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Drivers of Spatiotemporal Variability in Drinking Water Quality in the United States

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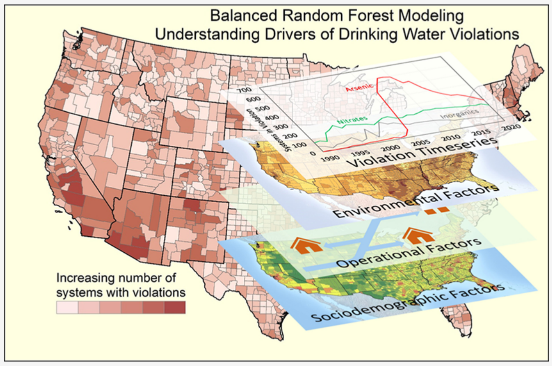

ABSTRACT: Approximately 10% of community water systems in the United States experience a health-based violation of drinking water quality; however, recently allocated funds for improving United States water infrastructure ($50 billion) provide an opportunity to address these issues. The objective of this study was to examine environmental, operational, and sociodemographic drivers of spatiotemporal variability in drinking water quality violations using geospatial analysis and data analytics. Random forest modeling was used to evaluate drivers of these violations, including environmental (e.g., landcover, climate, geology), operational (e.g., water source, system size), and sociodemographic (social vulnerability, rurality) drivers. Results of random forest modeling show that drivers of violations vary by violation type. For example, arsenic and radionuclide violations are found mostly in the Southwest and Southcentral United States related to semiarid climate, whereas disinfection byproduct rule violations are found primarily in Southcentral United States related to system operations. Health-based violations are found primarily in small systems in rural and suburban settings. Understanding the drivers of water quality violations can help develop optimal approaches for addressing these issues to increase compliance in community water systems, particularly small systems in rural areas across the United States.

KEYWORDS: *drinking water, water quality, violations, Safe Drinking Water Act, regulatory compliance, random forest modeling*

1. INTRODUCTION

Ensuring safe drinking water across public water supplies is an increasing priority in the United States and globally.[1] The majority of the United States population (≥286 million people out of a total population of 331 million [2021]) is served by community water systems (CWSs) regulated under the Safe Drinking Water Act (SDWA)[2] with an estimated 7% of systems experiencing some type of health-based (HB) violation.[3] Additionally, other studies estimate that ~40 million people rely on domestic (private) wells for drinking water with contamination reported in ~13% of these wells.[4,5] Increasing reports of drinking water contamination, particularly lead contamination (e.g., Flint, Michigan; Newark, New Jersey),[6,7] have garnered wide concern over the safety of drinking water. Waterborne disease outbreaks are also of concern with pathogens, such as Giardia, Legionella, Norovirus, Shigella, Salmonella, and Cryptosporidium, listed in the top 10 causes of outbreaks in public water systems.[8]

SDWA regulations include inorganics (16 contaminants), organics (53), radionuclides (4), disinfectant and disinfection byproducts (DBPs: 7), and microorganism categories (7) based on maximum contaminant levels (MCLs). In situations where quantifying contaminant concentrations is technically or economically infeasible, treatment techniques (TTs) are prescribed, such as the Surface Water Treatment Rules (SWTRs) and Ground Water Rule (GWR), which were designed to reduce illnesses related to pathogens in water (Supporting Information, Section 1.1). Many previous studies of US water quality have focused on specific contaminants, such as arsenic,[9−11] fluoride,[12] nitrate,[13−17] DBPs,[18] and the total coliform rule (TCR).[19] Allaire et al. (2018)[20] evaluated a range of SDWA violations but emphasized total coliform rule (TCR) violations. Many studies conducted by the United States Geological Survey focused on unregulated private domestic well water.[10] Analysis of groundwater quality by the USGS within the National Water Quality Assessment (NAWQA) program shows that more than 20% of sampled wells had at least one constituent that exceeded SDWA MCLs with the primary contaminant sources being geogenic arsenic and radionuclides.[21]

Numerous previous studies have evaluated drivers or controls on SDWA violations. Comparison of community water system (CWS) vs private well water arsenic levels shows generally good agreement with elevated arsenic in the Southwest, central

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Midwest, and Northeast United States.[22] Annual precipitation and groundwater recharge were found to be important drivers of elevated arsenic levels in the United States based on the application of machine learning approaches to private wells.[23] Another study showed that arsenic MCL (10 μg/L) violations were found mostly in the Southwest United States, primarily in groundwater systems (95%), serving small populations (mean ~1,100 people).[24] Dominant drivers of nitrate MCL (10 mg/L) violations were found to be land attributes (e.g., cropland, irrigation), N surplus inputs, and surplus precipitation based on random forest modeling.[16] DBPR violations were highest in Southcentral United States and were linked primarily to small CWSs (serving 500−3,300 people), long residence times associated with large distribution systems or storage tanks, and consecutive connections (i.e., CWS receiving some or all water from a wholesale system with purchase agreements) based on a detailed EPA study.[18] The Total Coliform Rule (TCR) violations constituted ~50% of all HB CWS violations (1991−2015).[19] However, revision of the TCR (RTCR) in 2016 greatly reduced HB violations from 32% (TCR in 2015) to 11% (RTCR violations in 2017) with most violations (ca. 83−93%) in very small systems (≤500 people).[19] A national assessment of all CWS SDWA violations shows that total CWS violations were linked to increased rurality and low-income minority populations, whereas compliance was associated with purchased water and private ownership.[20] These studies provide an indication of the wide variety of controls that can impair drinking water quality, including environmental, operational, and sociodemographic attributes.

The objective of this study was to assess the spatiotemporal variability in CWS violations and evaluate drivers of these violations considering all SDWA HB violations using data from 1990 to 2020 (Figure 1). Novel aspects of this work include the comprehensive assessment of all types of HB SDWA violations rather than individual regulations or contaminants and use of advanced data analytics and machine learning to rank potential drivers of system violations (balanced random forest modeling and Shapley analysis). A variety of drivers were considered, including environmental (e.g., climate, landcover, soil type, geology), operational (water source, CWS size and ownership, and consecutive connections), and sociodemographic (population density, social vulnerability). This work is particularly timely as the United States recently passed the Bipartisan Infrastructure Law, providing \$50 billion to improve water infrastructure over the next 5 years.[25] Implementing this law underscores the need to better understand the spatiotemporal distribution and drivers of CWS violations. Output from this analysis can help guide efforts to achieve compliance in CWSs.

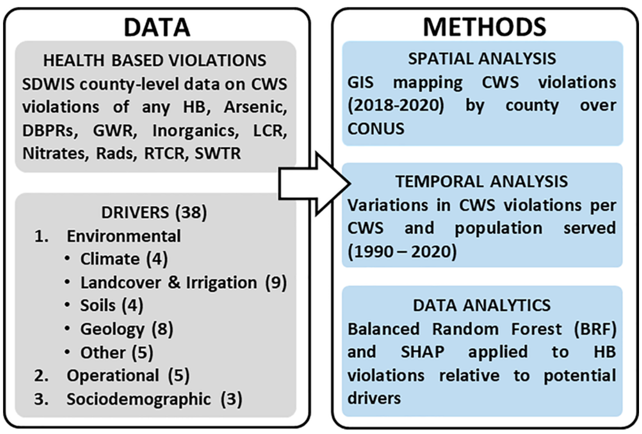

Figure 1. Flowchart describing primary data and methods applied. Safe drinking water information system (SDWIS); health-based violations (HB); disinfectant and disinfection byproducts rule (DBPR), ground water rule (GWR); lead copper rule (LCR); radionuclides (Rads); revised total coliform rule (RTCR); surface water treatment rule (SWTR); community water system (CWS); contiguous United States (CONUS); SHapley Additive exPlanations (SHAP).

2. MATERIALS AND METHODS

2.1. Data Sources. This study evaluated all SDWA violations of CWSs in the contiguous US (CONUS) that were listed active on April 15, 2021 (time of data download). Analysis focused on 48,215 CWSs, which represent 34% of PWSs (the remaining being transient and nontransient CWS) (Table S2b). This dataset shows that CWSs served ~94% of the population (~308 of 329 million, 2021) in the CONUS. This analysis examined all HB violations, excluding monitoring, reporting, and notification violations (Table S3c). The number of CWSs with HB violations was considered along with population served by CWSs.

Data on CWS attributes were mostly obtained from the Safe Drinking Water Information System (SDWIS) database, including location, State ID, ownership (private or public), number of consecutive connections, and CWS population served (Supporting Information, Section 1.2). Locations of CWSs are limited to the county level and were assigned to county centroids because data on actual CWS service area locations are only available for certain states.[26] Models of the drivers of SDWA violations considered 38 potential explanatory variables, including environmental, operational, and sociodemographic variables (Figure 1 and Supporting Information, Section 1.2). General environmental parameters (30 parameters) included parameters for climate (4), landcover and irrigation (9), soil type (4), lithology (8), and other (5). Operational parameters included 5 parameters (e.g., water source, etc). Sociodemographic factors included State ID, Social Vulnerability Index (SVI) from the Centers for Disease Control (CDC), and population density as a proxy for rurality. The explanatory variables were aggregated to the county level to compare with county-level CWS data.

2.2. Spatiotemporal Variability Analysis. Spatial variability in SDWA violations was mapped based on the population served by any CWS with HB violations at the county level under different SDWA rules using the most recent three years of data (2018−2020) (Table S2). These maps provide qualitative information on the distribution of SDWA violations. Temporal variability included SDWA violations from 1990 to 2020, considering both the number of CWS violations and also populations served (Table S8).

2.3. Balanced Random Forest Model Selection and Implementation. A variety of data analytics approaches have been applied to assess drivers or controls and predict contaminant distributions. In most analyses a binary dataset is evaluated which includes the presence/absence of SDWA violations with the majority of CWSs having no violations. Examples of previously applied approaches include logistic regression,[10,27] probit regression,[20] classification and regression tree analysis,[13] and random forest modeling.[16,28]

We tested logistic regression, probit regression,[20] random forest (RF), and balanced random forest (BRF)[16] approaches to determine the best-suited methodology for analysis of SDWA

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violations based on data from 2018 to 2020 considering any HB violation as well as specific violation types (e.g., inorganics, DPBR, etc.) (Supporting Information, Section 1.3).[29,30] BRF was selected because it performed slightly better than logistic regression, probit regression, and standard RF models as discussed in Section 3.3. In addition, BRF can also deal with colinear explanatory variables.[31] The BRF model used in this study was implemented in Python using the Balanced Random Forest Classifier (Supporting Information, Section 1.2). The BRF binary classification approach was used to relate the presence/absence of SDWA violations to various potential explanatory variables, including environmental, operational, sociodemographic variables (Supporting Information, Section 1.2). BRF was applied to 80% of the data, termed training data, and results were applied to the unbalanced 20% holdout test data to assess model performance. Metrics considered to assess the relative performance of the different models include percentage correctly classified (PCC), percentage with violations (sensitivity, true positives), percentage without violations (specificity, true negatives), and area under the receiver operating characteristic curve (AUC).[32] Values of 1.0 for PCC, true positives, true negatives, and AUC indicate a perfect model. Partial dependence plots were used to assess the directions and magnitudes of linkages between predictors and response variables (SDWA violations).

Once the BRF classifier was built, output from BRF was used with SHapley Additive exPlanations (SHAP) to assess the contribution of explanatory variables on the predicted probability of a CWS having a violation or not.[33] SHAP is based on the Shapley value, defined in cooperative game theory as the average marginal contribution of one player across all possible combinations of other players.[33,34] The advantages of SHAP relative to BRF variable importance metrics include the fact that SHAP is model agnostic and offers a better measure of variable importance that is consistent and locally accurate,[35,36] allowing us to investigate the modeled impact of each variable on violation incidence. SHAP values represent the change in probability beyond 0.5 associated with each explanatory variable or driver. In other words, the SHAP value represents the absolute change in probability attributed to each explanatory variable. Model output data, including the testing datasets, variable importance rankings, and selected partial dependence plots, can be found in Tables S10−S20.

3. RESULTS AND DISCUSSION

3.1. Spatial Variability in System Violations. Incidences of HB violations were found throughout much of the Southwestern, Southcentral, and Northeastern United States based on recent data on CWS populations served (2018−2020) (Figure 2). California ranked number 1 in terms of population served by CWSs with any HB violation, followed by Texas, and Pennsylvania (Figure S3b). EPA also lists “Serious Violators” referring to systems with unresolved serious, multiple, and/or continuing violations. Results for 2018−2020 indicate that Texas had the highest number of serious violators (616 CWSs out of ∼3,600 in the United States), ∼3× greater than the number in Louisiana which ranked second (Table S5).

DBPR violations comprised the largest percent of any HB violation, both in terms of the number of CWSs with DBPR violations (41%) and population served (39%; 2018−2020 data; Figure S2, Table S3c). DBPR violations occurred mostly in Southcentral United States, extending to the Northeast but also including Florida (Figure 3a). This is consistent with previous

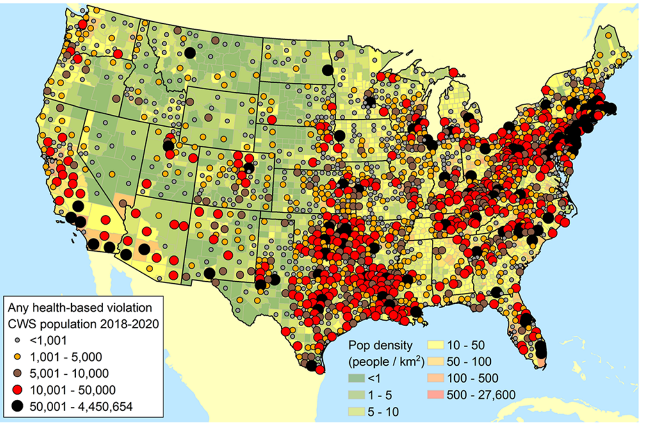

Figure 2. Spatial variability in any health-based community water system (CWS) violation (2018−2020) overlain on county-level population densities. Circles of different colors represent populations served by noncompliant CWSs at the county level. Data are provided in Table S6.

findings showing that the Southcentral United States to mid-Atlantic states have the highest DBPR violation rates.[18]

Spatial variability in any inorganic (combined arsenic, nitrate, and inorganics rules) and radionuclide rule violations generally reflect naturally occurring (geogenic) contamination of groundwater found in the Southwest and Southcentral United States (Figure S5 and S8). California and Texas ranked highest in terms of the number of CWSs with any inorganic violation (Figure S3e). Populations impacted by violations of arsenic, nitrate, and radionuclides show similar spatial patterns to the general distribution of any inorganic violation (Figures 3b,c, S5, and S8). Arsenic and radionuclides are naturally occurring contaminants derived from geogenic sources, whereas nitrate is primarily derived from agricultural activities[21] as further described in Section 3.3.

Revised total coliform rule (RTCR) violations were highest in Arizona and dispersed throughout counties in Nevada, New Mexico, and Texas with large populations impacted in the Northeast (Figure S9). Violations related to SWTRs were focused in the Northeast (e.g., West Virginia and Pennsylvania) and in Southcentral United States (e.g., Oklahoma and Texas), with the highest populations impacted in the Northeast (Figures S10 and S11). GWR violations were concentrated in individual states with the largest number of violations and populations served in Louisiana, followed by Pennsylvania (Figures S3q,r and S12). Populations served by CWSs violating the Lead and Copper Rule (LCR) were primarily located in the Northeast, Great Lakes region, and Southcentral United States (East Texas and Louisiana) (Figure 3d). LCR system violations ranked highest in Texas, followed by Louisiana and Illinois in terms of the number of violating systems and populations served (Figure S3s,t). Organic violations were limited to isolated urban locations scattered in the Northeast and Southeast (Figure S13).

3.2. Temporal Trends. HB violations varied markedly over time in response to regulatory changes, with spikes in the number of violating systems occurring in response to different regulatory changes: LCR in 1994, DBPR Stage 1 in 2005 and Stage 2 in 2015, and arsenic rule in 2006 (Figure 4). Enforcement of the more stringent arsenic rule (MCL reduction from 50 to 10 μg/L) resulted in CWS violations increasing from ∼70 in 2005 to ∼470 in 2006, peaking at ∼600 in 2008−2009 and gradually declining to 226 CWSs in 2020 (Figures 4, S6a,b,

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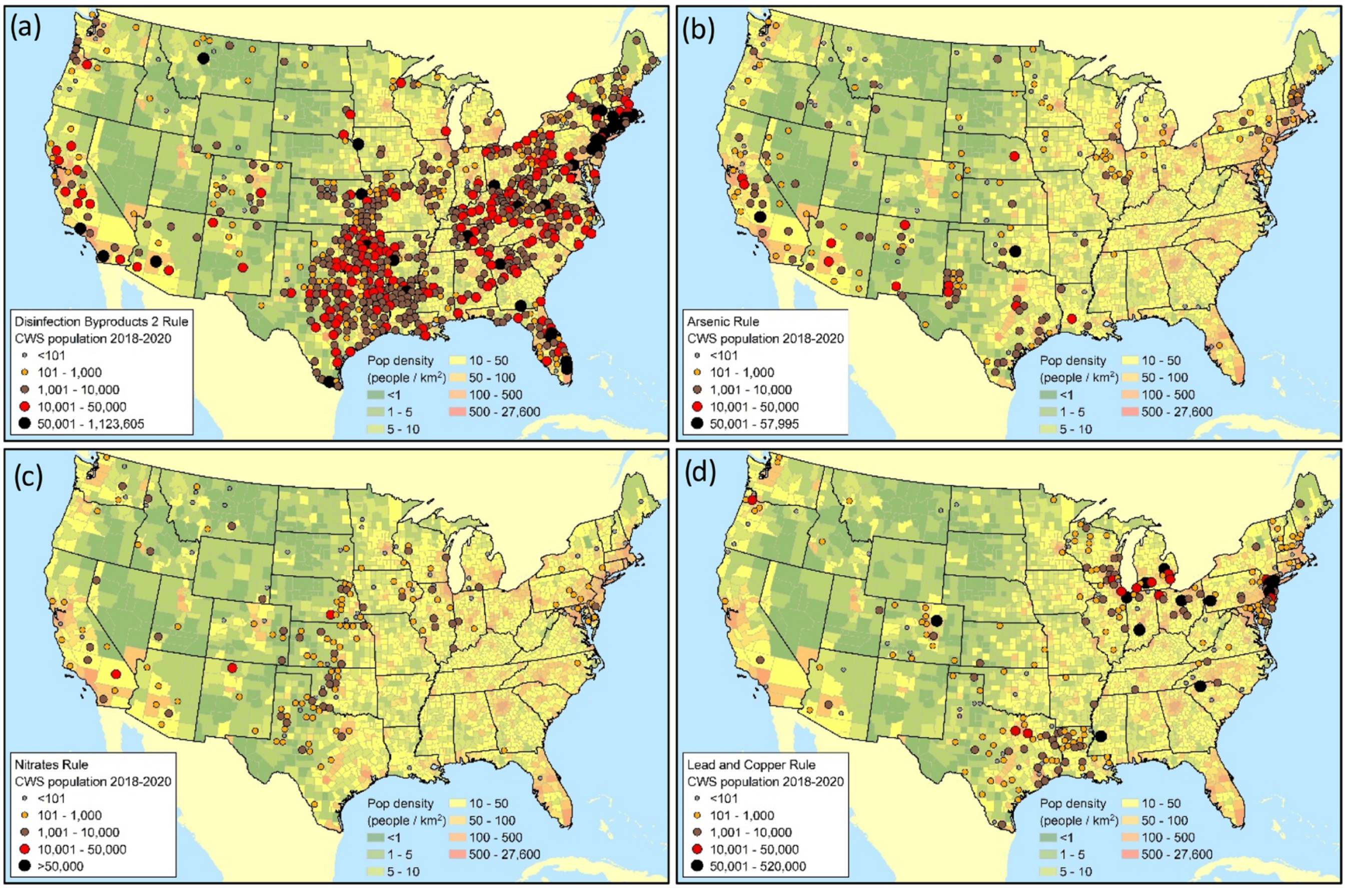

Figure 3. Maps of health-based violations based on 2018−2020 SDWIS data overlain on county-level population densities for (a) disinfectant and disinfection byproducts rule (DBPR) stage 2 violations, (b) arsenic rule violations, (c) nitrates rule violations, and (d) lead and copper rule violations. Circles represent county-level populations served by noncompliant systems. Data are provided in Table S6.

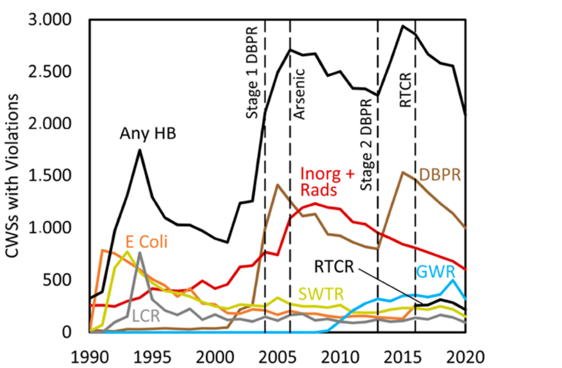

Figure 4. Time series of community water system health-based violations grouped into any health-based (HB) violation, disinfectant and disinfection byproducts rule (DBPR), any inorganic and radionuclides (combined arsenic, nitrate, inorganics, and radionuclides rules), *Escherichia coli* and revised total coliform rule (RTCR) after 2015, surface water treatment rule (SWTR), ground water rule (GWR), and lead copper rule (LCR). Dates of rule revisions are shown for arsenic in 2006, stage 1 DBPR in 2004, stage 2 DBPR in 2012 and RTCR in 2016. CWS peaks in violations are related to LCR in 1994 (∼760 CWSs violating), DBPR stage 1 in 2005 (∼1,400 CWSs), DBPR state 2 in 2015 (∼1,300 CWSs), and arsenic rule in 2006 (∼600 CWSs). More detailed time series are provided in Figure S15. Data are provided in Table S8.

and S15b). The decline in arsenic violations has been attributed to increases in CWS treatment and decreases in arsenic releases to the environment from chemical and hazardous waste sectors.[11] While time series of HB violations generally reveal a rapid decline in violations after rules were enforced, some rules, most notably nitrate, have relatively stable violations since the mid-1990s (Figures S7a,b and S15b). The largest impact of regulatory change can be seen in the RTCR with the number of TCR violations peaking at ∼3,800 in 1993 and declining from ∼1,800 systems in 2015 to ∼240 in 2016 with the implementation of the RTCR in 2016 (Figure S15d).

Time series of populations served by CWSs in violation show the predominance of SWTRs because surface water-sourced systems are much larger than groundwater-sourced systems (Figure S16). The spikiness in impacted populations reflects large systems going in and out of compliance. Populations served were also highly impacted by DBPR regulations with peaks in 2003 and 2015 (Figure S16a) which, similarly, are attributed to changes in compliance status of large surface water-sourced systems.

3.3. Drivers of Spatiotemporal Variability in System Violations.

3.3.1. Balanced Random Forest Model Performance and Data Limitations. Data analytics revealed that BRF performed better than unbalanced random forest, logistic regression, and probit regression, as indicated by higher values of AUC, sensitivity, and selectivity for models of the incidence of any HB violation against an unseen imbalanced dataset (Table S9d). BRF models of specific rule violations (e.g., arsenic, DBPR, nitrate) show a reasonable classification power (AUCs ∼0.80s) given the limitations associated with spatially aggregated, county-level data assigned to CWSs (Table 1). The classification model for any HB violation (Figure 5a) had among the lowest AUC values (0.67) compared to models of specific types of rule violations (Tables 1 and S9). In general, provided there is sufficient violation data, higher AUC values were attained for models of violations focused on specific contaminants or rules (e.g., arsenic, nitrate, DBPR, GWR) compared to violation categories that lumped together multiple contaminants (e.g., any HB violation) (Table 1). This reflects the relatively lower classification power when lumping together various contaminants and treatment requirements due to the varying importance of different drivers on specific water quality processes. For example, geogenic contaminants are mobilized to groundwater under certain geochemical conditions while DBPs result from disinfection processes.

Table 1. Performance of Balanced Random Forest for SDWA Rules[a]

	holdout dataset			full dataset		
rule	no. of viol.	PCC	AUC	no. of viol	PCC	AUC
any HB	1,035	66	0.67	5,041	72	0.81
arsenic	90	79	0.80	500	80	0.88
DBPRs	359	78	0.82	1,882	77	0.86
GWR	231	82	0.82	1,046	82	0.89
inorganics	16	82	0.66	86	82	0.88
LCR	61	73	0.77	343	72	0.84
nitrates	55	79	0.79	308	80	0.88
rads	67	78	0.71	335	78	0.86
RTCR	161	66	0.69	730	67	0.80
SWTR	104	79	0.76	486	79	0.87

[a]No. of viol.: number of health-based (HB) violations; percent correctly classified (PCC); area under receiver operating curve (AUC); disinfectant and disinfection byproducts rule (DBPRs); ground water ruleb (GWR); lead and copper rule (LCR); radionuclides (Rads); revised total coliform rule (RTCR); surface water treatment rules (SWTR).

This study relies heavily on the SDWIS data; however, there are limitations to these data, including potential under-representation of violations due to monitoring and reporting violations[15,37] which may disproportionately impact very small and small CWSs that are often characterized by under-regulation and high SDWIS violations.[38,39] This is particularly problematic given that the majority of CWSs experiencing HB violations are in very small (≤500) and small (501−3,300) systems in mostly rural and suburban regions (Figure 6). Additionally, due to poor reporting of treatment data and a lack of raw source water quality data, our analysis is not able to distinguish whether a lack of violations reflects the absence of a contaminant exceeding an MCL in the water source or the result of contaminant removal via treatment. Many CWS violations, with some exceptions (e.g., DBPR), require water source contamination as a necessary, but not sufficient, condition for a violation. DBPR violations reflect treatment conditions, whereas LCR violations primarily result from distribution system issues.

3.3.2. Disinfectant and Disinfection Byproducts Rule. DBPR violations are linked primarily with Stage 2 DBPRs, accounting for 84% of CWSs with DBPR violations (Figures 3a and S4a,b). Analyses of DBPR violations indicate that

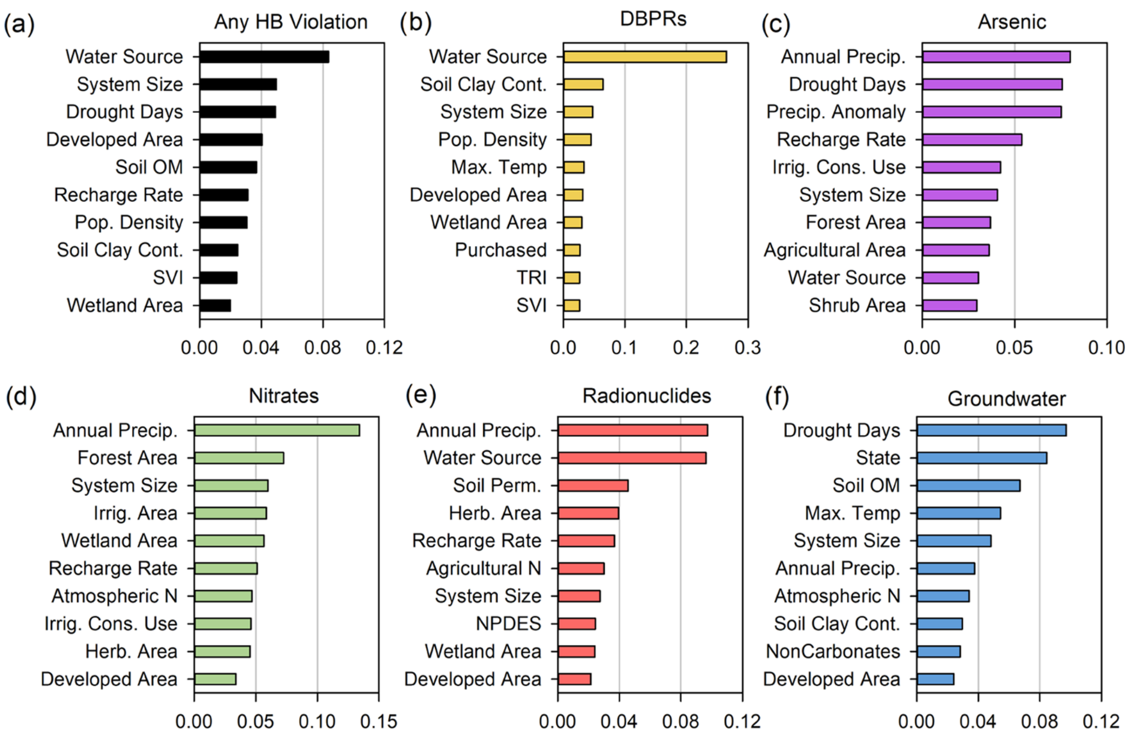

Figure 5. SHAP values showing top 10 drivers of (a) any health-based (HB) violation, (b) disinfectant and disinfection byproducts rule (DBPRs), (c) arsenic, (d) nitrates, (e) radionuclides, and (f) ground water rule (GWR). SHAP values for other regulations are shown in Figure S18. The drivers are shown in the *y* axis. The drivers are described in Supporting Information, Section 1.2. Acronyms: irrigation (Irrig); consumptive (Cons); content (Cont); precipitation (precip); herbaceous (Herb), organic matter (OM); Nitrogen (N); Pop. Density, population density; social vulnerability index (SVI); toxics release inventory (TRI); permeability (Perm); national pollutions discharge elimination systems (NPDES). Data are provided in Tables S10−S13, S15, and S18.

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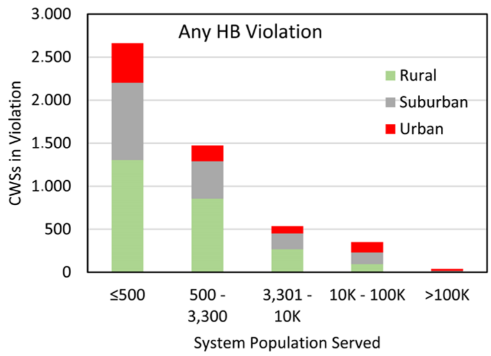

Figure 6. Number of community water systems (CWSs) with any health-based (HB) violation relative to the population served by the CWS for rural, suburban, and urban counties. Data and similar plots for all regulations, including number of CWSs and populations served, are provided in Figure S6.

operational and environmental drivers had the highest impact on the likelihood of a violation with water source ranked highest followed by soil clay content, system size, population density, and maximum temperature (Figures 5b and S18b). Most CWSs with DBPR violations were based on surface water sources (67% of CWSs and 82% of population served, Table S6c) although Pennsylvania requires disinfection of all groundwater systems.[40] Water source, system size, and population density as drivers of DBPR violations reflect the predominance of DBPR violations in very small to small systems, sourced by surface water, and serving mostly rural and suburban populations (Figure S17c). The importance of clay content on DBPR violations could be attributed to the influence of adsorption capacity of catchment soil type on dissolved organic carbon (DOC) concentrations in surface water[41] because DOC is necessary for DBP formation during disinfection. Alternatively, the high rank of soil clay content in the SHAP analysis may be an artifact of the spatial clustering of DBPR violations in Southcentral United States where regional clay content is high. Several Southcentral states have higher residual chlorine requirements due to elevated temperatures in the region. While the majority of states have requirements no more stringent than the federal standard (0.2 mg/L free chlorine), Louisiana requires 0.5−1.0 mg/L (depending on pH) and Oklahoma requires 1.0 mg/L (Table S22).[42,43] About half of the CWSs with DBPR violations were consecutive connections with almost 3 times higher violation rates in consecutive versus nonconsecutive systems (7.3 vs 2.6%) (Table S6d), consistent with recent EPA findings.[18] Additional factors impacting DBPR violations include longer disinfection residence time and limited ability to control treatment processes managed by wholesalers.[18]

3.3.3. Arsenic. Arsenic violations are primarily driven by environmental factors including annual precipitation, number of drought days, precipitation anomalies, effective recharge rates, and irrigation water withdrawal (Figure 5c). The ranking of SHAP values is consistent with previous studies which determined that precipitation and recharge have the strongest influence on arsenic concentrations in groundwater.[10] This leads to elevated arsenic in the arid and semiarid Southwest and Southcentral United States attributed to crystalline and volcanic source rocks, low recharge in arid climates, and long groundwater residence times.[10,21] Specifically, climate and recharge influence hydrogeochemical processes controlling the mobilization of geogenic arsenic, including evaporative concentration, increasing pH, increasing total dissolved solids along flow paths, and shifts in redox conditions.[10,44−46] Additionally, prolonged drought can increase the probability of arsenic concentrations in groundwater exceeding the 10 μg/L MCL[23] which is consistent with the relatively high ranking of the number of drought days (Figure 5c). Drought-induced increases in arsenic concentrations have been attributed to lowering water tables promoting initial oxidation of arsenic-bearing sulfide minerals[47] and subsequent recharge events reducing and releasing dissolved arsenic.[48] Arsenic concentrations increased in response to land subsidence attributed to aquifer over-pumping during dry periods in the San Joaquin Valley, California.[49] This mechanism of arsenic release from clay layer porewater by land subsidence may partially explain the importance of irrigation water withdrawal as a driver of arsenic violations. Given the strong association between CWS arsenic violations and private well concentrations,[22] the drivers identified in this analysis likely also exert control on arsenic exposure from private wells. Inorganics rule violations exhibited similar variable rankings to arsenic violations with annual precipitation, number of drought days, and effective recharge having the highest SHAP values (Figure S18d).

3.3.4. Nitrate. Nitrate violations had higher SHAP values for environmental features including annual precipitation, landcover, and irrigated area (Figure 5d) relative to other contaminants which captures the relationship with agricultural sources (Figure 5d). Additionally, the size of the CWS was the third highest ranking driver reflecting the predominance of nitrate issues in very small (≤500 people served) water systems.[15] The spatial distribution of nitrate contamination (Figure 3c) may reflect variations in nitrate contamination in the water source or variations in nitrate treatment. Higher incidences of nitrate violations were found in California, Texas, the Midwest, and North Atlantic and are consistent with previous findings.[15,16] Geographic trends in nitrate violations are driven by high N input (fertilizer and/or animal waste) and hydrogeologic conditions that promote transport and limit denitrification, including unconfined aquifers, shallow groundwater, well-drained and permeable soils, and patterns in irrigation and precipitation.[15] The lack of nitrate violations in much of the Southeast United States (Louisiana, Mississippi, Alabama) is surprising given the high fertilizer input in the Mississippi River Basin and has generally been attributed to high denitrification rates.[13] In addition, recent work has shown decreasing trends in total N flux rates in watersheds in the Lower Mississippi River Valley.[50] To further assess these findings, we examined SDWIS treatment data to explain the distribution of nitrate contamination. Treatment for iron and manganese removal is much more widespread in the Midwest and Southeast United States than inorganics removal that could include nitrate, suggesting anoxic conditions and denitrification in the water source (Table S23). For example, reported numbers of CWSs with treatment for removal of iron and manganese in the Midwest exceed reported inorganics removal category in the SDWIS database by factors of 5× (Ohio), 8× (Indiana), 12× (Illinois), 18× (Iowa), and in the Southeast (9×, Arkansas; 11×, Missouri, 69×, Mississippi) (Table S23). The high level of iron and manganese treatment suggests either (1) nitrate input to the system likely denitrified under these reducing conditions or (2) deeper GW is being used which is often associated with reducing environments.

3.3.5. Radionuclides. The importance of environmental drivers (annual precipitation, soil permeability, landcover) (Figure 5e) on radionuclide violations reflects the prevalence

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of these violations in the Southwest and Southcentral United States (Figure S8), similar to the spatial distribution of arsenic violations. Water source is a key driver as groundwater sources accounted for ≥95% of CWSs with radionuclide violations (Table S6c). Agricultural nitrogen inputs ranked fifth in SHAP value which is likely attributed to mechanisms of geogenic uranium mobilization in agricultural areas. Specifically, uranium mobilization is known to occur in aquifers in California's Central Valley, Texas Gulf Coast, and High Plains and is attributed to elevated nitrate and carbonate concentrations which promote oxidation of uraninite and subsequent formation of dissolved uranyl-calcium-carbonato species.[51−53] Unlike other SDWA rule violations analyzed in this study, radionuclides are impacted by the density of National Pollution Discharge Elimination System (NPDES) sites, which suggests a linkage with anthropogenic sources of radionuclides (e.g., radium or uranium from mining-influenced waters).

3.3.6. Treatment Technique Rules. State identification (ID) ranks in the top ten drivers (second for GWR and tenth for SWTR) for these rule violations and is evident in the maps with high violations restricted to specific states (Figures 5f and S20c). State ranking of incidences of GWR violations include Louisiana, followed by Pennsylvania and New Mexico (Figure S3q). In accordance with the GWR, state-specific definitions of significant deficiencies in groundwater systems account for variations across states. For example, GWR violations in New Mexico and Louisiana likely depend on state-specific definitions of treatment 'deficiencies' and resources available to address deficiencies prior to incurring a violation. Similarly, unlike other states, Pennsylvania requires 4 log virus removal of all CWSs, including groundwater systems;[40] the high incidence of GWR violations in the state is likely attributed to the more stringent disinfection requirements.[54]

Notably, the number of drought days has the largest impact on GWR violations (Figure 5f). One possible explanation is the increased use of groundwater during drought periods which could result in an increase in groundwater-sourced systems in violation. RTCR violations are more prevalent in groundwater systems (83% of systems, 2018−2020 data (Table S6)) with Pennsylvania having the highest number of violations (Table S7b).

3.4. Implications for Achieving Compliance of Community Water Systems. The comprehensive assessment of HB violations in this study provides valuable insights for optimizing infrastructure investments in the United States considering the proposed marked increases in infrastructure funding ($50 billion). To effectively achieve compliance in CWSs, infrastructure investments will need to consider spatiotemporal distribution of various SDWA rule violations across the United States and the underlying drivers of each type of rule violation. This is particularly important given the difference in underlying drivers and potential trade-offs associated with addressing specific types of rule violations. For example, remedying high RTCR violations by requiring increased disinfection or higher residual chlorine concentrations may decrease RTCR violations at the expense of increasing DBPR violations.

Additionally, to achieve long-term compliance, infrastructure investments must account for future environmental stressors rather than relying solely on historic observations of climate conditions. Notably, the incidence of many SDWA violations evaluated in this study may be vulnerable to climate change as seen by the importance of precipitation, drought, and temperature variables on arsenic, nitrate, DBPR, GWR, radionuclides, and inorganics violations. For example, increasing ambient temperatures cause faster chlorine decay, subsequently requiring a higher chlorine dosage to achieve free chlorine residual targets and potentially increasing DBP formation.[55] Similarly, prolonged droughts may accelerate degradation of groundwater quality by nitrate[56] and increase arsenic and GWR violations (Figure 5). Recent studies have highlighted the importance of other climate hazards that threaten water quality including post-wildfire increases in hexavalent chromium concentrations in soils,[57] and volatile and semivolatile organic compounds (VOCs and SVOCs),[58] and arsenic, nitrate, and DBPs in public drinking water systems.[59]

Infrastructure investments must also consider potential impacts of future regulatory changes to anticipate which systems are most vulnerable to changes in compliance status. Regulatory changes rapidly shift the distribution of drinking water quality violations over time. For example, more stringent arsenic regulations greatly increased system violations in the mid-2000s. In contrast, TCR violations dominated HB violations until 2016 when the implementation of the revised TCR (RTCR) caused a substantial reduction in violations. However, these regulatory changes can disproportionately impact socially vulnerable communities. For example, while very small water systems had the greatest number and severity of TCR violations, the RTCR amplified this disparity despite the fact that the overall number of violations decreased.[19] Similarly, development of more protective standards and associated increases in treatment technology can exacerbate issues of affordability as indicated by an increase in household cost of water for small systems before and after the revised arsenic rule[60] and the negative relationship between median household income and compliance with the arsenic rule.[61] Future compliance issues will likely be shaped by new regulatory decisions on emerging contaminants, such as per- and poly-fluoroalkyl substances (PFAS). While many of these regulatory decisions occur at the federal level, state-specific practices in implementing rules and providing resources to address violations can markedly impact compliance, as seen in the spatial distribution of GWR violations (Figure S3q and Section 3.3.6).

Understanding drivers of spatiotemporal variability in violations allows for targeted investments in infrastructure. Upgrading aging drinking water infrastructure for underserved communities and rural areas provides an opportunity to address issues of persistent violations and prevent future noncompliance. Future investments in treatment systems may involve purchasing systems with higher capital costs if they have lower maintenance issues or require less technical oversight. Additionally, smart water technologies have the potential to provide real-time data and enhance water quality monitoring.[62] Many CWSs with HB violations, particularly inorganic and radionuclide violations, occur in very small and small CWSs, which can face increased challenges in applying for assistance. Infrastructure funds should extend beyond initial capital costs for purchasing treatment systems and also finance operational costs of maintaining treatment systems and building local technical and managerial capacity. As an example, California's recent Safe and Affordable Funding for Equity and Resilience (SAFER) program provides $130 million per year until 2030 to address gaps and provide solutions for water systems, particularly in disadvantaged communities. SAFER uses short- and long-term models, which emphasize the need to quickly

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provide an interim source of safe, reliable drinking water while developing long-term, sustained solutions.

Ultimately, designing interventions will require rigorous system-specific evaluations and the comprehensive, large-scale analysis presented in this work highlights overarching trends in violations to guide more refined analyses.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.est.1c08697.

All data and scripts used in the model validation and balanced random forest modeling analysis, detailed information on regulatory background, timeline of regulatory changes, data definitions and sources, and detailed information on data analytics methodology, list of acronyms, breakdown of CWS violations by type, state rankings for highest violations for each rule, bubble maps of United States for violations of DBPR, any inorganic, arsenic rule, nitrates, radionuclides, RTCR, SWTR, long-term enhanced 1 SWTR, long-term enhanced 2 SWTR, GWR, LCR, time series for each rule violation, bar plots of each rule violation by system size, and bar plots of SHAP values for each rule violation (PDF)

Supporting Information Data Tables (XLSX)

SDWIS All Systems HB Violations 2018-2020 (XLSX)

Model Code (ZIP)

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Notes

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