This relationship is seen because high water temperatures are generally associated with higher levels of predation and higher levels of solar radiation, both of which decrease the survival of FIB (Sinton 2005). However, there are often seasonal variations in the importance of water temperature, air temperature, and water column mixing on FC survival and transport that complicate modeling and prediction efforts (Lipp et al. 2001; Chigbu et al. 2005).

Given the complex web of processes contributing to fecal contamination in coastal waters, the management of shellfish sanitation requires consideration of many factors that are formalized in a standardized process overseen by the U.S. Food and Drug Administration's National Shellfish Sanitation Program (NSSP; NSSP 2019). The NSSP requires state agencies to classify waters based on point source and nonpoint source pollution potential and baseline FC or Total Coliform concentrations. Coastal waterways are broken up into growing areas which are assigned management classifications. Sanitary surveys are routinely conducted every couple of years and reviewed annually to summarize the bacteriological water quality, meteorologic, and hydrologic characteristics in each growing area. Based on these sanitary surveys, the classifications of the growing areas can be approved, conditionally approved, restricted, or prohibited. Approved and conditionally approved areas are managed through water quality sampling programs designed by states within the overall guidelines provided by the NSSP, with program structures varying depending on the resources available, locally specific ecologies, and potential pollution sources. Given the importance of stormwater runoff as a driver of elevated FC concentrations in coastal waters, precipitation and river stage are often used to inform closures of areas that are conditionally managed. The NSSP currently provides two sampling strategies to utilize when collecting data for areas that require routine monitoring.

The first strategy is systematic random sampling, which aims to capture baseline FC measurements across a range of environmental conditions. A minimum of six water quality samples are collected at random time points throughout the year. While the aim is to capture FC concentrations over a range of conditions, in practice, the available resources of the regulatory agency can limit the timing of sampling (Hunt 1980). This can result in a dataset that doesn't necessarily capture the full range of conditions, especially during and immediately following events that lead to elevated fecal coliforms, but rather captures baseflow conditions (NSSP 2019).

The second strategy is adverse pollution condition sampling, which calls for sample collection during periods when point source pollution events or elevated rainfall and river stage have reached levels that are known to degrade water quality in specific areas. The dataset generated by the adverse pollution condition sampling method captures conditions when the contamination is near or at its highest levels. The states that utilize this sampling strategy must collect a minimum of five annual samples from spatially fixed water quality sampling stations (NSSP 2019).

Both systematic random sampling and adverse pollution condition sampling generate long-term datasets of FIB concentrations and oftentimes contain other water quality parameters such as water temperature, turbidity, and salinity. Regulatory data generated from shellfish sanitation management presents an opportunity for developing decision-support tools to aid in better management of shellfish growing area closures and reopenings.

The regulatory shellfish sanitation datasets that are produced by these sampling strategies vary by state and region (Nelson et al. 2022). Each state collects data pertaining to FCs at a minimum as well as water temperature, salinity, dissolved oxygen, pH, air temperature, and tidal stage. There are prior studies that utilize this regulatory data to relate FC concentrations to environmental parameters (Chigbu et al. 2004; Leight et al. 2016; Souedian et al. 2021). However, there are few that address the feasibility for using shellfish sanitation specific regulatory data for non-fisheries motivated water quality modeling. In the realm of prediction, it is common to use this monitoring data for building models (Schmidt et al. 2018; Zimmer-Faust et al. 2018; Wang and Deng 2019). However, prior studies that utilize regulatory data for prediction often make predictions over small spatial scales, do not incorporate forecasted predictors, or utilize methods that are not feasible for implementation into current management practices.

The research presented in this thesis aims to repurpose long-term FC observations for both historical water quality trend testing and predictive modeling by coupling regulatory shellfish sanitation datasets with relevant land use, meteorological, and hydrological characteristics.

1.1.1 Historical Trend Analysis

The purpose of the historical FC trend analysis is to utilize regulatory shellfish sanitation data to infer long-term spatiotemporal trends in water quality while accounting for variation in routine sampling and environmental landscapes. This is broken down into specific objectives including (1) assessing the feasibility of utilizing monitoring data to infer long term trends, (2) analyzing spatiotemporal trends in FC concentrations, and (3) identifying possible management and environmental drivers of these trends. For this study, we used North Carolina as a representative study system. The results of the historical trend analysis will help states with regulatory shellfish sanitation datasets to analyze the water quality trajectories in these shellfish growing waters. This can immediately help prioritize impaired waterways for water quality improvement projects and help understand more localized drivers of FC impairment over time.

1.1.2 Predictive Modeling

The purpose of the predictive FC modeling presented here is to utilize regulatory shellfish sanitation data to predict FC concentrations in shellfish growing waters. This is broken down into specific objectives including (1) using relevant watershed, hydrological, and meteorological characteristics to predict FC concentrations in shellfish growing areas, (2) updating these predictive models using forecasted precipitation inputs as well as antecedent measurements, and (3) identifying the key drivers of FC dynamics used in the prediction models. For this study, we used Florida as a representative study system. The results of the predictive FC modeling study can be used to develop nowcast and forecast tools. These tools can help shellfish growers make informed decisions for their businesses and can help management agencies make efficient decisions about the timing and spacing of sampling efforts.

CHAPTER

2

HISTORICAL TREND ANALYSIS

2.1 Introduction

Healthy estuarine environments are critical for maintaining ecological stability, coastal economies, and human health standards. In order to maintain and even improve these habitats, metrics of current and past conditions must be evaluated to inform proper management. Water quality measurements can be used to indicate overall estuarine health and can aid in understanding increasing coastal threats such as rising sea levels, increased salinities, and urbanization. Long-term water quality analysis is key for developing target thresholds for future management action as well as assessing the efficacy of past management measures (Cloern et al. 2016). The value of historical observations in advancing understanding of estuarine water quality has been demonstrated by multi-decadal studies of several systems, including the San Francisco Bay area (Beck et al. 2018; Cloern et al. 2016), May River, South Carolina (Souedian et al. 2021), Texas's coastline (Bugica et al. 2020), and the Chesapeake Bay area (Zhang et al. 2018; Harding et al. 2019). Most notably, long-term water quality monitoring in the Chesapeake Bay has led to the identification of climatic and anthropogenic drivers for certain water quality parameters and subsequent evaluation of the effectiveness of past management and restoration efforts (Kemp et al. 2005; Leight et al. 2011; Zhang et al. 2018; Harding et al. 2019).

Datasets used for prior longitudinal water quality studies are commonly a product of governmental agencies developing localized programs, like the Chesapeake Bay Program (Chesapeake Bay Monitoring Program 2022), in response to increasing population and significant degradation of vital estuarine ecosystems. While national and regional efforts have attempted to provide unbiased, sustained monitoring, these programs currently lack the spatial extent needed to capture coastwide water quality trends. The National Estuarine Research Reserve System (NERRS) is one of the few organizations with dedicated coastal water quality monitoring stations, which are included as part of the NERRS System Wide Monitoring Program (SWMP) that maintains 355 coastal water quality monitoring stations across 29 designated coastal reserves along the USA coastline (NERRS 2022). Compared to the over 13,500 freshwater monitoring stations maintained by the United States Geological Survey (USGS 2022), the relatively small number of water quality monitoring stations across coastal and estuarine waters (NOAA Tides & Currents 2022; US EPA 2006) are likely not representative of the variations in environmental conditions that we observe across the tens of thousands of miles of shoreline along the United States.

Because of the limited number of unbiased monitoring programs, the ability to use water quality data from regulatory operations presents a potentially valuable resource for assessing long-term estuarine conditions. Regulatory programs differ from monitoring programs by collecting water quality samples to meet regulatory requirements and inform short-term decision-making. For example, in North Carolina (NC), there are four NERRS SWMP monitoring stations and eight coastal stations with water quality data available through the USGS (South Atlantic Water Science Center, North Carolina Office, 2022) and fifty stations from the NC Ambient Monitoring System (Water Quality Portal 2021), but the NC Division of Marine Fisheries (NCDMF) shellfish sanitation program maintains 1,924 water quality monitoring stations. In fact, state shellfish sanitation programs across the USA collect an abundance of water quality observations, and often have for decades. Shellfish mariculture is highly dependent on water quality monitoring due to the direct influence that ambient conditions have on the safety of shellfish meat consumption. The U.S. Food and Drug Administration's National Shellfish Sanitation Program (NSSP) was developed in 1925 to maintain public safety and human health standards in relation to the consumption of shellfish grown in potentially polluted waters (NSSP 2019). The implementation of the NSSP has resulted in systematic sampling of water quality for day-to-day fisheries regulation, specifically for Fecal Indicator Bacteria (FIB), a group of bacteria that are commonly used as a proxy measure for harmful pathogen loads in the waterway that could potentially be incorporated into shellfish meat through filter feeding. Thus, fecal coliforms (FC), a type of FIB, and other environmental factors that contribute to FC load and water quality, are regularly measured in shellfish growing waters due to the food safety implications. As a product of this regular testing, fisheries operations have accumulated decades of data with the potential to provide insights on historical trends with wide spatial extents, potentially filling gaps in long-term water quality monitoring capacity.

However, because of the limited resources and industry specific priorities, regulatory data can maintain underlying biases as a result of the sampling methodology used to collect the water quality sample. Often, the collection of a sample can be motivated by day-to-day operational decisions, such as weather, the availability of field technicians, and ease of collection. These operational decisions lead to non-random sampling that provides observations that are not always representative of the system's true dynamics. Engaging regulatory personnel to understand their fisheries management and sampling decisions is necessary to properly analyze the observations collected by shellfish sanitation programs.

For example, the NSSP permits states to employ one of two sampling strategies when collecting regulatory water quality data in shellfish growing waters: adverse pollution condition sampling and systematic random sampling. The adverse pollution condition sampling strategy describes sampling in periods when known contamination events (commonly due to point-source pollution events or rainfall events) have degraded the water quality, and data collected under these conditions are expected to capture peak contamination. States must collect "a minimum of five samples… annually under adverse pollution conditions from each sample station in the growing area" (NSSP 2019) to meet NSSP sampling requirements. In contrast, the systematic random sampling strategy describes the collection of data across "a statistically representative cross section of all meteorological, hydrographic, and/or other pollution events" (NSSP 2019), resulting in the data collection under varied environment and climactic conditions. For state programs that use systematic random sampling, the NSSP requires samples be collected at least 6 times throughout the year (NSSP 2019). As a result of the requirements for the conditions under which the two systems of sampling can take place, the resulting data may be biased and impact their utility for use in long-term water quality assessments. With our growing reliance on aquaculture and the expanding value of shellfish production driving the development of fisheries management infrastructure (Azra et al. 2021), long-term datasets available through shellfish sanitation programs will become increasingly valuable. Realizing the potential of regulatory datasets to inform long-term water quality trends is a vital next step for assessing the health of our coastal ecosystems, but research is needed to determine the utility of these data for water quality analyses.

The goal of this study was to utilize shellfish management data to infer long-term spatiotemporal trends in water quality parameters, including FC and salinity, while accounting for variation in routine sampling conditions and environmental landscapes. Study objectives included (1) analyzing spatiotemporal trends from multidecadal fecal coliform concentration observations collected by a shellfish sanitation program, (2) identifying possible management and environmental drivers of fecal coliform trends, and (3) assessing the feasibility of using these monitoring data to infer long-term water quality dynamics. We focused on North Carolina's shellfish waters as a representative study system due to the availability of public, digitized multidecadal data, and the region's rapidly growing population, wide variety of land use characteristics along the coast, presence of the second largest estuarine system in the contiguous USA, and growing shellfish industry. Ultimately, this study demonstrates the application of shellfish management data for long-term water quality trend analysis in estuaries, informs future resource management strategies, and reveals new insights into the functioning of coastal systems.

2.2 Methods

2.2.1 Study Area Description: Shellfish Waters in North Carolina, USA

The study area spanned all marine and estuarine waters in coastal North Carolina, which are subdivided into shellfish growing areas (SGAs) (Figure 2.1a,b). SGAs are subdivisions of waterways used to support shellfish harvest through delineating administrative boundaries for regulatory purposes. SGAs spatially cover North Carolina's shoreline from Currituck Sound in the north to Brunswick County in the south. These SGAs are named with alphabetic letters (e.g. "A", "B", etc.; Figure 2.1b), and further categorized through a letter-number system (ex. "A01"). There are 9 SGA letter groups along North Carolina's coast and these groups of SGAs have similar ecological features and approximately correspond to County jurisdictions. This study excludes the northernmost SGA ("I") due to the lack of open shellfish growing areas and discontinuous water quality data. SGAs vary in environmental and managerial conditions across the NC coast. These variations manifest as differences in estuarine type which can be defined using physical measures of area, depth, volume, freshwater flow, and salinity within the estuary (Engle et al. 2007).

SGAs can contain multiple classifications including approved, conditionally approved, restricted, and prohibited areas. These classifications use the risk of pollution potential in an area to properly regulate the harvesting of shellfish from those waters. Of the 9,208 km^2 of shellfish waters, 5,910 km^2 (64.18%) are approved or conditionally approved. Observations collected through routine monitoring programs are used to help establish the classifications within SGAs. The NCDMF Shellfish Sanitation and Recreational Water Quality Section has jurisdiction over the classification of coastal waters for shellfish harvest, and also regulates closures and openings of conditionally approved SGAs. A majority of the NCDMF sampling stations included in this analysis are within the approved and conditionally managed SGAs (Figure 2.1a).

Sampling Strategies

In accordance with the NSSP, NCDMF routinely samples all shellfish growing areas on a regular basis (6 times annually) using the systematic random sampling strategy, meaning samples for each station are collected at randomly scheduled timepoints throughout the year; however, there are some constraints as to when sample collection is permissible. Specifically, samples are only collected during conditions when the SGAs are open for harvest or assumed to be unimpacted by unsafe FC levels, resulting in the subsequent data not capturing peak FC concentrations. Because freshwater input and runoff are tied to increased FC concentrations in estuarine waters, precipitation intensity is used as a management indicator for closures of conditionally approved waterways (NSSP 2019; Leight et al. 2016). In North Carolina, rainfall closure thresholds in conditionally approved waters range from 1-3 inches of rainfall within a 24-hour period (Figure 2.1c) and dictate if a managed shellfish area will be closed for harvesting after a meteorological event. The "emergency closure" of additional areas can occur after higher rainfall amounts are noted and, for the purposes of this analysis, those areas will be represented by a 4 inch threshold. Rainfall thresholds are assigned to conditionally managed areas. To reopen closed areas that have been temporarily closed following exceedances of those rainfall thresholds, NCDMF tests the water, and reopening will only occur after samples confirm safe harvest conditions, which is defined by waters that do not exceed a FC density of 14 MPN (Most Probable

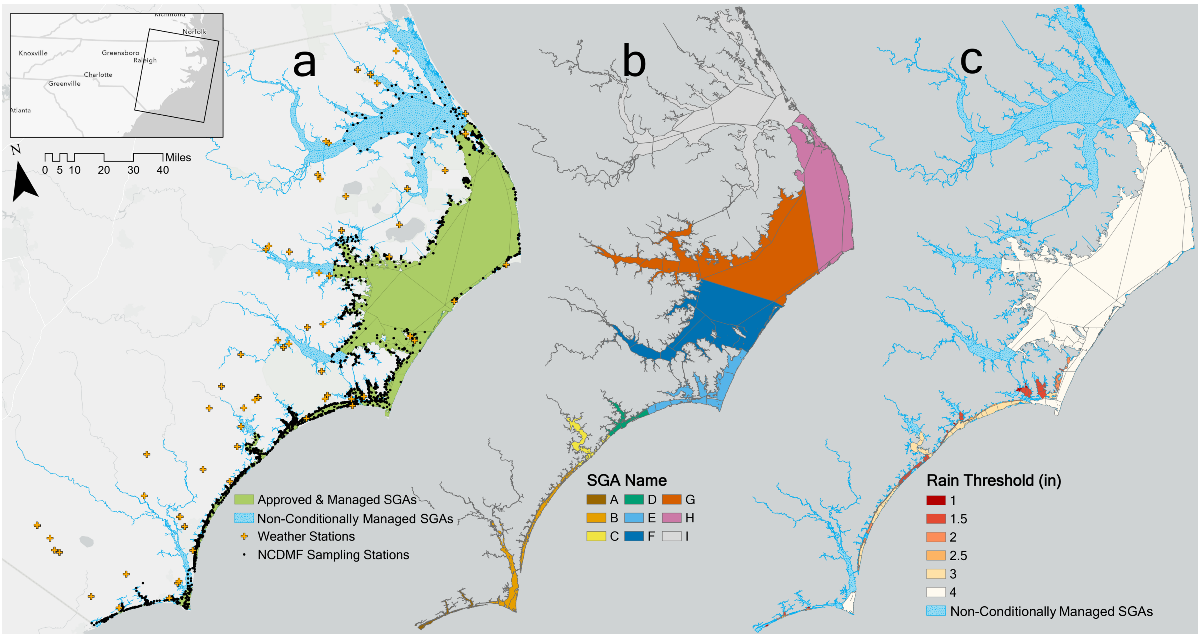

Figure 2.1: Leftmost map (a) illustrates NCDMF conditional management units with water quality sampling stations. Blue waters correspond to waters that are not approved for shellfish growing and harvesting, while the green areas correspond to the conditionally managed shellfish growing waters. The black points indicate the exact locations of the NCDMF water quality sampling stations and the orange crosses indicate the locations of the weather stations used to gather the precipitation time series data. The middle map (b) illustrates the NCDMF SGAs colored by the first letter of their SGA name. The rightmost map (c) illustrates rainfall thresholds (as of July 2021) for NCDMF conditionally managed areas measured in inches. Dark red indicates a rainfall closure threshold of 1 inch where the lightest white indicates areas with a rainfall closure threshold of 4 inches. Study area maps were created in ArcGIS Pro version 2.8.

Number) per 100 mL of sample (NSSP 2019); sampling for reopening is hereafter referred to as "conditional sampling". MPN is a statistically based unit of measure to determine the concentration of FCs from a counted number of test tubes with microbial growth during a serial dilution. NCDMF balances its limited resources with speed of reopening by only conditionally sampling when the organization suspects the FC concentrations will be low enough to support reopening. SGAs A, C, D, E, and the northern half of B are characterized by moderate to low rainfall thresholds (i.e., 1-3 inches) whereas SGAs F, G, H, I, and the southern half of B have high rainfall thresholds (i.e., 4 inches; Figure 2.1c).

Under systematic random sampling, routine sampling in conditionally approved waters must occur when the SGA is open and not during a temporary closure. Accordingly, this stipulation creates bias in the routine monitoring data. As such, areas with a 1 inch rainfall threshold will close more often than areas with 4 inch thresholds, resulting in more restrictive sampling conditions and more homogeneous water quality samples in the long-term. Furthermore, NCDMF will change rainfall thresholds or exclude stations for areas with persistently poor water quality, resulting in the longest-standing monitoring stations typically being located in growing areas that are known to be productive with relatively good water quality, contributing another source of bias to the data.

2.2.2 Data Description

To analyze shellfish sanitation program data, water quality observations were compiled for the study area along with additional environmental variables believed to be potential descriptors of FC trends including salinity, precipitation, land use, and sampling station distance to closest shoreline. These variables have been established as relevant to FC concentrations in estuarine waters (Chigbu et al. 2004, 2005; Campos et al. 2013; Leight et al. 2016).

Water Quality

During each sampling event, a grab sample is collected for FC analysis. To enumerate FC, NCDMF uses a five-tube decimal dilution, method SM 9221 (NSSP 2019). Data records also include monitoring type to indicate the type of sampling (either conditional or routine), coded SGA designation (i.e., names listed in Figure 2.1b), station name, date of the sample, tide at the time of sample, salinity, and water temperature. The data are publicly available through NCDMF, and have been reorganized into a normal form database called “Shell-Base”, which is freely available through the Southeast Coastal Ocean Observing Regional Association’s Data Portal (SECOORA 2022).

In our study, the data were filtered to only include routine samples from stations that had 20 years of continuous water quality sampling data from 1999 to 2021. These conditions were met by 466 stations. We chose the time period of 1999 to 2021 due to changes in management procedures in the NCDMF in the 1990’s. Throughout the 1990’s, NCDMF progressively introduced conditional management plans to many of the growing areas. Therefore, by confining the dataset from 1999 to 2021, we are safely ensuring that the conditional management plans have been introduced and that the sampling would be reflective of that. Observations collected through conditional sampling were not considered in the analysis because the varied conditions under which conditional sampling occurs results in skewed FC concentrations and is not as representative of the system as the data collected through routine sampling design.

Salinity

Because data collected through the NCDMF monitoring program may have preferential sampling bias, we sought to analyze additional salinity data collected from an unbiased monitoring program in order to understand how the NCDMF observations compared to an independent dataset. We accessed the North Carolina Division of Water Resources (NCDWR) Water Quality Portal (Water Quality Portal 2021). The NCDWR dataset consists of 17 monitoring stations that had at least 10 years of salinity data between the years 1999 and 2021 and were within proximity to the NCDMF water quality sampling stations (Figure 2.2); stations with fewer than 10 years of data or in portions of the estuary that did not overlap with NCDMF stations (e.g., fresh headwaters) were not considered in the analysis. However, data from NCDWR sites in SGAs D and E were still considered despite being relatively distant from NCDMF monitoring locations as these were the only NCDWR sites present in SGAs D and E.

Precipitation

The precipitation data was gathered through the North Carolina State Climate Office (North Carolina State Climate Office, NC State University 2021) for weather stations (n = 70) that

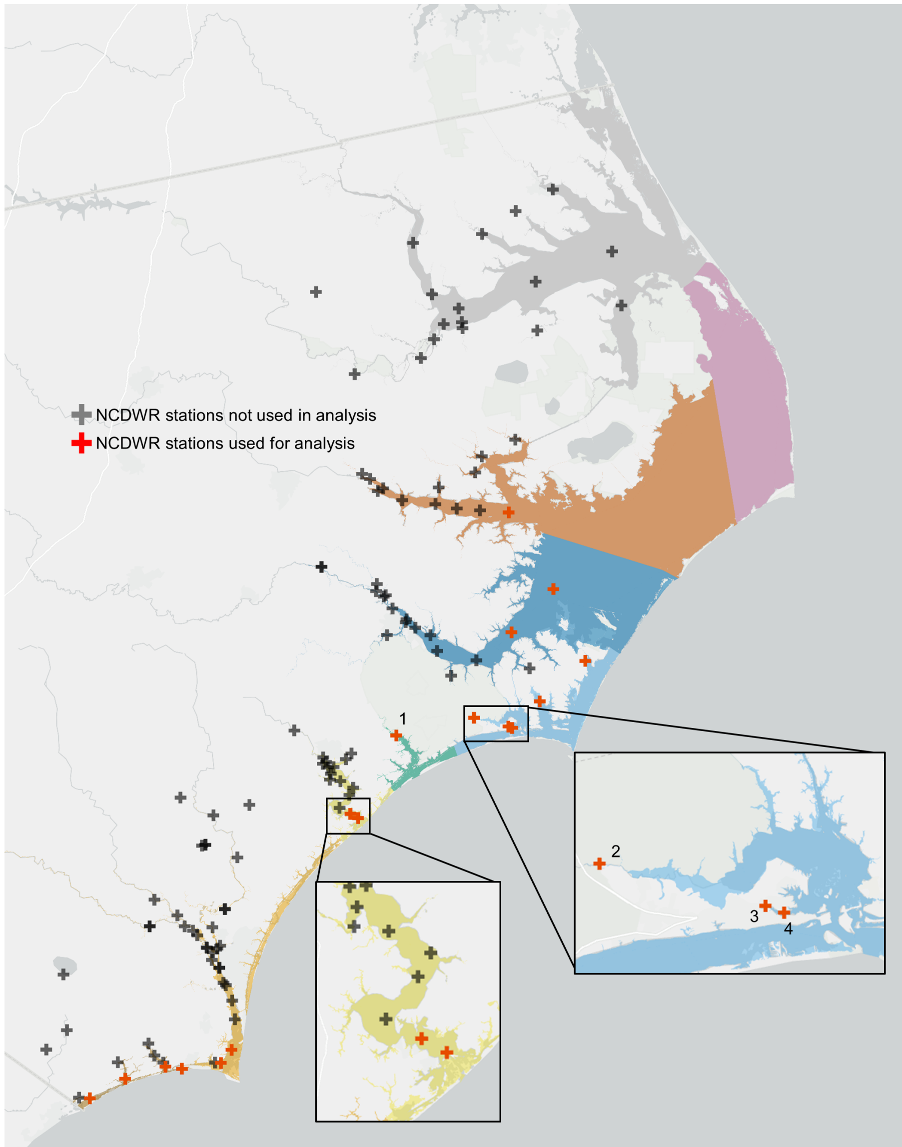

Figure 2.2: Map of NCDWR water quality sampling stations along the coast of North Carolina. Numbers 1 – 4 are added to annotate stations referenced in Figure 2.5. Stations are colored by their use in the analysis. Study area maps were created in ArcGIS Pro version 2.8

contained continuous data for 1999 to 2021 (Figure 2.1a). Precipitation data were related to water quality sampling locations as a function of proximity.

Geographic Context

Land Use and Land Cover (LULC) data for North Carolina in 2001 and 2019 were compiled from the National Land Cover Database (Dewitz and U.S. Geological Survey 2021) created by the Multi-Resolution Land Characteristics Consortium (MRLC). LULC categories were consolidated into “Developed”, “Barren”, “Cultivated”, “Vegetated”, and “Wetlands” classes and summarized for each coastal watershed, defined by USGS 12 digit Hydrologic Unit Codes (HUC12; Figure 2.3).

We calculated percent changes within each consolidated LULC class for all coastal watershed areas from 2001 to 2019 in R version 4.1.0 (R Core Team 2021). We then related water quality stations to watersheds based on distance, with stations being assigned to the nearest watershed. Because of the variation in flow volumes of contributing tributaries to these estuaries it is difficult to generalize the exact transport distance of non-point sources of FCs in coastal systems. It is known that FCs are generally sourced from surrounding watersheds and their survivability in the water is dependent on a wide range of environmental factors (Weiskel et al. 1996; Cho et al. 2016; Korajkic et al. 2019). For context, Weiskel et al. (1996) demonstrated that even point source discharges of FC being diluted to near-background levels within 15 meters of the source (Weiskel et al. 1996). Each station’s distance to shoreline was also calculated, which was done through nearest feature geoprocessing in R using the estuarine shoreline data layer from the NCDMF Estuarine Shoreline Mapping Project (NC Division of Coastal Management 2007).

2.2.3 Data Analysis

The 20-year trends in water quality variables were analyzed to allow for (1) comparison against different environmental variables to understand possible drivers of change and (2) evaluation of spatial variability in water quality trends. Mann-Kendall (MK) testing and Sen Slope Estimators were calculated and applied to annual average FC concentrations and annual average salinity values for the water quality sampling stations, and total annual precipitation for the terrestrial weather stations. Fecal indicator bacteria concentrations are highly variable in space and time, with samples collected consecutively over the span of a

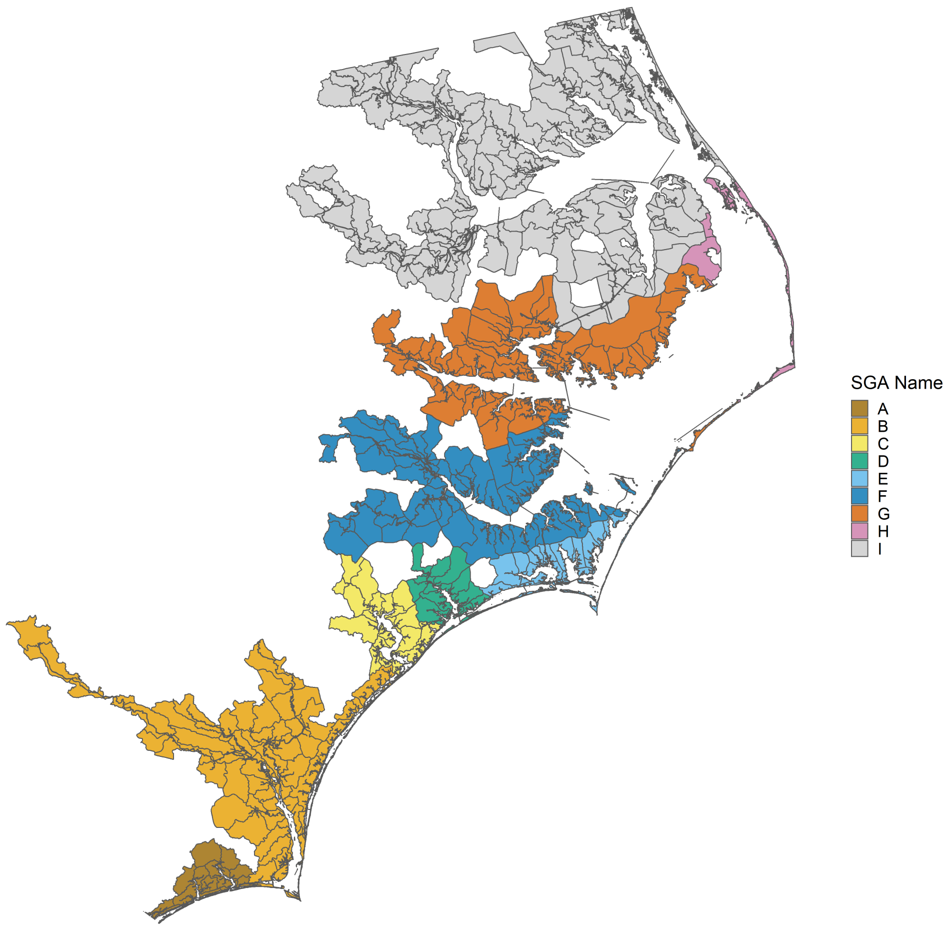

Figure 2.3: Map of coastal North Carolina HUC12 watershed areas that were used to summarize land use change between 2019 and 2001. The watersheds in this map are colored by the SGA name that the watershed is closest to and therefore associated with. Study area map was created in R version 4.1.0 with the 'sf' version 0.9 package.

few minutes sometimes varying by an order of magnitude over a few minutes (Boehm 2007). Accordingly, the annual arithmetic mean was selected to represent the central tendency in long-term FC data, with the annual time step selected to average out the effects of seasonal variation. Similarly, using total annual precipitation informed us of the overall freshwater load over the years and allowed us to explore long-term drivers of baseflow FC concentrations. MK testing and Sen Slope Estimation analysis have been used in numerous environmental, hydrological, and water quality studies (Hirsch et al. 1982; Cailas et al. 1986; Hipel et al. 1988; Zetterqvist 1991; Burn and Hag Elnur 2002; Meals et al. 2011; Mustapha 2013) due to their robustness against non-normal data with missing values. Statistical analyses and mapping were conducted in R with the 'trend' package version 1.1.4 (Pohlert 2020) and the 'sf' package version 0.9 (Pebesma et al. 2022).

Mann-Kendall Trend Test

The MK trend test is a nonparametric test for monotonicity of trends in time series data (Mann 1945; Kendall 1975). By ranking the time series observations and measuring the later observations (j) against earlier observations (i), MK testing allows us to understand the monotonicity of an upward or downward trend in a time series. A perfectly monotonic trend consistently increases or decreases. For example, a perfectly increasing monotonic function is never decreasing at any point along the function. Using pairwise comparison of ranked values from all data points, the test statistic (S) is calculated through either adding or subtracting 1 for every value that is larger or smaller than the later value (Equation 1). This results in a test statistic (S) that characterizes the directionality and monotonicity of a trend in a given time series. S is then used to calculate the τ test statistic (Equation 2), which is a measure of correlation that ranges from -1 to +1 with the sign indicating the direction of the value's change over time. This test determines whether there is a significant, monotonic trend in a value over time in either a positive or negative direction.

$$S = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \mathrm{sign}(y_j - y_i) \qquad \mathrm{sign}(y_j - y_i) = \begin{cases} 1 & y_j > y_i \\ 0 & y_j = y_i \\ -1 & y_j < y_i \end{cases} \tag{2.1}$$

$$\tau = \frac{S}{n(n-1)/2} \tag{2.2}$$

In Equations 1 and 2, n is the number of observations in the time series, i is the earlier value in the time series sequence, j is later value in the time series sequence, and y represents the measurements at times i or j. The value of τ is also known as the Mann-Kendall trend test statistic.

Sen Slope Estimator

While the MK test statistic (τ) value denotes direction and how well a time series fits a monotonic model, the Sen slope estimator (β) determines the rate of change for the resulting MK trends. The resulting β is based on a median of all possible slopes calculated (Equation 3).

$$\beta = \text{median}\left(\frac{y_j - y_i}{x_j - x_i}\right) \tag{2.3}$$

The Mann-Kendall trend test and Sen slope estimators provided us with FC τ (τ_{FC}), FC β (β_{FC}), salinity τ (τ_{Sal}), salinity β (β_{Sal}), precipitation τ (τ_{Precip}), and precipitation β (β_{Precip}) for each water quality sampling station.

Correlations

Pearson's correlation coefficients (r) were calculated to evaluate the relationships between the FC, salinity, and precipitation trends as well as the LULC class percent change for the consolidated classes and distance to shore.

2.3 Results

2.3.1 Coastwide Trends

The results of the MK testing and Sen slope estimation of FC concentrations were mapped alongside the developed land use change for each coastal watershed (Figure 2.4). The spatial distribution of τ_{FC} varied along the coast with defined areas of similar τ_{FC} values. From the most southern coastal area, we observe higher, positive τ_{FC} values for stations down estuary of areas with very high proportions of developed change. Within the south-central portion of the coast, we can see more negative τ_{FC} values. Farther north, in the area characterized by the large, Albemarle-Pamlico sound which spans SGAs F, G, H, and I, there is a mixture of lower positive and lower negative τ_{FC} values. The developed land use change is fairly uniform along a majority of the state's coastline, with higher proportions of developed land change being located in the watersheds associated with SGA C and E and the most intense increase in proportion of developed land being in central watersheds associated with SGA B.

The Pearson correlation coefficients for the water quality and environmental trends along the full coastal area are summarized in Table 2.1. These correlations include the relationships between τ_{FC}, β_{FC}, τ_{Sal}, β_{Sal}, τ_{Precip}, β_{Precip}, developed land percentage, barren land percentage, wetlands land percentage, vegetated land percentage, cultivated land percentage, and distance to shore. We observed a strong negative relationship between both τ_{FC} & β_{FC} and τ_{Sal} & β_{Sal} (r values from -0.281 to -0.304); both significance, direction, and magnitude of change of temporal trends between FC and salinity were inversely related. There was a weak positive relationship between β_{FC} and τ_{Precip} & β_{Precip}. The positive relationship between τ_{Sal} & β_{Sal} and all land use classifications with wetlands had the strongest positive coefficients (r = 0.393 and r = 0.401, respectively). Distance to shore was weakly correlated with overall FC trends.

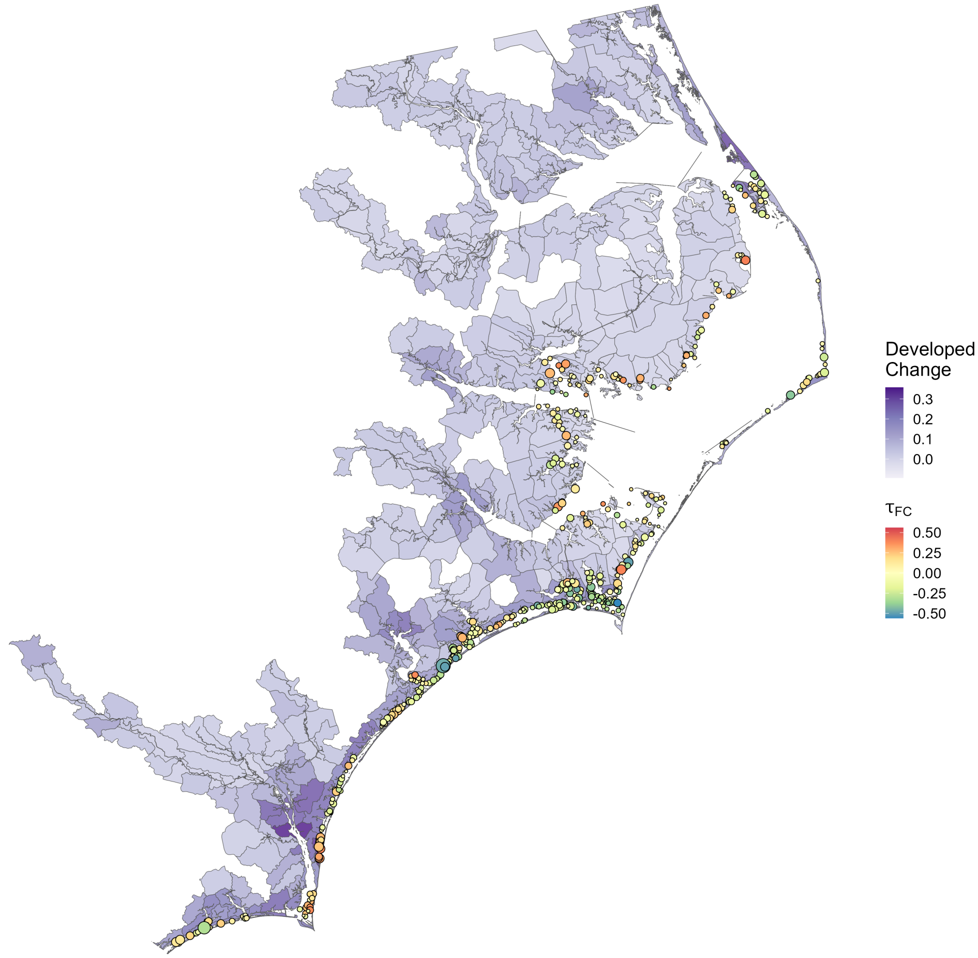

Figure 2.4: Map of the 20-year FC trends for all 466 water quality stations (points) along North Carolina's coast alongside the developed change percentage of the HUC12 watershed areas (purple fill). The points representing the water quality station FC trends are colored by the τ_{FC} value with the red and orange colors illustrating the positive trends in FC concentrations while the green and blue colors indicate a negative trend in FC concentrations. These points are also sized by the magnitude of their β_{FC} values (i.e., larger points represent steeper slopes in the FC trends and smaller points represent more gently sloping FC trends). The light purple watershed areas represent smaller proportions of developed land increase whereas dark purple areas represent a more intense increase in developed land proportions from 2001 to 2019; white, unfilled areas between watersheds correspond to watersheds that do not directly connect to a waterway. This map was created in R version 4.1.0 with 'sf' version 0.9 package.

Table 2.1: Pearson's correlation matrix representing relationships between water quality trends (FC concentration and salinity) and environmental parameters (LULC change, precipitation, shore distance) for all stations along North Carolina's coast included in the MK trend testing.

	Wetland LULC	Cult. LULC	Veg. LULC	Barren Change	Develop LULC	Shore Dist.	β_{Salinity}	τ_{Salinity}	β_{Precip}	τ_{Precip}	β_{FC}	τ_{FC}
τ_{FC}	0.006	-0.029	0.087	0.062	0.127	0.057	-0.304	-0.304	0.095	0.108	0.751	1.000
β_{FC}	-0.072	-0.047	0.017	0.021	0.044	0.013	-0.281	-0.260	-0.023	-0.012	1.000	
τ_{Precip}	-0.192	-0.070	-0.023	0.020	0.067	-0.033	-0.304	-0.371	0.920	1.000		
β_{Precip}	-0.315	-0.149	-0.048	-0.024	0.004	-0.103	-0.368	-0.397	1.000			
τ_{Salinity}	0.393	0.174	0.100	0.119	0.111	0.144	0.908	1.000				
β_{Salinity}	0.401	0.189	0.078	0.120	0.116	0.117	1.000					
Shore Dist.	0.187	0.017	0.174	0.087	0.318	1.000						
Develop LULC	0.282	-0.005	0.193	0.099	1.000							
Barren LULC	0.299	-0.070	0.179	1.000								
Veg. LULC	0.198	-0.004	1.000									
Cult. LULC	-0.082	1.000										
Wetland LULC	1.000											

When aggregated to annual averages, the NCDWR salinity data is insufficiently short (n ranging from 10 to 14 between stations) and limits our ability to apply trend testing. However, the NCDWR salinity time series (Figure 2.5) largely follow the same trends as the NCDMF salinity data; exceptions include sites in growing areas E and D, where several NCDWR stations were located in the upstream, fresher portions of the estuaries. While we generally selected stations in locations similar to NCDMF stations, these are presented due to lack of stations in the more brackish and marine waters within these areas. Given that the NCDWR data is collected through an unbiased monitoring program, the agreement between the NCDWR and NCDMF salinity observations indicates the NCDMF observations may not be severely affected by sampling bias.

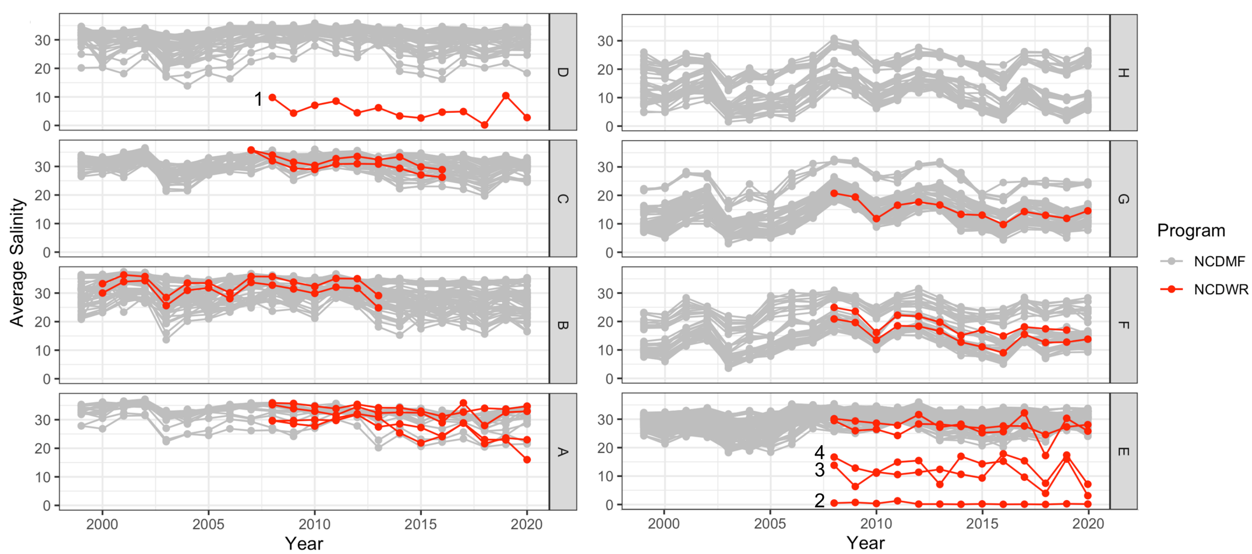

Figure 2.5: Time series of NCDMF salinity results (grey lines) with the NCDWR salinity results (red lines) from the chosen representative stations along North Carolina's coast. Line graphs are grouped by their SGA area. Locations of NCDWR stations labeled as 1-4 are annotated in Figure 2.2.

2.3.2 SGA Specific Trends

To further understand spatial relationships within the results, the data for stations within SGA name groups were pooled. There are 8 total SGA groups (A, B, C, D, E, F, G, H) that were used to aggregate the station results. Correlations between all considered variables were calculated for each SGA (Table 2.2). From the correlations describing FC trends with LULC changes, we saw strong negative correlations between FC trends and developed land use change in SGA letters C and A despite the weak positive correlation represented by the coefficient calculated from all data (i.e., full coast). Negative correlations between FC trends and wetlands land use change were also observed, being especially strong in southern SGAs (A, B, C, D). β_{Precip} and β_{FC} had negative relationships for most SGAs, with the exception of SGA A and SGA B. The correlation between β_{Precip} and β_{FC} was broken down further for SGA C (Figure 2.S1), which revealed a strong correlation attributed to negative β_{FC} values occurring in conjunction with high β_{Precip} values. Shore distance had a fairly positive to fairly negative relationship with β_{FC} moving from the southern SGAs (A, B, C, D) to the northern SGAs (F, G, H). The relationship between shore distance and β_{FC} is shown in Figure 2.S1. Salinity trends were negatively correlated with β_{FC} along each SGA with the exception of SGA E (Table 2.S2). Due to the ecological importance of salinity when it comes to water quality and predicting FC concentrations (Souedan et al., 2021; Florini et al., 2020; Liu et al., 2012), our understanding of salinity integrating the effects of both land use and precipitation, and the consistent directionality of the correlation coefficients, we analyzed this SGA-specific relationship further (Figure 2.6).

Table 2.2: Pearson's correlation coefficients broken down by SGA letter (rows) for the relationships between β_{FC} and LULC class change, β_{Sal}, β_{Precip}, and shore distance. SGAs are listed in geographic order across the rows from H to A, with H being the northernmost SGA and A being the southernmost.

	β_{FC} and LULC Classes					β_{FC} & Other Parameters		
	Barren	Cultivated	Developed	Vegetated	Wetlands	β_{Sal}	β_{Precip}	Shore Distance
H	0.311	-0.043	0.278	0.255	0.158	-0.04	-0.032	-0.105
G	-0.141	0.014	-0.006	-0.066	0.234	-0.147	-0.345	-0.094
F	0.188	-0.056	-0.219	-0.105	-0.178	-0.363	-0.031	-0.099
E	0.003	-0.207	0.052	0.015	0.123	0.161	-0.151	0.045
D	0.254	-0.324	-0.180	-0.500	-0.267	-0.088	NA	0.244
C	0.040	0.252	-0.497	-0.006	-0.514	-0.561	-0.827	0.335
B	-0.042	0.034	0.128	0.167	-0.253	-0.055	0.094	0.099
A	-0.223	0.394	-0.355	0.31	-0.386	-0.510	0.071	0.417
Full Coast	0.021	-0.047	0.044	0.017	-0.072	-0.281	-0.023	0.013

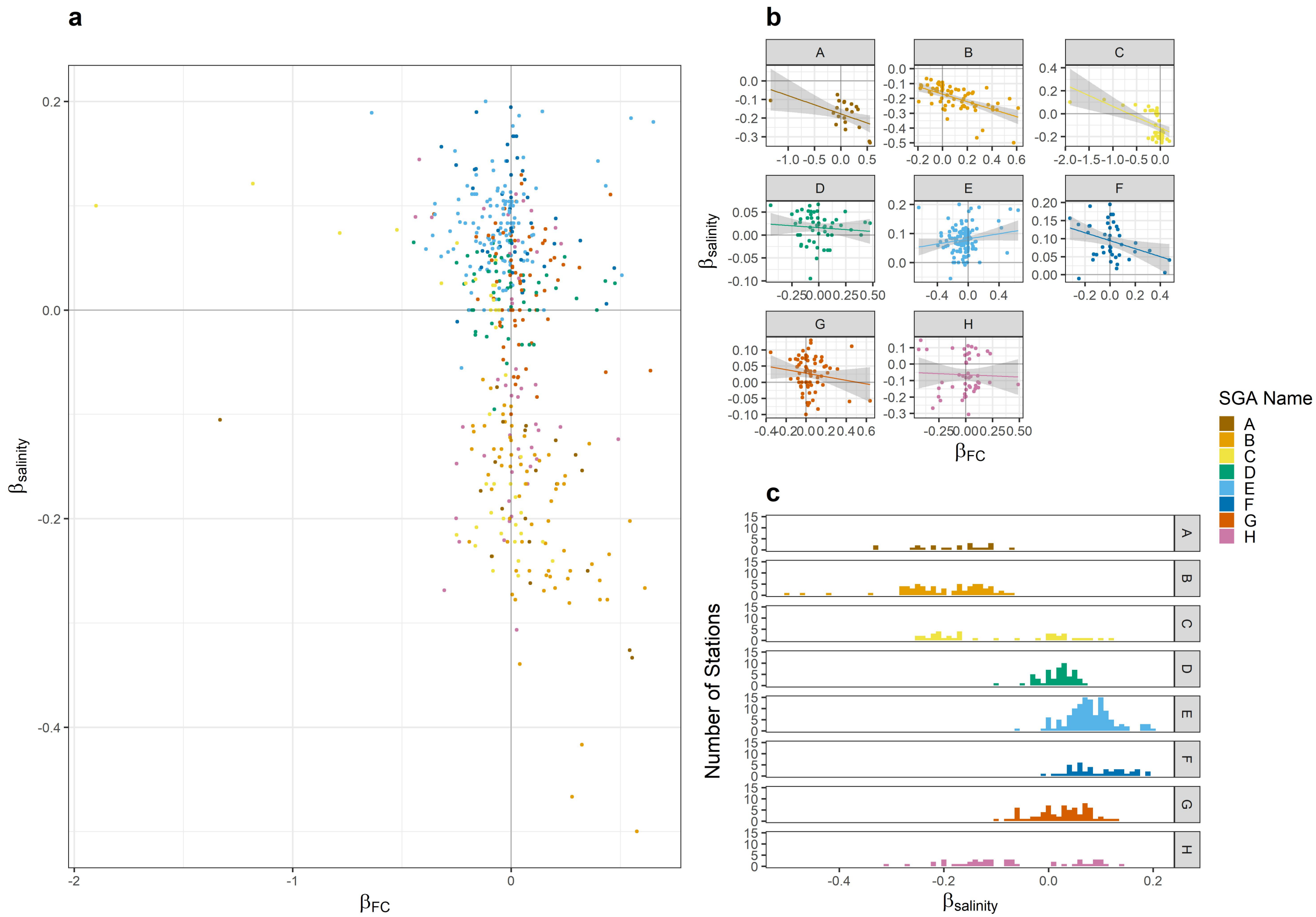

Figure 2.6: Leftmost scatterplot (a) illustrates the relationships between β_{FC} and β_{Sal} for each station colored by the station's associated SGA letter. The top right scatterplots (b) illustrate β_{FC} and β_{Sal} for each station within the SGA. The lower right histograms (c) show the distributions of β_{Sal} values broken down by SGA letter. Both (b) and (c) further demonstrate the spatial variation in salinity trends and relationships between β_{FC} and β_{Sal} across the coast.

There were weakly correlated, somewhat grouped relationships between β_{FC} and β_{Sal} along the full coast (Figure 2.6a), with strongly negative correlations in SGA B and somewhat in C, weakly correlated relationships in SGAs D, F, G, and H, and a positive correlation in SGA E (Figure 2.6b). When broken out by SGA (Figure 2.6c), the β_{Sal} distribution varied from lower negative values with higher spread in the southern SGAs A, B, and C, to higher positive β_{Sal} values with more narrow spread in the central SGAs D, E, and F. SGAs G and H had lower β_{Sal} values than the more central areas, but higher than the more southern areas (Figure 2.6c).

2.3.3 Representative Focal Areas

To explain some of the variation seen within the North Carolina coastal system, we detailed the trends seen under locally specific management and environmental conditions in SGAs B, E, and G (Figure 2.7). SGAs B, E, and G were selected because they captured different modes of estuarine and management variation, described in more detail in the following sections. More specifically, they represent different classes of estuarine drainage areas as defined by Engle et al. (2007), different shellfish lease distribution, and different levels of developed land change within the surrounding watersheds. Estuary drainage area classifications were originally created by NOAA's Coastal Assessment Framework to incorporate tidal influence into watershed delineation (NOAA, 2003). Engle et al. (2007) uses these areas to reclassify areas through a system that includes area, depth, volume, freshwater flow, and salinity to define an estuary type. This results in a coded class system ranging from 1 to 9 (Engle et al. 2007). By using a variety of different estuarine drainage area classes, we are effectively capturing a variety of physical and hydrological conditions, which enriches the interpretation of our results.

Focal Area B

SGA B (Figure 2.7c) is associated with waters at the mouth of the major river cutting through this region, the Cape Fear River, and lagoonal estuaries. SGA B is a class 6 estuary (Engle et al. 2007) characterized by large area, moderate volume, high freshwater flow, and moderate depth and salinity. This area contains higher rainfall thresholds ranging from 2 to 4 inches indicating that coastal FC concentrations within conditionally approved or approved portions of these growing areas do not respond as intensely to rainfall as compared to other

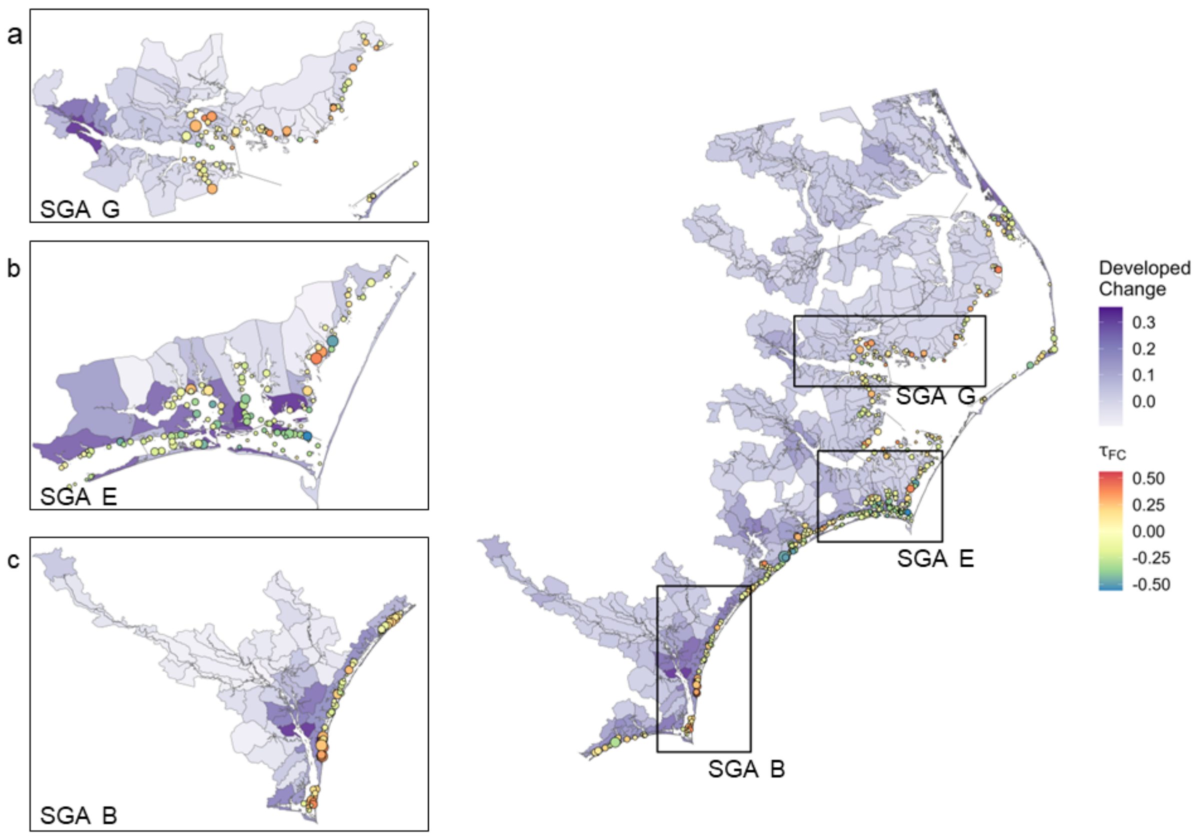

Figure 2.7: Full map of coastal North Carolina depicting the τ_{FC} values sized by the magnitude of their β_{FC} alongside HUC 12 land areas and their respective percent change in developed land use. SGAs B (a), E (b), and G (c) are used as focal areas to understand how management planning, increase in developed land, and estuary type affect the variation in FC trends.

areas of the coast with lower rainfall thresholds. Prior studies have reported poor water quality in SGA B (ALFORD et al. 2016; NCDEQ 2022), likely correlated with a high increase in the developed land up-river. Based on the changes in land use observed over the study period, watersheds adjacent to SGA B were associated with increased urbanization along the NC coast (Figure 2.4). SGA B is also characterized by consistently negative β_{Sal} values indicating decreasing salinity values for the samples that have been taken over the past 20 years (Figure 2.6c).

FC trends support our prior understanding regarding declining water quality in this region (Figure 2.7c), as demonstrated by high τ_{FC} and β_{FC} values across most of the study sites. However, some spatial variation in FC trends were observed. The more southern areas within this SGA, associated with the mouth of the Cape Fear River, have higher τ_{FC} values than the lagoonal areas located in the northern portion of the region, which are not generally directly affected by the Cape Fear River. The southern Cape Fear River can experience diverted flow through a man-made waterway under some high tide conditions, resulting in river flows discharging directly into the lagoonal estuaries. This tidal overflow effect might explain the similar trends in β_{FC} from the southern Cape Fear River area to the southern lagoonal estuary area despite being very separate geographies. While there are negative τ_{FC} values in the lagoonal areas, the β_{FC} is higher in the areas where τ_{FC} is positive, meaning that the FC concentrations towards the mouth of the Cape Fear River are increasing at a faster rate than the decreasing, lagoonal FC concentrations.

Focal Area E

SGA E (Figure 2.7b) represents a trunk and tributary estuarine system surrounded by moderate urban development in the past 20 years. SGA E contains systems classified as class 2 estuaries (Engle et al. 2007) indicating moderate area with low volume, moderate freshwater flow, and high salinity. SGA E supports a large number of up-estuary shellfish leases within the tributary systems. This area responds strongly to rainfall events in terms of FC load, as demonstrated by the low rainfall thresholds (i.e., 1 inch to 4 inches), with the lowest rainfall thresholds located up-estuary. This watershed, similar to SGA B, experienced a moderate increase in developed land use within the past 20 years (Figure 2.4). However, the τ_{FC} values in this region were generally negative with a few very positive τ_{FC} values within the river systems, suggesting an improvement in baseflow water quality. This area has also shown more positive β_{Sal} values (Figure 2.6c), indicating an increase in salinity measured for the samples taken over the past 20 years.

Focal Area G

SGA G (Figure 2.7c) contains the Pamlico and Pungo Rivers. SGA G is a class 4 estuary (Engle et al. 2007), which is characterized by moderate area, moderate depth, low volume, and high freshwater flow. This area is associated with the back-barrier Albemarle-Pamlico Estuary to the east, which is a class 9 estuary (Engle et al. 2007) indicating very large area, deep bathymetry, high volume, and high salinity environment. This area is also characterized by low increase in surrounding development and relatively fewer shellfish leases, demonstrating that this system is relatively unimpacted by human activity as compared to focal areas B and E. Accordingly, rainfall thresholds within SGA G are all at the highest limit of 4 inches, indicating FC concentrations in these waters are not highly sensitive to precipitation and stormwater runoff. There was a variety of negative and positive τ_{FC} values in this area with a majority of the stations exhibiting negative τ_{FC} values. The β_{Sal} values in this area are also variable, exhibiting a range of both positive and negative trends.

2.4 Discussion

In this study, we assessed the feasibility of utilizing estuarine monitoring data from a representative regulatory program (i.e., shellfish sanitation) to infer long term water quality trends. We used these data to look specifically at the spatial and temporal trends in FC concentrations and identified possible management and environmental drivers of these trends. Our study system, coastal North Carolina, exhibited a variety of trends in both the 20-year FC concentrations and the considered environmental drivers. While the resulting water quality trends and their relationships with environmental factors were complex, there were emergent patterns that we found to offer key insights.

We found that shellfish sanitation data collected routinely through a systematic random sampling strategy as defined by the National Shellfish Sanitation Program (NSSP) could cautiously be used for long-term water quality trend analysis when used alongside NCDWR salinity measurements. By comparing salinity measurements collected by the NCDWR, which maintains an unbiased monitoring program, and NCDMF, which only samples when shellfish waters are open for harvest, we were able to assess whether the sampling constraints imposed on the NCDMF measurements influenced the trend testing results.

We found that the NCDMF and NCDWR salinity time series behaved similarly across all SGAs (Figure 2.5). However, the NCDWR data only spanned 10 years while the NCDMF data spanned 20, and the difference in time series length limits our ability to extensively compare the NCDMF data using NCDWR observations. Additionally, though not strongly evident in the salinity data analyzed here, the risk for sampling bias to affect routine monitoring data collected by shellfish sanitation programs exists and should always be considered when analyzing regulatory water quality measurements.

We expect sampling bias risk to be greatest in conditionally approved waters with low rainfall thresholds (i.e., 1 to 2 inches), such as SGA E given the underlying conditions in which routine monitoring data can be collected. In contrast, in areas with relatively high rainfall thresholds (e.g., 4 inches), routine FC samples can typically be collected at any time during the year since these waters remain open unless an exceptional event, such as a hurricane or major frontal storm, has occurred. Because waters with high rainfall thresholds largely remain open, the six annual samples are collected under a wider range of environmental conditions, and there is less risk of sampling bias potentially affecting FC trends quantified from the routine monitoring data. For example, SGA G represents an area with high rainfall thresholds (4 inches). These high rainfall thresholds create less restrictive conditions for routine sampling, effectively increasing the variety of conditions captured in the sampling. Accordingly, FC trends determined from shellfish sanitation data from these stations are likely representative of the true improvement or degradation in water quality observed in the system, which also helps to explain why the FC trend results we reported corroborate findings from other studies that have evaluated water quality in this region. In contrast, areas that are more restricted in the time and conditions that routine sampling is able to occur (i.e., areas that are conditionally managed with low rainfall thresholds), such as SGA E, are associated with routine observations that have higher risk of being biased, and there is increased complexity in terms of interpreting these data to infer general water quality trends. Low rainfall thresholds dictate higher rates of closures for even mild meteorological events, which effectively restricts the open times available for routine sampling. However, we demonstrated that the use of an external water quality dataset, in this case for salinity, can be used to assess how sampling bias may have affected measurements collected by shellfish sanitation programs.

Nonpoint source runoff is considered a major contributor to FC loads in estuaries located near developed landscapes (Mallin et al. 2000; Coulliette et al. 2009; Kirby-Smith and White 2006; Campos et al. 2013). Therefore, the increasing trends we documented in

FC concentrations in SGAs B, E, and H align with the known relationship between FC and development. Specifically, the positive relationship between change in developed land cover across a watershed and increasing FC trends was seen in SGAs B, E, and H, while A, C, D, F, and G were associated with negative correlations (Table 2.2). Relationships between developed land use change and FC trends could potentially be clarified further by using population density change over watersheds, stormwater management, or differentiating impervious surfaces (Mallin et al. 2000; Carle et al. 2005; Cahoon et al. 2016; Freeman et al. 2019).

The negative correlation between FC and salinity along all SGAs (Table 2.2) was consistent with established water quality relationships except for a few contradictory results. The inverse relationship between FC and salinity could be a result of the coupled effect of increased freshwater input that comes with increased precipitation (Campos et al. 2013; Coulliette et al. 2009). It is known that FC concentrations increase following runoff after rainfall events, especially in more developed areas (Mallin et al. 2000; Carle et al. 2005; Cahoon et al. 2016; Freeman et al. 2019). These same rainfall events that increase the FC concentrations also decrease salinity, which is illustrated in the inverse relationships reported in this study across each SGA, with the exception of SGA E (Table 2.2, Figure 2.6). However, the inverse relationship between FC concentration and salinity trends was often noisy (Figure 2.6b), with the correlation coefficient between FC concentration and salinity trends being in the range of [-0.147, 0.161] for 5 out of 8 SGAs (Table 2.2). In the case of SGA E, where a positive correlation between salinity and FC trends was observed, the correlation appears to have been influenced by outlying values (Figure 2.6b), particularly since most of the β_{Sal} values reflected increases in salinity (Figure 2.6c) while the β_{FC} values showed there were FC concentration decreases across most sampling locations (Figure 2.6a, 6b).

The noisy relationships between FC concentration and salinity trends (Figure 2.6) in our results could be explained by our dataset not capturing short-term FC concentration increases following storm events and instead capturing FC during baseflow conditions. Because the data analyzed in this study was produced from routine systematic random sampling, which is collected when waters are open for harvest to capture baseline fecal coliform loading, the observations will not capture changes in storm-driven FC concentrations. Instead, the measurements may reveal if there is chronic loading in an area (e.g., due to continuously failing septic systems or poorly performing wastewater treatment plants). Therefore, the trends from this analysis are representative of baseflow conditions. Accordingly, had the routine sampling data captured post-storm conditions, we expect stronger correlations between FC and salinity trends would have been observed. Instead, we believe that factors such as increases in tidal flushing (e.g., due to inlet dredging) and changes in baseflow FC loads in these systems play a larger role in explaining the negative relationship between FC and salinity than changes in rain and runoff.

In addition to providing insights on long-term water quality trends, shellfish sanitation data can be used to assess the efficacy of current management practices. For example, a conditionally managed area with low rainfall thresholds that still show a trend towards increasing FC concentrations could indicate a decline in water quality that has not been met with intense enough action by the current management plan. As a result, trends in fecal coliform observations could be used as an "early warning system" to pinpoint areas where more intense management measures need to be taken. For example, the way in which these data could be used as an "early warning system" is demonstrated by focal SGA B (Figure 2.7c), where the mouth of the Cape Fear River likely shows increasing FC concentrations due to degradation of water quality that may need to be met with new management actions.

Although our results demonstrated opportunities of using shellfish sanitation data for inferring long-term water quality trends, our study was limited by several factors. Firstly, we did not account for tidal circulation due to the major modeling effort that would be required to include tidal circulation and flow patterns at this spatial and temporal scale. Future research may include factors that capture the marine flushing of an area such as inlet maintenance or distance to the nearest intracoastal waterway. Secondly, there was a lack of unbiased FC concentration datasets for trend validation, and we relied on findings from prior published studies to "ground truth" FC trends calculated from monitoring data. Regions outside of our study area may not have access to the type of information used to help diagnose the reliability of shellfish sanitation monitoring data for water quality inference. As new monitoring programs are introduced to track changes in marine systems, opportunities to pair sites with existing shellfish sanitation program monitoring locations could help to create data needed to characterize potential sampling bias effects and increase the ability for long-term shellfish sanitation data to be used for water quality analyses. Finally, because of variation in sampling protocols across state programs, shellfish sanitation data are nuanced and challenging to interpret. This study offers context and an approach for confronting nuance in the data. However, directly engaging with shellfish sanitation program managers is essential to accurately interpreting trend results like those presented here, as local expertise provides invaluable insight into the state and function of these estuarine systems and their management.

CHAPTER

3

PREDICTIVE MODELING

3.1 Introduction

The shellfish mariculture industry is becoming an increasingly important part of supporting global food systems because of the cost effective and sustainable nature of its farming practices (Theuerkauf et al. 2019; Botta et al. 2020; FAO; Azra et al. 2021). Bivalve shellfish farming ranges from very intensive, to very simple. Factors such as seed sourcing, farm costs, labor input, and yield will depend on the culturing methods. Farming bivalves begins with attaining larval stage organisms. These larvae can come from natural recruitment, collection of wild sources, or from land-based nurseries (Sturmer 2019). Once the free-floating larvae settle, they are called "spat" and can be moved out to the "grow-out" phase. Methods for growing oysters in the grow out stage include intertidal culture, water column culture, and subtidal culture in uncontrolled estuarine environments. To contain the harvest, farmers use equipment such as floating bags, racks or cages to keep their stock contained and keep out predators. Clams can be cultured in bottom trays, soft bottom bags, or bottom exclusion nets. Depending on the source and ploidy of the spat, it takes between 12 to 36 months for oysters to reach optimal market size and 12 to 18 months for hard clams to reach optimal market size (University of Florida, 2019; Sturmer, 2019; FDACS, 2022). Regardless of culturing methods, adult shellfish are placed in uncontrolled estuarine environments until they are harvested.

The ability to grow bivalves in open estuarine waters without providing additional inputs (e.g. feed, chemicals) is a key reason why bivalve production is considered exceptionally sustainable and cost effective, but results in farmed bivalves being exposed to changes in ambient estuarine conditions. In particular, bivalve shellfish are filter feeders and therefore sensitive to changes in ambient water quality, as they can ingest contaminants from the water column while feeding (Jørgensen 1990). Once consumed, bivalves can concentrate contaminants from the water column in their tissues, necessitating that water quality in shellfish growing areas be managed to ensure harvested shellfish are safe for human consumption. Specifically, public health officials are primarily concerned about the presence of fecally-associated pathogens in shellfish tissues, as many such pathogens cause severe human illness if consumed.

In the USA, regulatory agencies use fecal indicator bacteria (FIB) concentrations, specifically of fecal coliforms (FC), as proxies for the overall load of fecally-associated pathogens that could threaten human health if present in shellfish. Regulatory programs operate under the assumption that shellfish harvested from waters with elevated FC concentrations are contaminated. Chronic FC contamination in coastal waters is driven by persistent increases in development in the surrounding watershed, livestock production, and point source pollution episodes such as septic tank failures (Campos et al. 2013). Short-term contamination events are primarily driven by rainfall and subsequent stormwater runoff transporting the FC bacteria from their terrestrial sources to the adjacent waterways (Jeng et al. 2005; Coulliette et al. 2009; NSSP 2019). State shellfish sanitation programs, under the guidance of the U.S. Food and Drug Administration's National Shellfish Sanitation Program (NSSP 2019), classify and manage shellfish growing waters as a function of FC concentrations. Shellfish growing areas can be classified as approved, restricted, prohibited, conditionally approved, and conditionally restricted based on sanitary surveys of an area describing the environmental factors that are current or potential pollution sources, microbiological sampling trends, and stock within the area (NSSP 2019). Conditionally approved waters are commonly assigned rainfall thresholds, which are 24-hour rainfall depths associated with FC concentration exceedances. Rainfall thresholds are determined through observational studies and modified over time as needed. Some states will also use river stage thresholds in tandem with rainfall.

As a protective measure to prevent harvesting contaminated product, temporary closures of conditionally approved shellfish growing areas are issued immediately and without warning once rainfall thresholds are met. This policy of immediate closures causes shellfish growers to have little time to react to the closure and allocate resources efficiently. In fact, shellfish sanitation closures constitute a major reason for economic loss within the industry and can be especially detrimental to smaller businesses (National Sea Grant Law Center, 2019; Evans et al., 2016; Landrum et al., 2000). The prediction of shellfish sanitation closures would enable growers to make more informed management decisions to mitigate the effects of immediate closures on their shellfish harvest. Examples of management actions include harvesting their stock early, deciding to wait until the area reopens, or focusing on leases located in open growing waters.

Currently, state shellfish sanitation programs maintain long-term water quality monitoring programs through which to periodically reevaluate the harvest classification of shellfish growing waters, and the data generated from shellfish sanitation management presents an opportunity for developing decision-support tools to aid in better management of shellfish growing area closures and reopenings. The NSSP currently provides two sampling strategies to utilize when collecting this data for areas that require continuous management.

The first strategy is systematic random sampling, which aims to capture baseline FC measurements across a range of environmental conditions. While the aim of this strategy is to capture FC concentration over a range of conditions, in practice, depending on the available resources of the regulatory agency, this can result in a database that doesn't necessarily capture the conditions after events that lead to elevated fecal coliforms and rather capture baseflow conditions (Chazal, 2023 [Chapter 2]). The second strategy is adverse pollution condition sampling, which calls for sample collection during periods when point-source pollution events or elevated rainfall and river stage have reached levels that are known to degrade water quality in specific areas. The dataset generated by the adverse pollution condition sampling method captures conditions when the contamination is near or at its highest levels. While both sampling strategies were intended for shellfish growing area management, the data generated from adverse pollution condition sampling captures more conditions in which the water quality is degraded, and therefore has more utility for predicting similar degraded water quality conditions.

There is growing interest in leveraging these regulatory data to make decision support tools. Zimmer-Faust et al. (2018) utilized this type of regulatory shellfish sanitation data to develop and compare predictive models for three of Oregon's shellfish growing areas. With Firth's Binary Logistic Regression and Classification Tree approaches performing the best within this ecosystem, Zimmer-Faust et al. (2018) was able to provide insights into both predictability of closures in certain shellfish growing areas and easily interpretable parameter estimates to suggest better management criteria and more targeted sampling strategies. Wang et al. (2019) utilized shellfish sanitation regulatory data to create predictive models for shellfish growing areas along Louisiana's Gulf coast. They used Artificial Neural Networks with relevant input parameters selected through stepwise regression analysis to predict daily and seasonal variations in fecal coliform levels. Schmidt et al. (2018) used generalized linear models and generalized additive models to successfully forecast one week threshold exceedances of E. coli concentrations in Cornwall, UK. While all of these models were successful in predicting log transformed FC values, they were limited in their spatial extent, with Schmidt et al. (2018) using 2 study sites within areas relatively close together in Cornwall, UK, Zimmer-Faust et al. (2018) using 13 sampling stations within a single bay in Oregon, and Wang et al. (2019) using 3 beaches all within 20 km of each other on the coast of Lake Erie. While there are small-scale drivers of FC concentrations for local prediction, this study will aim to broaden the model application by spanning multiple different watersheds along the coastline of an entire US state. Another limitation of the previous studies that leverage monitoring data for FC prediction is the lack of forecasted meteorological values as predictors. Updating models with forecasted rainfall data will potentially allow for more accurate predictions of FC concentrations due to the mechanistic importance of stormwater runoff in contributing to elevated FCs in coastal systems.

While there are many other data-driven statistical models for predicting Harmful Algal Blooms and other biotoxins in shellfish growing areas (Cruz et al. 2022), and FC concentrations for recreational beaches (Parkhurst et al. 2005; Park et al. 2018; Searcy and Boehm 2021; Li et al. 2022), the predictive models developed for FC concentrations in shellfish growing areas remain limited in their ability to directly support the management of coastal resources. These limitations include a lack of data availability for models that require fine-scale temporal or spatial resolution for training, models that are too computationally intensive given the limited resources of management agencies, and models whose relationships between the predictor and response variables are convoluted. Within predictive models that exist, there are even fewer that utilize machine learning methods to account for the complex and often non-linear relationships that occur in estuarine environments (Schmidt et al. 2018;

Zimmer-Faust et al. 2018; Grbčić et al. 2022).

The purpose of this study was to develop predictive FC models that could be used to create regional decision-support tools for shellfish-growers and estuarine resource managers. Our objectives were to (1) develop predictive FC concentration models for shellfish growing areas using watershed characteristics and antecedent hydrologic observations as predictors, (2) test the change in model performance associated with using forecasted, as opposed to observed, rainfall inputs in the models for day-of to two-day-ahead prediction, and (3) identify the most important variables in the models and evaluate whether they align with shellfish sanitation management criteria. We also compared the forecasted and observed rainfall amounts to assess the uncertainty tradeoffs associated with using predicted estimates as model inputs.

3.2 Methods

3.2.1 Study Area

Florida, USA, is home to 8,127 hectares of shellfish growing areas (SECOORA 2022)) that span diverse ecoregions.The Florida Department for Agriculture and Consumer Services (FDACS) implements the NSSP in Florida and manages the state's shellfish sanitation program. The state's conditionally approved shellfish growing waters are managed through temporary closures dictated by threshold exceedances of antecedent rainfall and, in some areas, river stage. There are 1,285 spatially fixed sampling water quality stations across five management areas: West Gulf, Central Gulf, Big Bend, South Gulf, and Atlantic (Figure 3.1). FDACS uses management areas to group areas under similar harvesting pressure and each area is overseen by a local office (FDACS correspondence). Though defined for administrative purposes, the FDACS management areas also capture differences in physiography, coastal geomorphology, and resource management needs (Hapke et al. 2019).

3.2.2 Data Acquisition and Pre-Processing

FDACS FC monitoring data between 2012 and 2021 were used in this analysis. Although FDACS's publicly available digitized dataset extends past 2012, data collected prior to 2012 were not considered because of a shift in FDACS lab procedures that occurred in 2012

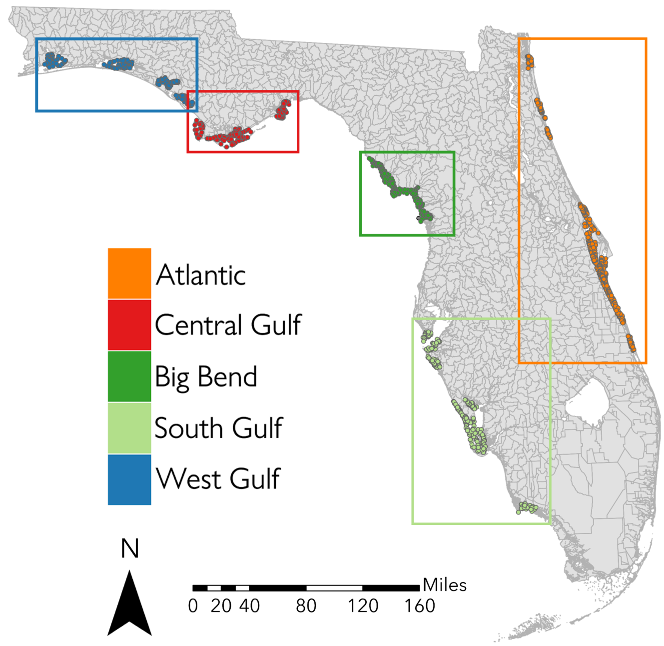

Figure 3.1: Study area map of Florida coastline depicted with the FDACS water quality sampling stations colored by the management areas used to split up data for modeling.

resulting in measurement units changing from most probable numbers (MPN) to colony forming units (CFU), which are not directly comparable (Noble et al. 2003; Gronewold and Wolpert 2008; Cho et al. 2010).

The NSSP currently allows states to choose from one of two sampling strategies to use in their ambient water quality monitoring programs: systematic random sampling and adverse pollution condition sampling (NSSP 2019). Florida uses the adverse pollution condition sampling strategy, resulting in their monitoring data being expected to capture conditions when FC contamination is near or at the highest expected concentrations. Per the NSSP, the state is required to collect at least 5 samples annually from each of the spatially fixed water quality sampling stations, amounting to 407,136 total FC observations in the dataset.

3.2.3 Environmental Predictors

To predict daily FC concentrations, we included environmental parameters that may be associated with FC dynamics in regards to the non-point sources of FC, transport of FC into water bodies, and system mediators contributing to decay times of FC (Table 1). All associated parameters were included in the initial models and were then reduced during the variable selection process.

Radar-based, continuous precipitation data was gathered from NEXRAD, and totaled over subwatershed areas (HUC12 as defined by U.S. Geological Survey). These totals were included for 1 day, 3 days, 5 days, and 7 days prior. Rainfall was aggregated over the watershed area to estimate the volume of water expected to runoff into the downstream estuary and transport FC. River stage was measured from USGS gauge sites that had adequate data spanning the 2012 to 2021 range. Additionally, other variables considered in the model that relate to FC transport included watershed channelization characteristics, specifically the length of natural channelization and the length of artificial channelization within the watershed area, calculated from the USGS National Hydrography Dataset (USGS NHD). Increased channelization creates greater opportunity for rapid drainage and transport of stormwater runoff from land to downstream estuarine waters (Falbo et al. 2013), thus also increasing the opportunity for FC transport. Other meteorological and hydrological parameters including wind speed, wind direction, water temperature, and air temperature were gathered from NOAA Co-Ops Stations and were also aggregated on 1 day, 3 day, 5 day, and 7 day totals. Wind is widely reported in the literature as an important variable for explaining coastal circulation patterns (Chigbu et al. 2004; Ufnar et al. 2006; Lewis et al. 2013; NSSP 2019), particularly since winds blowing onshore can increase estuarine residence times. Wind speed and direction were aggregated to their latitude (u) components, longitude (v) components, speed, and combined vector components (Grange, 2014). Water and air temperature were considered because of the key role temperature plays in determining the survivability and therefore persistence of FC in the marine environment (Sinton 2005; Lipp et al. 2001; Chigbu et al. 2005). Watershed characteristics, including total area, were summarized on a HUC12 watershed scale and included as predictors to capture potential FC sources. Percent land use was obtained from Multi-Resolution Land Characteristics Consortium's National Land Cover Database (Dewitz and U.S. Geological Survey 2021); classes were aggregated from 20 relatively narrow classes into five broad categories: open water, wetlands, developed, cultivated, and vegetated. The land cover data were aggregated to reduce the total number of variables associated with land cover while still capturing variation in areas that are primarily dominated by natural versus human systems. We associated the FC data to the temporally closest land use dataset which includes 2011, 2013, 2016, and 2019 data. Soil drainage was gathered from the USGS NRC SSURGO dataset and were

Table 3.1: Environmental variables and their features used to predict FC concentrations. Also indicated is the variables type which represents the mechanism that relates that variable to FC concentrations in coastal waters, the spatial resolution of the dataset used, the features used for each observation, the units of the variable, and the source of the variables datasets.

Type	Variable	Spatial Resolution	Features	Units	Data Source
Response	FC Concentration	Discrete Station		CFU	FDAC
Transport	Rainfall	HUC12	1,2,3,5,7 day prior	kg/m^2	NEXRAD
	River Stage	Discrete Station	1,2,3,5,7 day prior	ft	USGS
	Wind Speed	Discrete Station	1,2,3,5,7 day prior	m/s	NOAA Co-ops
	Wind Direction	Discrete Station	1,2,3,5,7 day prior	Deg. True	NOAA Co-ops
	Channelization (natural)	HUC12		m	USGS NHD
	Channelization (artificial)	HUC12		m	USGS NHD
	Watershed Area	HUC12		acres	FDEP
Source	Land Usage	HUC12	2011, 2013, 2016, 2019	% acreage	NLCD MRLC
	Soil Drainage	HUC12	C, D, B/D, C/D	% acreage	NRCS SSURGO
System Mediators	Air Temperature	Discrete Station	1,2,3,5,7 day prior	° F	NOAA Co-ops
	Water Temperature Month	Discrete Station	1,2,3,5,7 day prior	° F	NOAA Co-ops

categorized by USGS groups C, D, B/D, and C/D which correspond to levels of drainage and infiltration that affect runoff potential. The month time component was included to account for seasonal differences in rain and wind patterns.

3.2.4 Modeling

We developed 5 models with different predictor structures (Figure 3.2) for each of the 5 management areas along Florida's coast (Figure 3.1) for a total of 25 different models. All of the models included the same static variables (eg., land cover, soil drainage characteristics), but differed in terms of the temporally-dynamic variables considered (i.e., rainfall, wind, river stage). The first model, referred to as the null model (N), used all antecedent rainfall predictors (3-day, 5-day, 7-day) as well as day-of rainfall (1-day). We refer to this model as "null" as it captures an impossible predictive modeling scenario in which the observed day-of rainfall is known. Because the N model includes day-of observed rainfall, we assumed it included the best possible predictor and would have the lowest error. The second model, referred to as the observed model (O), contains all antecedent predictors, and excludes day-of rainfall. This model is representative of the information that a resource manager or grower would have available to them when tasked with making a management decision, and corresponds to the data that could be used to create an operational predictive model as part of a decision-support tool. The final three models all excluded day-of rainfall, but included antecedent predictors as well as forecasted rainfall. Specifically, day-of rainfall forecasts (f_1), 2-day (i.e., next-day) rainfall forecasts (f_2), and 3-day (i.e., in two days) rainfall forecasts (f_3).

Random Forest models were used to predict daily FC concentrations. Random Forest is a type of machine learning algorithm used commonly for both regression and classification problems (Breiman 2001). Broadly speaking, Random Forest models work by creating many decorrelated and individually uninformative decision trees using random subsets of the full dataset to create an ensemble, or "forest", that works together to generate a prediction (Breiman 2001). The Random Forest algorithm was chosen for its ability to handle the nonlinear relationships between predictors and responses that are commonly seen in estuarine/marine systems (Fan et al. 2015; Zhang et al. 2020), and because of its suitability and robustness with "medium" dataset sizes (Hastie et al. 2009). Models were built in R with the random forest method 'rf' within the 'caret' package version 6.0.90 (Kuhn et al., 2022). We used a randomized 80% training 20% testing split with hyperparameter, mtry,

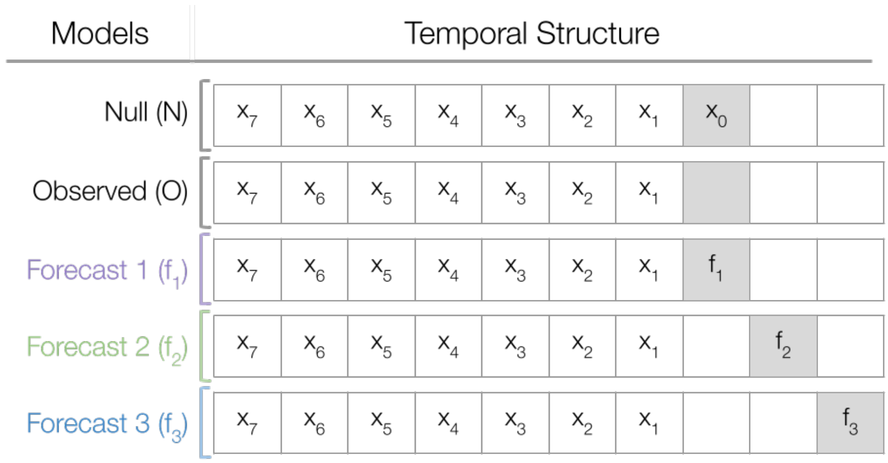

Figure 3.2: Dataset alignment schematic showing the antecedent predictors x_1, x_2,...x_7, day-of predictors x_0, and the forecasted rainfall f_1, f_2, f_3. The gray boxes represent the day of the FC observation.

tuned automatically using the optimal mtry value from five searches (tuneLength = 5). Mtry dictates the number of variables that are randomly chosen as candidate features to split data in one of the many trees used to create Random Forests. All model results are reported for the testing split only.

In total, 67 candidate predictor variables were compiled. However, to ensure variables did not include redundant information, we applied a variable screening procedure from which to reduce the total number of predictors included in the models. Variable Inflation Factors (VIF) were iteratively used to reduce multicollinearity in the selected variables within the models using a threshold of 10. The VIF procedure was applied for each of the 5 management areas, and included only the observational data (i.e., forecasted rainfall variables were not included). While there are no standard practices for selecting VIF thresholds for multicollinearity, statisticians have suggested the use of 5 or 10 as reasonable maximum values (Montgomery et al. 1992; Zuur et al. 2007). To assess each of the models' goodness of fit, we used the coefficient of determination (R2). We reported root mean squared error (RMSE) to evaluate the error across the five models in the same area.

Random forest methods include incremental node purity scores for each of the predictors. The incremental node purity is used to rank features by how well a predictor splits the data in each of the trees that are used to train the Random Forest model. This is measured through the magnitude of decrease in the Gini Index before and after a feature is used to split the data.

3.2.5 Forecasted Rainfall

The rainfall forecasts, like the observed rainfall measurements, were radar-based, continuous precipitation data from NEXRAD. Forecasts for 1-day, 2-day, and 3-day over subwatershed areas (HUC12 as defined by U.S. Geological Survey) were gathered. This was done through determining the total rainfall for the 24 hour period within each of the HUC12 subwatershed areas. Because of the use of different observed and forecasted rainfall variables in the models, we explored correlations between the forecasted and observed rainfall values to characterize the uncertainty introduced to the models with the use of forecasted inputs.

3.3 Results

3.3.1 FDACS Monitoring Data

The FDAC FC observations used within this analysis were summarized with monthly means and total number of observations per month in each management area (Figure 3.3). Overall, the South Gulf area had the lowest means ($\bar{x} = 3.99$) while the West Gulf had the highest ($\bar{x} = 8.61$). The West Gulf and the South Gulf both had the highest mean monthly FC in 2018, the Central Gulf in 2017, the Atlantic in 2021, and the Big Bend in 2012 (Figure 3.3). Sampling in each of the management areas was generally consistent across the years with Big Bend having the most sampling effort overall and South Gulf having the least (Figure 3.3). We also explored the number of sampling stations in the Atlantic (n = 442), Big Bend (n = 242), Central Gulf (n = 192), South Gulf (n = 249), and West Gulf (n = 156).

Most management areas show peak FC concentrations during the winter months (November - February) with the exception of the South Gulf area which shows peak mean FC concentrations between August and October (Figure 3.4).

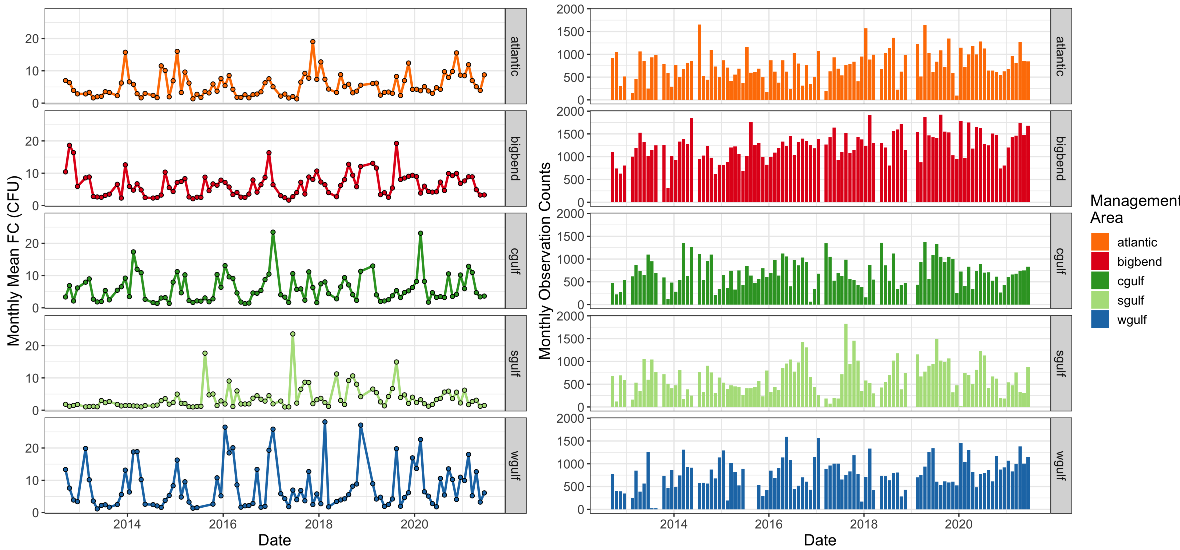

Figure 3.3: Summarized FDAC FC sampling results between 2012 and 2021. Summaries include mean monthly FC concentrations (CFU) represented for each management area (left) and the total number of FC samples taken within the management area for each month within the time series (right).

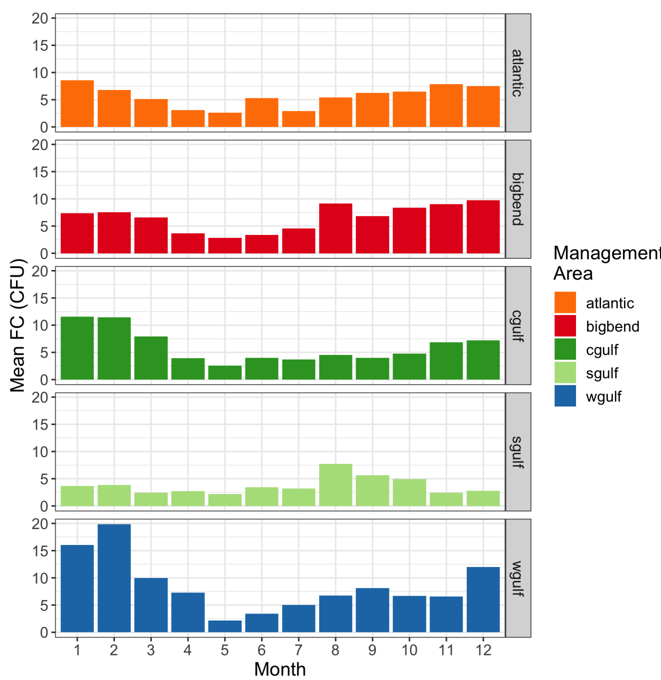

Figure 3.4: Summarized FDAC FC sampling results between 2012 and 2021 aggregated to a monthly scale. Mean FC (CFU) is indicated for every month for each management area.

3.3.2 Model Performance

The performance of the models varied between the 5 management areas (Table 3.2). The Central Gulf, Big Bend, South Gulf, and Atlantic management areas performed similarly with R^2 values ranging from 0.360 to 0.457. The best overall performance was seen in the O model in the West Gulf region ($R^2 = 0.720$). The overall worst performing model was the f_2 model in the South Gulf region ($R^2 = 0.360$). There is negligible change in RMSE across models within the same management areas.

Table 3.2: R^2, RMSE, and n values for each of the models built in this study for all of the study areas.

	Null (N)			Observed (O)			Forecast 1 (f_1)			Forecast 2 (f_2)			Forecast 3 (f_3)		
	R^2	RMSE	n	R^2	RMSE	n	R^2	RMSE	n	R^2	RMSE	n	R^2	RMSE	n
West Gulf	0.698	9.48	35,536	0.720	9.29	35,624	0.682	9.52	31,772	0.681	9.95	31,572	0.687	9.69	35,496
Central Gulf	0.413	8.48	43,036	0.444	8.61	43,072	0.433	9.09	39,732	0.415	8.55	39,700	0.438	8.01	42,748
Big Bend	0.404	10.4	53,996	0.427	10.4	54,264	0.380	11.5	49,964	0.457	10.1	48,900	0.438	9.94	53,216
South Gulf	0.385	6.61	26,784	0.403	6.53	26,896	0.427	6.36	24,420	0.360	6.22	23,816	0.383	6.16	26,296
Atlantic	0.417	9.14	40,148	0.395	9.17	40,340	0.383	9.05	36,680	0.400	9.36	35,948	0.418	9.06	39,668

Table 3.3: RMSE and n values for each of the models built in this study for all of the study areas, categorized by the data either exceeding (E) or within safe (S) regulatory threshold limits (14 CFU).

	Null (N)			Observed (O)			Forecast 1 (f_1)			Forecast 2 (f_2)			Forecast 3 (f_3)		
	Type	RMSE	n	Type	RMSE	n	Type	RMSE	n	Type	RMSE	n	Type	RMSE	n
West Gulf	E	21.7	965	E	21.5	949	E	20.9	885	E	22.6	906	E	21.7	984
	S	5.48	6,141	S	5.33	6,175	S	5.86	5,469	S	5.49	5,407	S	5.78	6,114
Central Gulf	E	24.9	714	E	25.7	700	E	27.3	665	E	25.4	635	E	23.6	678
	S	4.72	7,892	S	4.74	7,914	S	4.70	7,281	S	4.81	7,304	S	4.67	7,871
Big Bend	E	25.1	1,265	E	24.9	1,293	E	28.6	1,221	E	24.3	1,189	E	24.4	1,200
	S	6.22	9,533	S	6.17	9,559	S	6.05	8,771	S	5.94	8,590	S	5.93	9,433
South Gulf	E	29.8	195	E	28.5	210	E	30.4	165	E	29.6	146	E	28.9	173
	S	3.45	5,161	S	3.36	5,169	S	3.09	4,719	S	3.48	4,617	S	3.31	5,086
Atlantic	E	27.0	694	E	27.6	683	E	27.8	602	E	28.4	611	E	26.9	696
	S	4.75	7,335	S	4.62	7,384	S	4.49	6,733	S	4.54	6,578	S	4.52	7,237

To explore the model error further, we used the regulatory threshold of FC concentrations associated with shellfish harvest closures, 14 CFU (NSSP, 2019). The RMSE was reported for exceedances and safe levels for each of the models in each of the management areas (Table 3). To do this, the data was categorized based on the regulatory threshold for exceedence (14 CFU) and the RMSE was recalculated for each category. The exceedances consistently have a much higher RMSE than the safe levels. This indicates that the models are able to predict FC concentrations within the safe <14 CFU limit better than in exceedance conditions.

3.3.3 Variable Importance Scores

We used standardized, incremental node purity scores to summarize the feature importance for each of the models in each of the management areas (Figure 3.5).

Generally, the Atlantic, Central Gulf, South Gulf, and West Gulf management areas indicate antecedent precipitation as being the most important predictor of FC concentrations in the null and observed models. In the Big Bend management area, day-of river stage (River Stage 0 Day) was the most important predictor in the null model, while the antecedent, day before river stage was the most important predictor in the observed model. In both the Atlantic and the Big Bend management areas, there is an increase in importance in the antecedent, 7 days before wind component variables (Wind Lat. 7 Day, Wind Long. 7 Day). When we include the day-of rainfall forecasts for the 1 day forecast model (f_1), we see a slight change in the overall variables that are important in predicting FC concentrations. However, there are more differences seen in the 2 and 3 day forecast models, most notably the increased importance in water temperature and wind components in the 3 day forecast models (f_3). We see that 3 day forecasted rainfall is highly important in the Atlantic management area comparatively to the other management areas. In the Atlantic and Big Bend management areas in particular, there is increased importance distributed among the antecedent wind component predictors in the forecasted models. The increase in variable importance aside from wind is also seen in the remaining predictors in the forecasted models relative to the N and O models, but to a lesser extent.

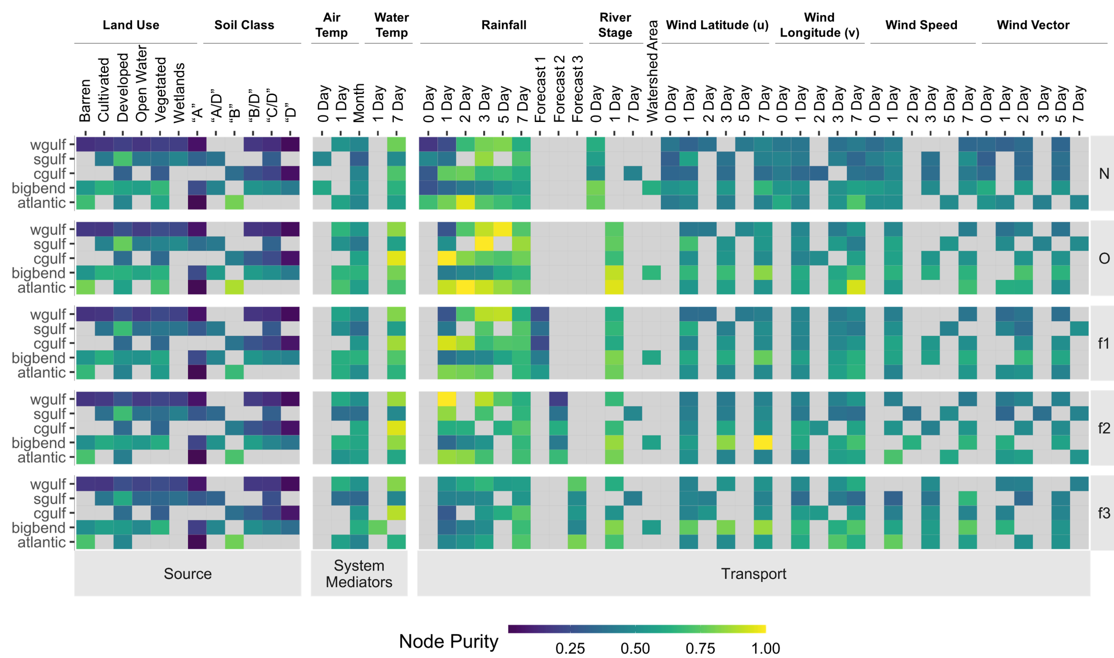

Figure 3.5: Heatmaps of the variable importance scores in all of the models. Areas are listed on the left, while model structure type is listed on the right. Columns correspond to candidate predictor variables considered in the analysis. Variables are organized by their mechanistic categories (Source, System Mediators, Transport). The gray cells are variables that were removed by pre-processing VIF procedures, or were not considered for a particular model structure (e.g., the forecasted variables were not considered in the N and O models).

3.3.4 Rainfall Discussion

Because the main differences within the models lie with the inclusion of rainfall forecasts, it is important to evaluate the error that these forecasts introduce into the models. We compared the day-of (x0) measurements, or the actual, observed values, and the predicted rainfall (f_1, f_2, f_3) measurements, or the forecasted values (Figure 3.6). All of these values are aggregated across the HUC12 watershed area.

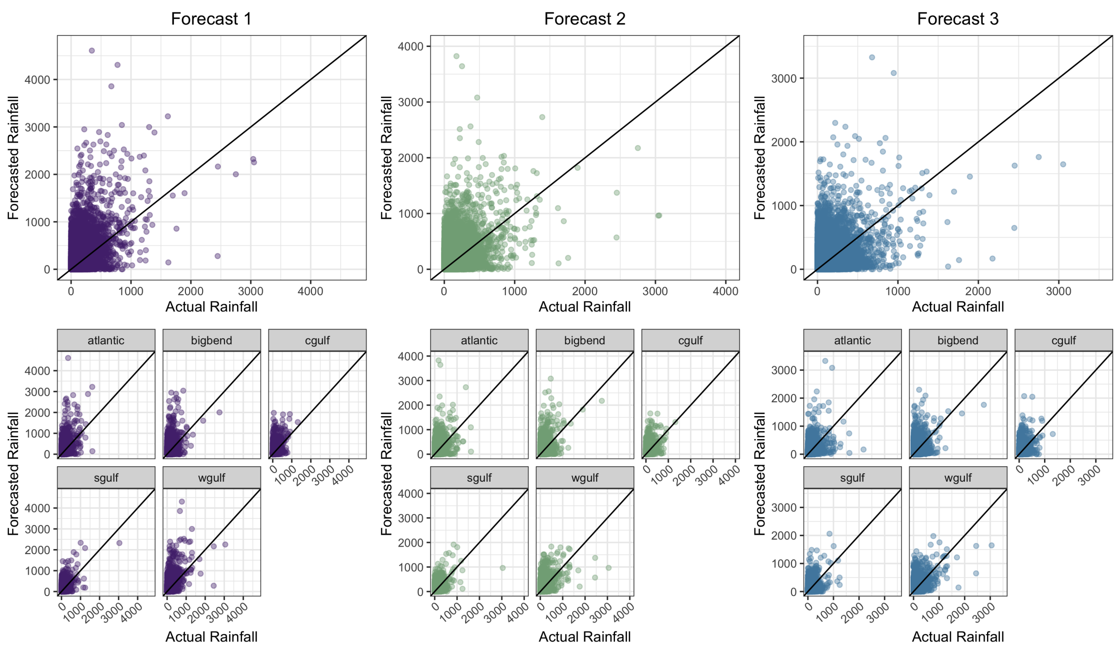

Figure 3.6: Actual measured rainfall values against forecasted rainfall values.

Pearsons correlation test revealed the relationship between actual and forecasted rainfall values for all data from f_1 models were relatively poor ($R^2 = 0.306$, RMSE = 153.3) with a decline in correlation between the observed and forecasted rainfall amounts for the 2-day ($R^2 = 0.236$, RMSE = 131.1) and 3-day ($R^2 = 0.207$, RMSE = 121.0) estimates.

3.4 Discussion

This study utilized random forest regression models for 5 management areas along the Florida coast to predict FC concentrations with a suite of different meteorological, hydrological, and geological predictors. We then updated these models with 1, 2, and 3 day rainfall forecast predictors to determine the performance as a short-term forecast tool. With both the forecast, and non-forecast models, we interpreted the variable importance scores to determine the main drivers of FC concentrations and FC forecasts across the 5 management areas in Florida.

3.4.1 Model Performance

The models created in this study performed sufficiently well to be integrated into decision-support systems. Compared to the few studies that utilize Random Forest regression models to predict raw densities of FC in coastal waters (Parkhurst et al. 2005), our models demonstrated better performance. Our models performed worse than studies that utilize $\log_{10}$ transformations of FC in Random Forest regression models (Jones et al. 2013; Brooks et al. 2016; Wang et al. 2021). However, the use of the $\log_{10}$ transformation in Random Forest models, similar to the use of geometric means, will generally be biased towards lower concentrations (Haas 1996; Crump 1998). Meaning that although overall performance is improved, the predictive performance in exceedance categories will be lower overall (Brooks et al. 2016).

Overall, the models in West Gulf performed better, with consistently higher R^2 values, than the Central Gulf, Big Bend, South Gulf, and Atlantic (Table 3.2). The West Gulf contained the highest percentage of exceedance data (Table 3.3) and demonstrated the highest means in the exploratory analysis (Figure 3.3). The dataset in that region may have been more balanced and therefore the predictions were not overly biased towards the non-exceedance, lower levels of FC.

Across models, updating the predictors to rainfall forecasts rather than measured values did not affect model performance. Because of the minimal benefits to using the f_1 models, day-of forecasting is best performed by the O models in each of the growing areas. We did not compare the use of only antecedent predictors for 2-day and 3-day forecasting, therefore the best recommendation for these forecasts is to utilize the f_2 and f_3 models.

We recommend that future work analyzes the effects of dataset imbalance on predictive performance and explores models that may improve prediction of exceedance values as well as normal, non-exceedance values of FC.

3.4.2 Variable Importance

Among the most important variables was antecedent rainfall and river stage. The importance of these transport mechanisms for predicting FC concentrations in coastal waters has been corroborated by other studies (Crowther et al. 2001; Chigbu et al. 2005; Jeng et al. 2005; Coulliette et al. 2009; Campos et al. 2013; NSSP 2019). FDAC sets rainfall and, in some cases, river stage thresholds for temporary closures of shellfish growing areas in Florida. The alignment of these study results with current management understanding suggests that these models are representing true FC dynamics within these systems.

The null model (N) was the only model to include day-of predictors without forecasted information (Figure 3.2). However, the day-of rainfall information was not as important as the antecedent 1 to 7 day rainfall measurements. This importance of lagged rainfall indicates a possible relationship between previous meteorological conditions such as drought or heavy rainfall conditions and FC concentrations. The models that used only antecedent rainfall (N and O models), performed similarly to the models that used forecasted and antecedent rainfall (f_1, f_2, f_3 models). Because of the poor correlation of forecasted rainfall with actual rainfall (Figure 3.4), the use of other variables becomes particularly important for the accurate prediction of FC concentrations. Wind components in particular become slightly more important during the 2 and 3 day forecast models. This could be due to the known relationship between wind and elevated FC concentrations in the Gulf Coast area (Chigbu et al. 2004; Ufnar et al. 2006; Lewis et al. 2013; NSSP 2019). With the removal of the more important variables (antecedent rainfall and river stage), and the introduction of more error in the forecasted rainfall variables (Figure 3.6), the secondary mechanism of elevated FC concentrations due to wind is revealed. Because of the understood importance of elevated river stage as a primary driver of elevated FC concentrations in addition to stormwater runoff from rainfall, (Faust 1976; Ahn et al. 2005; Chigbu et al. 2005; Wilkinson et al. 2006; Vidon et al. 2008; Kay et al. 2010) it is recommended that future work explores the addition of forecasted river stage in FC concentration prediction.

Overall, the variable importance scores in this study provided insight into the relationships between the environmental variables introduced in the model and FC concentrations. The changes between the importance of certain variables when aligned for forecasting as opposed to day-of and observed models can enrich our understanding of the environmental dynamics contributing to FC levels in coastal waters.

CHAPTER

4

CONCLUSIONS

This thesis presents two coastal water quality modeling studies that leverage shellfish sanitation data for historical analysis and future prediction of fecal coliforms.

Chapter 2 demonstrated that it is possible to utilize North Carolina's shellfish sanitation data for long-term, baseflow water quality analysis. Using salinity as a metric for monitoring program related bias, we found that sampling bias could exist in areas with lower rainfall thresholds. However, the similarities between trends in NCDMF datasets and unbiased salinity datasets show that generally, the risk of bias is limited in these systems for baseflow FC trends. Finally, representative focal areas were chosen in areas with high development, moderate development, and low development to provide regionally specific insights into FC and environmental dynamics. Although our results demonstrated the opportunities and challenges of using shellfish sanitation data for inferring long-term water quality trends, our study was limited by several factors. Firstly, there is a lack of unbiased FC datasets for trend validation. We relied on findings from prior studies to "ground truth" FC trends calculated from monitoring data. Regions outside of our study area may not have access to the type of information used to help diagnose the reliability of shellfish sanitation monitoring data for water quality inference. Engaging with program managers is essential to improving the interpretation of the trend results, as local expertise provides invaluable insight into the state and function of these estuarine systems and their management. Ultimately, this study informs future management strategies, provides a programmatic and statistical workflow for future trend analyses with regulatory data, and reveals new insights into the complexities of estuarine and coastal systems.

Chapter 3 utilized Florida's shellfish sanitation data to develop random forest regression models for 5 management areas along the coast to predict FC concentrations. Predictors included a suite of different meteorological, hydrological, and geological predictors to represent the mechanisms behind the sources of FC, transport of FC from the sources to the waterways, and the factors that affect survivability of FC in marine systems. We then updated these models with 1, 2, and 3 day rainfall forecast predictors to determine the performance as a short-term forecast tool. While the performance of the different management areas varied, we determined that the performance of the predictive models was adequate to inform decision support tools. With both the forecast, and non-forecast models, we interpreted the variable importance scores to determine the main drivers of FC concentrations and FC forecasts across the 5 management areas in Florida. As expected, rainfall and river stage were generally among the more important variables for predicting FC concentrations. However, in the forecasted models, the importance of the variables changed due to the uncertainty of the forecasted inputs.

This thesis explored both historical trend testing and short-term forecasting of FC concentrations in coastal waters. The modeling described in this thesis will play an important role in preserving coastal resources under increasing climate stressors and supporting shellfish farmers who are maintaining sustainable food systems.

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APPENDIX

APPENDIX

A

HISTORIC TREND ANALYSIS

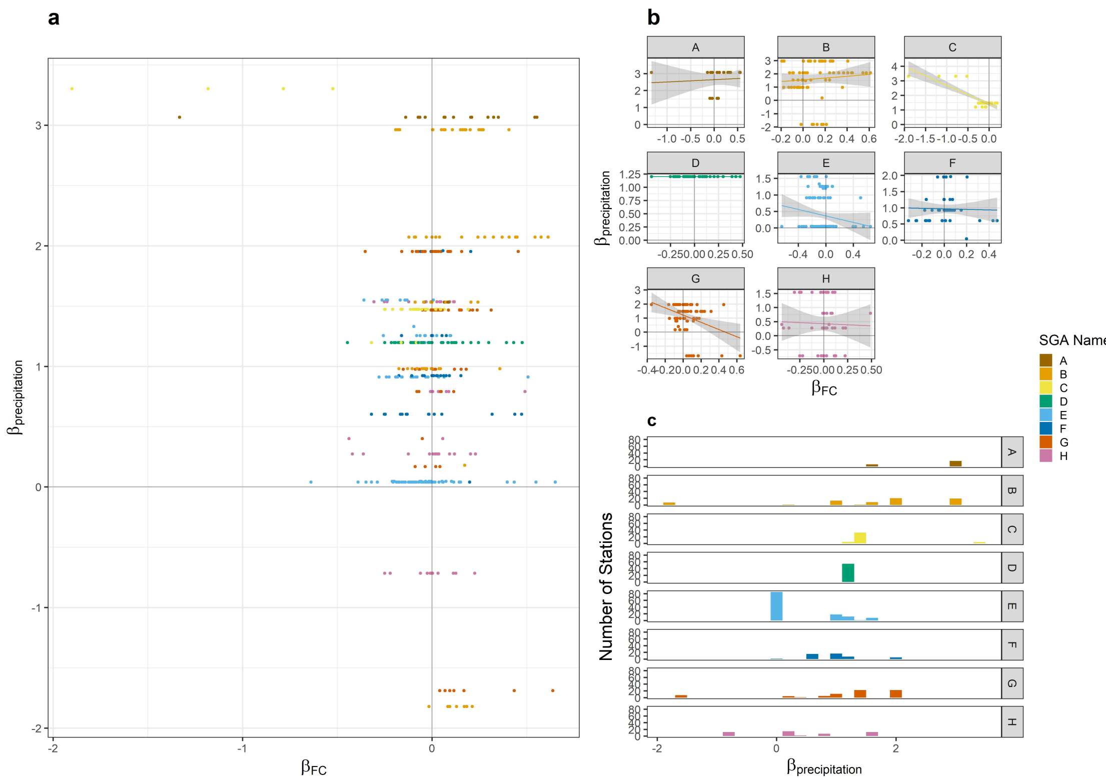

Figure A.1: Leftmost scatterplot (a) illustrates the relationships between β_{FC} and $\beta_{Precipitation}$ for each station colored by the station's associated SGA letter. The top right scatterplots (b) illustrate β_{FC} and $\beta_{Precipitation}$ for each station within the SGA. The lower right histograms (c) show the distributions of $\beta_{Precipitation}$ values broken down by SGA letter. Both (b) and (c) further demonstrate the spatial variation in precipitation trends and relationships between β_{FC} and $\beta_{Precipitation}$ across the coast.

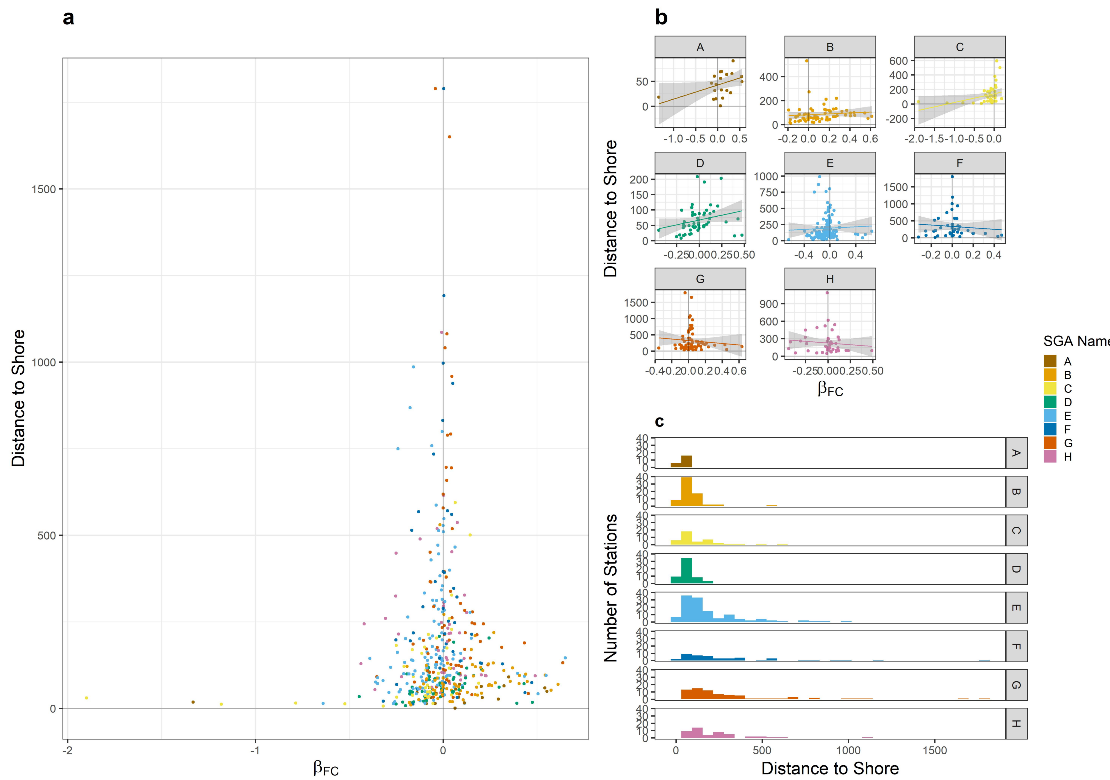

Figure A.2: Leftmost scatterplot (a) illustrates the relationships between β_{FC} and distance to shore in meters for each station colored by the station's associated SGA letter. The top right scatterplots (b) illustrate β_{FC} and distance to shore for each station within the SGA. The lower right histograms (c) show the distributions of distance to shore values broken down by SGA letter. Both (b) and (c) further demonstrate the spatial variation in distance to shore and relationships between β_{FC} and distance to shore across the coast.