Investigating the connections between the concentration-discharge, concentration-baseflow relationships of *E. coli* and watershed landscape

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Abstract:

Water quality research is crucial for safeguarding the health of both humans and ecosystems. *E. coli*, as a bacteria causing stomach cramps and diarrhea to more severe conditions, has raised significant concerns in water quality studies. Recent research highlights the relationships between concentration, discharge, and baseflow and how they correlate with attributes like catchment residence time, stream hierarchy, land covers, and so on. Landscape patterns and connectivity have reshaped natural hydrological cycles and *E. coli* biochemical processes, thereby changing the concentration-discharge (C-Q) and concentration-baseflow (C-B). However, the control mechanisms on concentration-discharge and concentration-baseflow patterns of *E. coli* are unclear, influenced by natural and anthropological factors, and the potential contrasting behaviors at low and high flow regimes. Our results illustrated that varying concentration-discharge and concentration-baseflow patterns have a particular relationship with the land use type of the site watershed.

Keywords:

Escherichia coli concentration, Concentration-Discharge relation, Baseflow, Land use, Landscape pattern.

1. Introduction:

To effectively manage water quality, it is crucial for us to understand the complex dynamics of watershed processes and the various external factors that influence water quality. Research indicates that the quality of stream water changes across different spatial and temporal dimensions, exhibiting statistically significant yet diverse relationships with prevailing flow conditions (Musolff et al., 2015; Moatar et al., 2017; Diamond & Cohen, 2018). The concentrations of water quality constituents and the relationships between concentration and flow (C-Q) are indicative of the hydrologic and biogeochemical processes within a watershed (Chorover et al., 2017; Lintern et al., 2018; Ebeling et al., 2021). These processes include the sources, storage, reactions, proximity, and transport of materials in catchments (Rose, L et al., 2018), interactions between groundwater and surface water (Kornelsen & Coulibaly, 2014; Hoagland et al., 2017; Guo et al., 2022), catchment residence time (Beven, 1987; Tetzlaff et al., 2009; Maher, 2011), and stream order (Creed et al., 2015). They also involve the properties (e.g., charge, solubility, reactivity) of individual water constituents (Moatar et al., 2017; Kaushal et al., 2018), the influence of topography (Liu et al., 2022), and the terrestrial and within-stream biogeochemical reactions (Kaushal et al., 2018; Markovic et al., 2020). Although other elements like hydrologic routing, total area, and land cover can influence C-Q relationships, their roles must be understood and exhibit significant variability (Diamond & Cohen, 2018). Additionally, establishing water quality standards for lakes, streams, rivers, and estuaries relies on comprehending contaminant loads estimated from the associations between streamflow and chemical fluxes (Diamond et al., 2018).

Concentration-discharge (C-Q) relationships often demonstrate non-linear or non-monotonic alterations in the Slope, signaling a distinct flow threshold at which the constituent under study may exhibit radically different behavior. This observation is supported by research that indicates such breakpoints (Moatar et al., 2017; Diamond & Cohen, 2018). These shifts suggest alterations in the dominant ecohydrological processes within the system (Chorover et al., 2017). Crossing these thresholds can activate additional hydrological pathways within the watershed (Diamond & Cohen, 2018) or prompt a transition from dominantly surface water to a more significant influence of groundwater (Hensley et al., 2019). Typically, negative logarithmic transformations of concentration (log(C)) against discharge (log(Q)) exhibit slopes indicative of dilution and are commonly observed with geogenic solutes. Conversely, positive slopes suggest an increase in concentration and are frequently associated with solutes linked to biological activity.

Numerous studies have investigated the connections between Concentration-Discharge (C-Q) relationships and baseflow indices on various scales (Ebeling et al., 2021; Moatar et al., 2017; Musolff et al., 2015). Research consistently shows that, within a given catchment, the dynamics of C-Q relationships—and consequently nutrient export patterns—are influenced by the proportion of streamflow that constitutes baseflow (Gorski & Zimmer, 2021; Knapp et al., 2020; Minaudo et al., 2019). Specifically, the extent of baseflow contributions can modify C-Q relationships by altering the interaction between surface water and groundwater (Minaudo et al., 2019). Additionally, baseflow fluctuations can impact nutrient removal efficiency by shifting the balance between hydrological and biogeochemical processes (Moatar et al., 2017).

The research questions of our project are analyzing the spatial distribution of the relationship between *Escherichia coli (E. coli)* concentration and discharge (C-Q) and *E. coli* concentration and baseflow (C-B) throughout the United States. Furthermore, this research examines how the spatial patterns of C-Q and C-B correlate with land cover within the HUC12 watersheds where measurements are taken. There are two significant research gaps in our fields: 1. Prior studies on the stream Concentration-Discharge (C-Q) relationships typically target short-term observations and are confined to small watershed areas (Basu et al., 2010; Godsey et al., 2009). Additionally, much of the existing research has focused on the role of baseflow in streamflow, examining the influence of the Baseflow Index on C-Q relationships within specific watersheds, predominantly in temperate climates (Guo et al., 2022). These gaps highlight the need for extended analysis across diverse climatic and geographical landscapes to better understand these ecological dynamics.

2. Methods:

2.1 The Ecoli concentration data and baseflow data:

First, our team downloaded the Discharge data from the USGS website. However, on various state websites, we obtained the *E.coli* data from many websites, including USGS, National Park Service Water Resources Division, and Environmental Management and Protection Division. In order to obtain these *E.coli* data, we used the corresponding R package to download the Ecoli data and corresponding traffic data on the website. After downloading, we found that the discharge data is suitable for USGS stations for statistics, but the Ecoli data is based on the USGS and other various measuring stations. In order to facilitate subsequent matching work, we need to combine the *E.coli* data with the discharge The data are uniformly matched so that they can all be counted at USGS stations. Therefore, we first plotted the *E.coli* and discharge measurement stations, and first completed the first part of matching by finding the closest discharge measurement station to each Ecoli measurement station within a radius of 1km in the HUC12 watershed. Then, if there are multiple measuring stations within a radius of 1km, the upstream and downstream, as well as the river map, are analyzed to find measuring stations on a river for matching. In this way, we obtained *E. coli* concentration and stream discharge in about 452 watersheds across diverse land uses in the United States. We leveraged these data with baseflow computed from discharge and other water quality indicators.

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2.2 Breakpoint and Trends Analysis:

In this step, we used the Davies Test in the Segmented Package with R studio (Muggeo, 2008) package segmented performs to estimate segmented regression models with a fixed number of breakpoints in the concentration discharge (C-Q, C-B, and C-BI) relationships. Here is the detailed workflow of the segmented package: First, the package will start with a base model, a Generalized Linear Model (GLM); GLMs are used to model relationships between a dependent variable and one or more independent variables. They are assuming that the model's parameters (like the Slope) might change at some potential breakpoint T. Second, the Maximum Likelihood Estimation (MLE) will be used to estimate the model parameter with MLE at each T point and get a set of model parameter estimates for each T point. Then, the Likelihood Ratio Statistic can compare the model parameters at each T point and determine whether the parameters have changed. The final step is significance Testing, which can obtain the p-value and ensure that we have sufficient to reject the null hypothesis at a significance level of 5%. (There is no change of the model parameters in the model)

$$\ln L_0(\theta) = -\frac{1}{2}\sum_{i=1}^{N}\left(T_i \ln(2\pi) + \ln\left|\Sigma_{0,i}\right| + \left(y_i - \beta_{0,i} - \beta_{1,i}x_i\right)' \Sigma_{0,i}{}^{-1}\left(y_i - \beta_{0,i} - \beta_{1,i}x_i\right)\right),$$

$$(\Sigma_{0,i})_{t,t} = \tau_0^2 + \sigma^2,$$
$$(\Sigma_{0,i})_{t,s} = \tau_0^2, \quad t \neq s,$$

$$\mathrm{LR}(\rho) \equiv 2\ln L\left(\hat{\theta}(\rho), \hat{\tau}_1^2(\rho), \rho\right) - 2\ln L_0\left(\hat{\theta}_0\right),$$

$$\mathrm{LR} \equiv \max_{\rho} \mathrm{LR}(\rho),$$

Equation 1: The major calculation process of segmented packages in R.

3. Results:

3.1 The matching results summary:

（1）Concentration - Discharge:

Table 1: The table of ANOVA results of climate and C-Q relationship

Have Breakpoints	11
Non-Breakpoints	87

（2）Concentration - Baseflow:

Table 2: The table of ANOVA results of climate and C-B relationship

Have Breakpoints	8
Non-Breakpoints	91

（3）Concentration - Baseflow Index:

Table 3: The table of ANOVA results of climate and C-BI(Baseflow Index) relationship

Have Breakpoints	5
Non-Breakpoints	110

We matched based on USGS's STAID, which obtained concentration and discharge data from 452 measuring stations across the United States and baseflow data from 1,000 measuring stations. According to table1-table3, we matched and obtained 99 sets of ecoli concentration-discharge data, 11 sets of data contained breakpoints, and 87 sets of measurement station data did not contain breakpoints. After matching, we obtained 99 groups of *Ecoli* concentration-baseflow data, 8 of which contained breakpoints, and the remaining 91 groups of data did not contain breakpoints. From Table 3, we can see that after matching and calculation, we obtained 115 groups of ecoli concentration-baseflow index data, of which five groups of data contain breakpoints, and the remaining 110 groups of measurement station data do not contain breakpoints.

Overall, we can see that from C-Q, C-B to C-BI, the number of measurement stations containing breakpoints decreases, and the number of measurement stations without breakpoints gradually increases, which means that the relationship between variables is more inclined to a Linear monotonic relationship.

3.2 The relationship between the climate and the C-Q and C-B relationship:

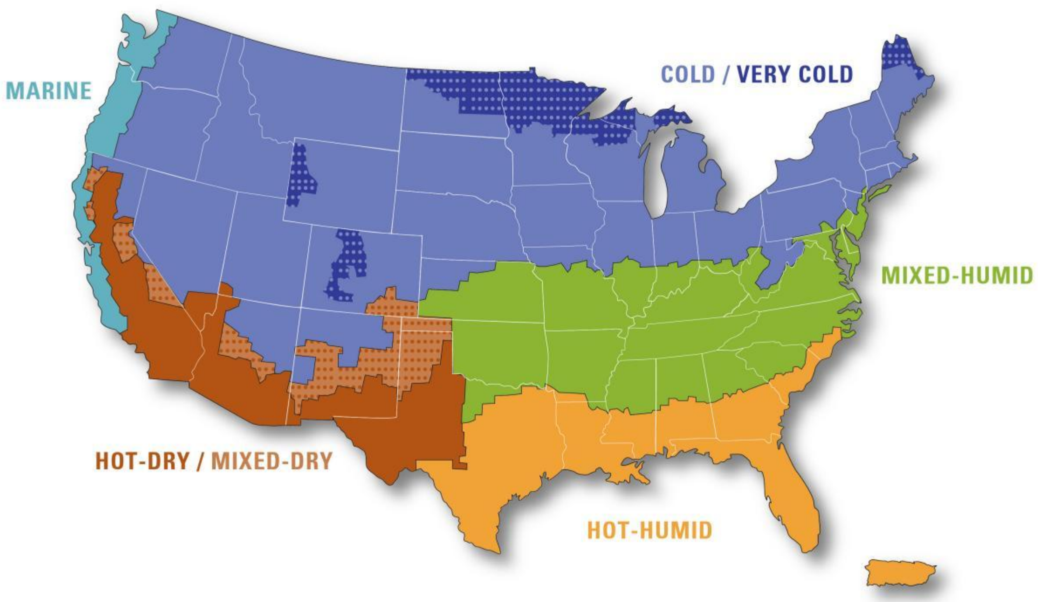

Figure 2: The climate zones of the U.S. Source: Pacific Northwest National Laboratory, PNNL, USDOE Office of Energy Efficiency and Renewable Energy, EEREk

	Df	Sum Sq	Mean Sq	F value	Pr (>F)
Climate	4	0.795	0.19879	3.672	0.00774
Residuals	103	5.575	0.05413		

Table 4: The table of ANOVA results of climate and C-Q relationship

	Df	Sum Sq	Mean Sq	F value	Pr (>F)
Climate	4	0.282	0.07044	1.302	0.274
Residuals	103	5.572	0.05410		

Table 5: The table of ANOVA results of climate and C-B relationship

After getting the matching results of C-Q and C-B, we used the seven major climatic regions in the United States to classify the current data and then conducted ANOVA analysis on the C-Q and C-B station data with climate, respectively, so that we could test the climate's spatial number of C-Q and C-B approximate distribution relationship. Based on the figure above, we can figure out that the C-Q has statistically significant evidence of a difference in means among the different climate groups. Compared with the C-Q relation, the C-B relationships don't have statistically significant evidence of a difference in means among the different climate groups.

3.3 The constant spatial distribution:

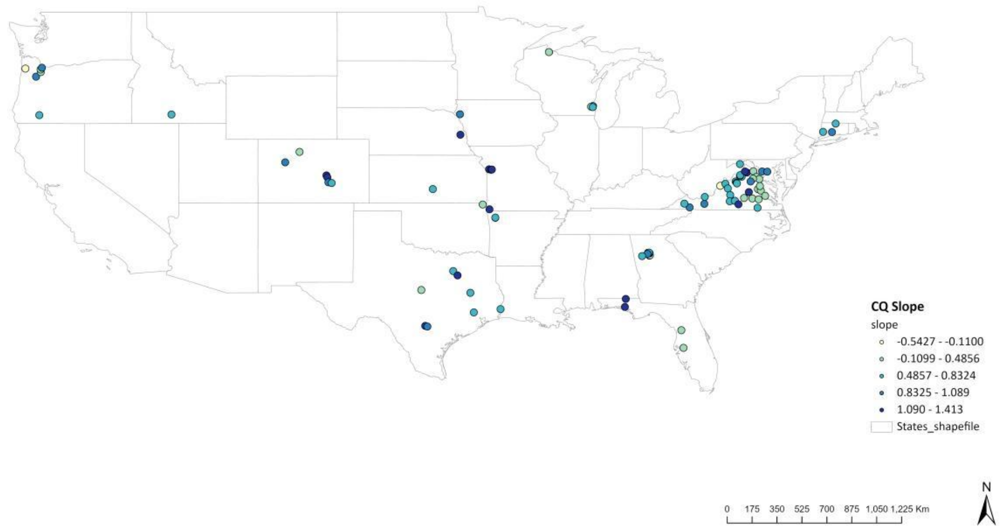

Figure 3: The layout of the Concentration-Discharge constant station distribution

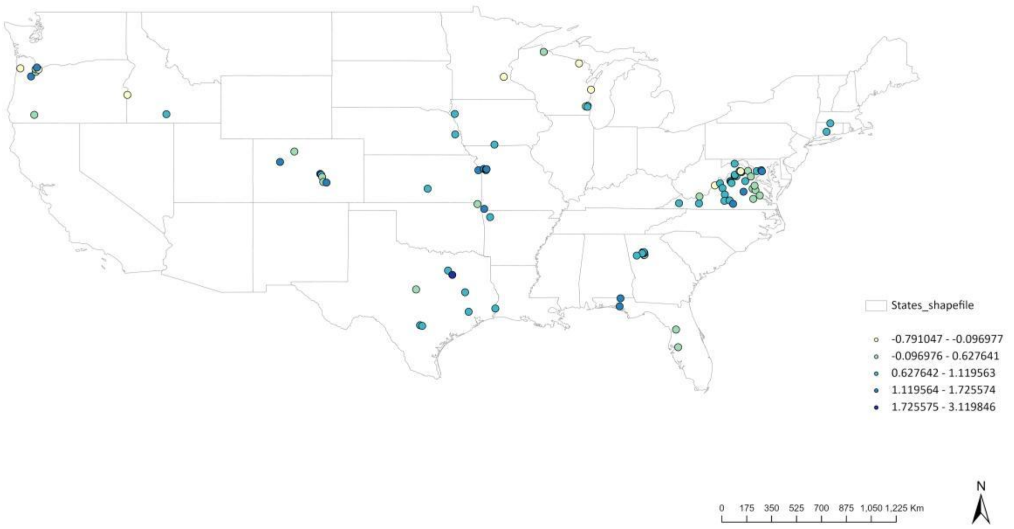

Figure 4: The layout of Concentration-Baseflow constant stations distribution

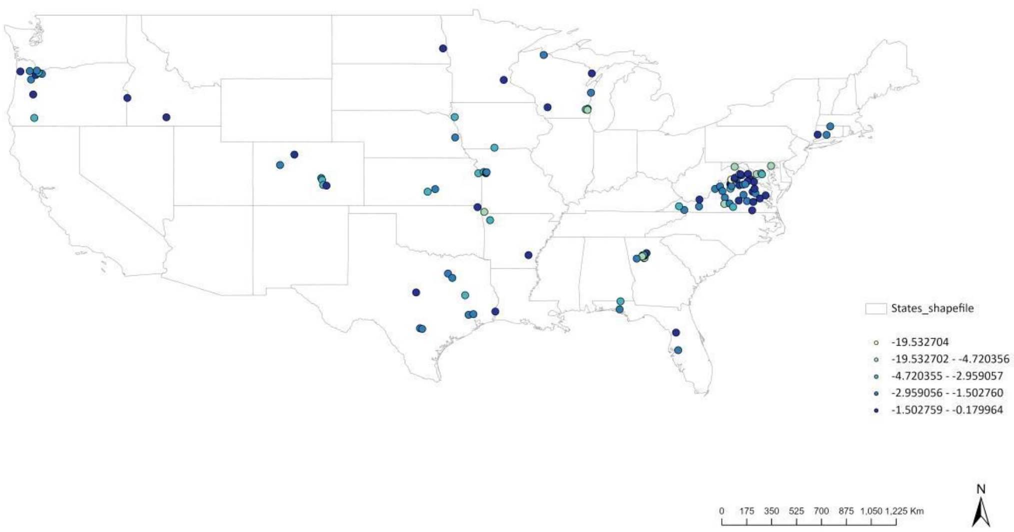

Figure 5: The layout of Concentration-Baseflow Index constant stations distribution

When classifying the results, we found that in the paired measurement station data, most of the measurement stations did not contain breakpoints. Therefore, we extracted the station data with constant Slope in the C-Q and C-B relationships as the main analysis goals. According to Figure 3, we can see that the darker the points, the higher the coefficient between C-Q. The stations along the eastern coast and the central and southern regions have a higher C-Q relationship, while those in the northwest and north have lower C-Q coefficients. The correlation is slightly lower. According to Figure 4, we can see that C-B in the northwest corner, south-central part, and southeastern part of the United States has a higher coefficient. Conversely, the correlation between C-B in the northern part of the site is lower. From Figure 5, we can see that the C-BI relationship is generally distributed evenly. The measuring stations in the central and southern parts of the site, the eastern coastal area, and the northwest corner generally have higher coefficients. On the contrary, the measuring stations in the northeastern and north-central parts of the site generally have higher coefficients. The C-BI relationship is less obvious.

When making horizontal comparisons, we found that there are specific differences in the color distribution of the three relationships. In the distribution diagram of the C-B relationship, the light color accounts for a larger proportion, which means that the C-B relationship accounts for a larger proportion at the measurement stations with weaker coefficients in the site. Many. On the contrary, the C-BI relationship has a higher proportion of dark-colored sites in the site, which means that the sites with larger C-BI account for a higher proportion, and the C-Q relationship has a color proportion in between the C-B and C-BI.

3.4 The Land cover Correlations:

Table 6: The table of Concentration-Discharge.

	A_	PERENNIAL_	DEVELOPED_	DEVELOPED1	DEVELOPE_1	DEVELOPE_2	BARREN_LAN	DECIDUOUS_	EVERGREEN_	MIXED_FORE	SHRUB_SCRU	HERBACEOUS	HAY_PASTUR	CULTIVATED	WOODY_WETL	Trend
A_	1	-0.04	0.06	0.09	0.08	0.09	-0.04	-0.04	-0.05	-0.02	-0.09	-0.08	0.02	0.09	0.03	-0.13
PERENNIAL_	-0.04	1	0.76	0.63	0.62	-0.05	-0.2	-0.21	-0.23	-0.27	-0.27	-0.32	-0.25	-0.09	-0.15	-0.13
DEVELOPED_	0.06	0.76	1	0.88	0.77	0.03	-0.35	-0.28	-0.35	-0.25	-0.19	-0.38	-0.19	-0.16	-0.04	-0.13
DEVELOPED1	0.09	0.63	0.88	1	0.92	0	-0.4	-0.24	-0.33	-0.22	-0.12	-0.41	-0.2	-0.15	0.03	-0.11
DEVELOPE_1	0.08	0.62	0.77	0.92	1	-0.02	-0.38	-0.19	-0.27	-0.2	-0.13	-0.39	-0.21	-0.18	-0.02	-0.09
DEVELOPE_2	0.09	-0.05	0.03	0	-0.02	1	-0.14	-0.03	-0.07	-0.04	-0.08	0.09	0.16	0.07	0.04	-0.06
BARREN_LAN	-0.04	-0.2	-0.35	-0.4	-0.38	-0.14	1	-0.22	0.29	-0.19	-0.29	0.21	-0.26	-0.32	-0.39	0.22
DECIDUOUS_	-0.04	-0.21	-0.28	-0.24	-0.19	-0.03	-0.22	1	0.31	0.13	-0.08	-0.24	-0.17	0.59	0	0.23
EVERGREEN_	-0.05	-0.23	-0.35	-0.33	-0.27	-0.07	0.29	0.31	1	-0.15	-0.21	-0.01	-0.23	0	-0.22	0.27
MIXED_FORE	-0.02	-0.27	-0.25	-0.22	-0.2	-0.04	-0.19	0.13	-0.15	1	0.22	-0.12	-0.09	-0.05	0.21	-0.01
SHRUB_SCRU	-0.09	-0.27	-0.19	-0.12	-0.13	-0.08	-0.29	-0.08	-0.21	0.22	1	-0.21	0.23	-0.11	0.62	-0.06
HERBACEOUS	-0.08	-0.32	-0.38	-0.41	-0.39	0.09	0.21	-0.24	-0.01	-0.12	-0.21	1	0.01	-0.16	-0.21	-0.13
HAY_PASTUR	0.02	-0.25	-0.19	-0.2	-0.21	0.16	-0.26	-0.17	-0.23	-0.09	0.23	0.01	1	0.01	0.11	-0.09
CULTIVATED	0.09	-0.09	-0.16	-0.15	-0.18	0.07	-0.32	0.59	0	-0.05	-0.11	-0.16	0.01	1	0.17	-0.09
WOODY_WETL	0.03	-0.15	-0.04	0.03	-0.02	0.04	-0.39	0	-0.22	0.21	0.62	-0.21	0.11	0.17	1	-0.1
Trend	-0.13	-0.13	-0.13	-0.11	-0.09	-0.06	0.22	0.23	0.27	-0.01	-0.06	-0.13	-0.09	-0.09	-0.1	1

Table 7: The table of Concentration-Baseflow

	A_	PERENNIAL_	DEVELOPED_	DEVELOPED1	DEVELOPE_1	DEVELOPE_2	BARREN_LAN	DECIDUOUS_	EVERGREEN_	MIXED_FORE	SHRUB_SCRU	HERBACEOUS	HAY_PASTUR	CULTIVATED	WOODY_WETL	Trend
A_	1	-0.01	0.1	0.11	0.06	0.05	-0.05	-0.08	-0.09	-0.04	-0.11	-0.07	0.03	0.06	0.07	0.14
PERENNIAL_	-0.01	1	0.77	0.65	0.63	-0.03	-0.25	-0.18	-0.26	-0.26	-0.26	-0.33	-0.27	-0.14	-0.12	-0.06
DEVELOPED_	0.1	0.77	1	0.89	0.75	0.07	-0.39	-0.23	-0.39	-0.25	-0.21	-0.38	-0.23	-0.2	0	-0.02
DEVELOPED1	0.11	0.65	0.89	1	0.91	0.03	-0.44	-0.2	-0.36	-0.22	-0.14	-0.42	-0.23	-0.17	0.05	-0.03
DEVELOPE_1	0.06	0.63	0.75	0.91	1	-0.02	-0.41	-0.15	-0.28	-0.2	-0.14	-0.41	-0.22	-0.19	0	-0.07

DEVELOPE_2	0.05	-0.03	0.07	0.03	-0.02	1	-0.15	-0.04	-0.08	-0.04	-0.08	0.12	0.11	0.04	0.01	-0.08
BARREN_LAN	-0.05	-0.25	-0.39	-0.44	-0.41	-0.15	1	-0.2	0.36	-0.17	-0.26	0.2	-0.25	-0.22	-0.37	0.11
DECIDUOUS_	-0.08	-0.18	-0.23	-0.2	-0.15	-0.04	-0.2	1	0.28	0.14	-0.07	-0.21	-0.21	0.52	0.01	0.01
EVERGREEN_	-0.09	-0.26	-0.39	-0.36	-0.28	-0.08	0.36	0.28	1	-0.13	-0.19	0.02	-0.24	0.02	-0.23	0.13
MIXED_FORE	-0.04	-0.26	-0.25	-0.22	-0.2	-0.04	-0.17	0.14	-0.13	1	0.23	-0.11	-0.1	-0.04	0.18	-0.1
SHRUB_SCRU	-0.11	-0.26	-0.21	-0.14	-0.14	-0.08	-0.26	-0.07	-0.19	0.23	1	-0.2	0.18	-0.1	0.56	-0.12
HERBACEOUS	-0.07	-0.33	-0.38	-0.42	-0.41	0.12	0.2	-0.21	0.02	-0.11	-0.2	1	0.07	-0.14	-0.2	-0.07
HAY_PASTUR	0.03	-0.27	-0.23	-0.23	-0.22	0.11	-0.25	-0.21	-0.24	-0.1	0.18	0.07	1	-0.03	0.09	0.09
CULTIVATED	0.06	-0.14	-0.2	-0.17	-0.19	0.04	-0.22	0.52	0.02	-0.04	-0.1	-0.14	-0.03	1	0.15	0.01
WOODY_WETL	0.07	-0.12	0	0.05	0	0.01	-0.37	0.01	-0.23	0.18	0.56	-0.2	0.09	0.15	1	0.12
Trend	0.14	-0.06	-0.02	-0.03	-0.07	-0.08	0.11	0.01	0.13	-0.1	-0.12	-0.07	0.09	0.01	0.12	1

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After exploring the spatial distribution relationships of C-Q, C-B, and C-BI spatial distribution in the site, we selected the C-Q and C-B relationships, extracted these measuring stations without breakpoints, and divided the HUC12 watershed. Then, the Land cover map of NLCD2021 is used to calculate the area proportions of different LandCovers in the HUC12 watershed where each site is located, and then the coefficient matrix is calculated with the status of the relevant Slope (positive, negative). According to Table 6, we can find that the Evergreen area, Deciduous planting area, and Barren landscape area have a high correlation with the C-Q relationship. From Table 7, we can find that the relationship between Land cover and C-B of Evergreen and woody wetlands shows a high correlation. In addition, from the overall effect, the coefficient between C-B and Land cover is generally smaller than the coefficient between C-Q and the proportion of Land cover in the basin.

4. Discussion & Conclusion:

4.1 The breakpoints of distribution：

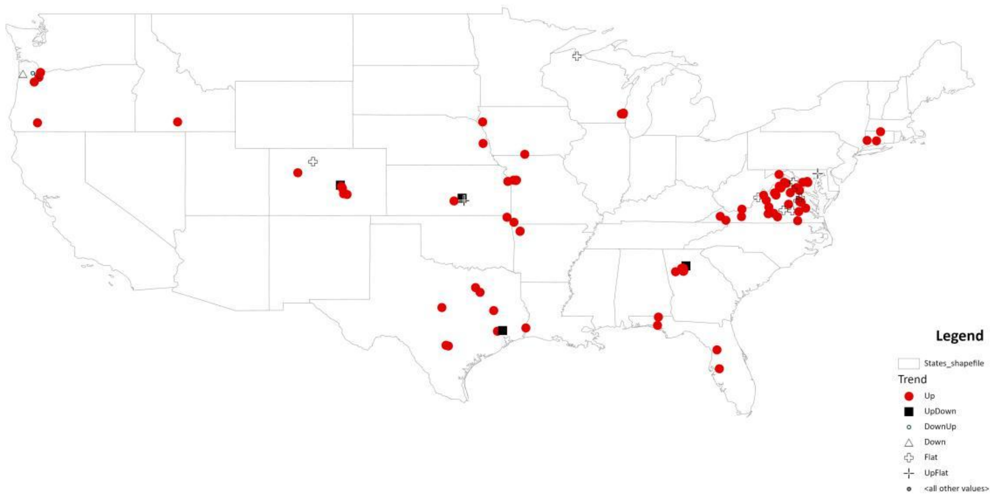

Figure 8: The layout of Concentration-Discharge stations distribution

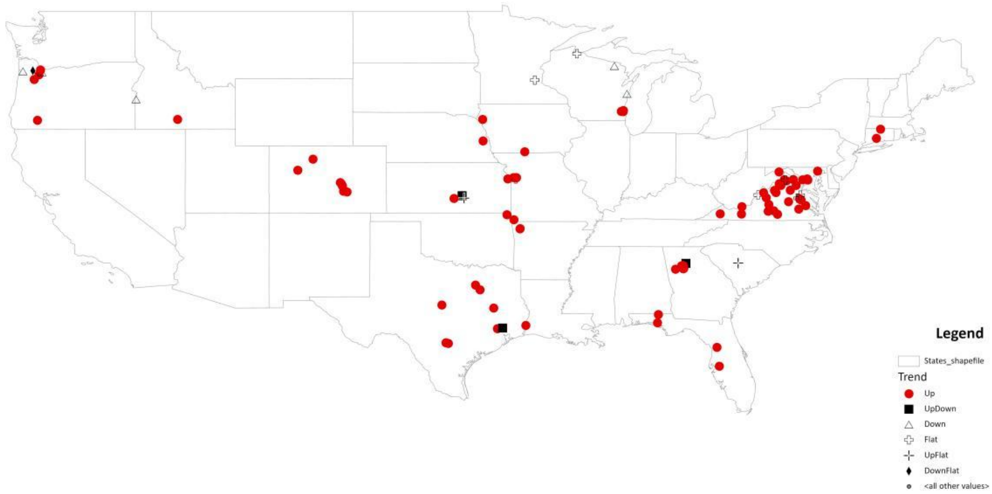

Figure 9: The layout of the Concentration-Baseflow stations distribution

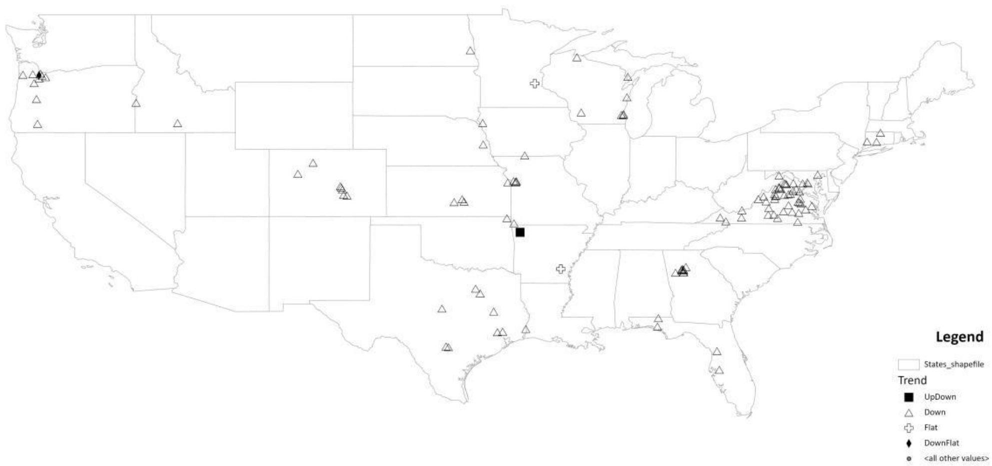

Figure 10: The layout of Concentration-Baseflow Index stations distribution

After analyzing the C-Q and C-B measurement stations without breakpoints, we added the C-Q, C-B, and C-BI measurement stations with breakpoints. In order to make shape classification more suitable for subsequent data processing, we position all slopes with an absolute value less than 0.3 as Flat. Then, plot the locations of all measuring stations. According to Figure 8, we can see that the C-Q relationship within the venue is mainly Up. Shape sites are also relatively evenly distributed in space. Flat sites are mainly distributed in the east and middle parts of the site. UpDown-shaped C-Q sites are mainly distributed in the middle of the site. The Down-shaped site is located in the northwest corner of the site. From Figure 9, we can see that the main shape of C-B in the site is also dominated by Up, which means that as Baseflow increases, the concentration of Ecoli also increases due to the cumulative effect. The Down and Flat shapes in the site are mainly concentrated in the central and northern areas. As Baseflow increases, the Ecoli concentration will be diluted or change slightly. The sites whose shape contains breakpoints are mainly concentrated in the south of the site. From Figure 10, we can see that the shape of C-BI within the production area is mainly distributed in the form of Down, which means that as the Baseflow index increases, the *Ecoli* concentration shows a downward trend. The sites containing breakpoints are mainly distributed in the southern and northwest corners of the site. Overall, there is an abnormal shape in the northwest corner of the site, which makes the shapes of C-Q, C-B, and C-BI somewhat different from those of the surrounding areas.

4.2 The Land cover results:

Figures 6 and 7 illustrate that both C-Q and C-B exhibit a significant correlation with the proportions of Evergreen, Deciduous, and Barren landscape areas in HUC12 watersheds. The relationship between C-B and Land cover is generally weaker compared to that between C-Q and LandCover, suggesting that *E. coli* concentrations are more strongly associated with agricultural areas. This indicates that agricultural activities and non-point source pollution in these areas are primary contributors to spikes in *E. coli* levels.

The analysis suggests that variations in land use and cover are key factors influencing *E. coli* concentrations in runoff, as supported by Gregory et al. (2019). The transition from natural landscapes to developed or intensively used areas typically leads to a decline in water quality, resulting in higher *E. coli* loads, as noted by multiple studies (Goto et al., 2011; Larned et al., 2004; Liang et al., 2013; Harmel et al., 2010). Both anthropogenic sources, such as wastewater, biosolids, livestock, and pets, and natural sources, including wildlife and feral animals, contribute to *E. coli* levels across different land covers (Pandey et al., 2012).

The presence of uncontrollable natural sources poses challenges to managing local *E. coli* pollution (Gregory et al., 2019). Effective management practices include delaying manure application to several days before expected rainfall to prevent runoff into water bodies, as recommended by Meals et al. (2006). Additionally, employing conservation tillage and maintaining higher vegetation on hayland at the time of application can significantly reduce microbial contamination from agricultural sources. It is also advisable to segregate crop-growing areas from livestock zones to prevent cross-contamination from pig manure. Where necessary, implementing isolated filter strips can help minimize the mutual contamination of water sources.

4.3 Conclusion:

Through this research project, we first realized that the relationship between *E.coil* concentration and Discharge distribution has a certain relationship with climate distribution. In addition, within the scope of the study, we found that the main pollution of *E. coli* is distributed in the planting area of the site; that is, non-point source pollution is the main form of *E.coli* pollution. In future research, we will introduce more soil, environmental, and agricultural variables to further study the correlation of *E. coli* contamination.

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