Assessing the Effect of Changing Ambient Air Temperature on Water Temperature and Quality in Drinking Water Distribution Systems

Supplemental Material

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Section A. Ambient air temperature observations and projections

The ambient air temperature observations and projections utilized in this work include the city-level historical observations compiled in Lai and Dzombak (2019) and location-specific temperature projections using an integrative technique with the autoregressive integrated moving average (ARIMA) model and global climate model (GCM) simulations (i.e., G-ARIMA model) developed in Lai and Dzombak (2021). General background information about the historical observations and projections is provided in this section. Further details and descriptions about the observations and the projections can also be found in previous work (Lai and Dzombak 2019, 2020, 2021). Alternatively, it is possible to apply downscaled GCM projections (e.g., Mearns et al. 2017; Pierce et al. 2014) for assessing future temperature changes. While some background information about the GCM projections is provided in this section, downscaled climate model projections and use of other regional climate projections were not applied in this work as the main focus was to assess the effect of air temperature change on water temperature and water quality in drinking water distribution systems (DWDS).

A-1. Historical ambient air temperature records

The historical air temperature records employed for the analyses in this work were obtained from Lai and Dzombak (2019), where long-term historical city-level observations starting as early as 1870s were compiled for 93 U.S. cities, including Washington, D.C., from U.S. federal agency sources. Two cities (Kansas City, MO and Marquette, MI) were removed the analyses because of weather station changes during critical periods of assessment for the particular analyses conducted, as will be further discussed. The compiled historical records for the cities were produced by combining records from local weather stations in each city based on the criteria

described in Owen et al. (2006), as cities can have multiple weather stations with different spatial locations during their historical periods of record [discussions about the limitations of such compilation are provided in Lai and Dzombak (2019)]. The original historical data used in the compiled point observations were from the Global Historical Climatology Network-daily database (GHCN-D; Menne et al. 2012).

The list of the 93 U.S. cities is provided in Table S1. These 93 cities were selected based on the length of existing temperature records, i.e., a data record starting earlier than 1900 and the percentage of years with missing values (a year was considered as "missing" if more than 10 daily data for that year are missing) during the period of record is below 5%.

Table S1. List of the U.S. cities used for the analyses. The IDs belong to the current weather stations for the individual cities and were assigned by GHCN.

#	Name	GHCN ID	Latitude	Longitude	#	Name	GHCN ID	Latitude	Longitude
1	Abilene	USW00013962	32.4106	-99.6822	48	Lander	USW00024021	42.8153	-108.7261
2	Albany	USW00014735	42.7431	-73.8092	49	Lansing	USW00014836	42.7803	-84.5789
3	Albuquerque	USW00023050	35.0419	-106.6156	50	Los Angeles	USW00093134	34.0511	-118.2353
4	Amarillo	USW00023047	35.2333	-101.7089	51	Louisville	USW00093821	38.1811	-85.7392
5	Atlanta GA	USW00013874	33.63	-84.4417	52	Lynchburg	USW00013733	37.3208	-79.2067
6	Augusta	USW00003820	33.3644	-81.9633	53	Madison	USW00014837	43.1406	-89.3453
7	Baltimore	USW00093721	39.1836	-76.6542	54	Marquette	USW00094850	46.5311	-87.5483
8	Bismarck	USW00024011	46.7708	-100.7603	55	Memphis	USW00013893	35.0564	-89.9864
9	Boise	USW00024131	43.5667	-116.2406	56	Meridian	USW00013865	32.3347	-88.7442
10	Boston	USW00014739	42.3606	-71.0106	57	Middletown	USW00014711	40.1936	-76.7633
11	Cedar Rapids	USW00014990	41.8833	-91.7167		Harrisburg			
12	Charlotte	USW00013881	35.2236	-80.9553	58	Milwaukee	USW00014839	42.955	-87.9044
13	Chattanooga	USW00013882	35.0311	-85.2014	59	Minneapolis	USW00014922	44.8831	-93.2289
14	Cheyenne	USW00024018	41.1519	-104.8061	60	Mobile	USW00013838	30.6264	-88.0681
15	Chicago	USW00094846	41.995	-87.9336	61	Moline	USW00014923	41.4653	-90.5233
16	Colorado Springs	USW00093037	38.81	-104.6883	62	Montgomery	USW00013895	32.2997	-86.4075
17	Columbia SC	USW00013883	33.9486	-81.1186	63	Nashville	USW00013897	36.1189	-86.6892
18	Columbus OH	USW00014821	39.9914	-82.8808	64	New York	USW00094728	40.7789	-73.9692
19	Concord	USW00014745	43.1953	-71.5011	65	Norfolk VA	USW00013737	36.9033	-76.1922
20	Concordia	USW00013984	39.5514	-97.6508	66	North Platte	USW00024023	41.1214	-100.6694
21	Corpus Christi	USW00012924	27.8	-97.4	67	Oklahoma City	USW00013967	35.3889	-97.6006
22	Dallas Fort Worth	USW00003927	32.8978	-97.0189	68	Omaha	USW00014942	41.3103	-95.8992
23	Denver	USW00003017	39.8328	-104.6575	69	Pensacola	USW00013899	30.4781	-87.1869
24	Des Moines	USW00014933	41.5339	-93.6531	70	Philadelphia	USW00013739	39.8683	-75.2311
25	Detroit	USW00094847	42.2314	-83.3308	71	Phoenix	USW00023183	33.4278	-112.0039
26	Dodge City	USW00013985	37.7608	-99.9683	72	Pittsburgh	USW00094823	40.4847	-80.2144
27	Dubuque	USW00094908	42.3978	-90.7036	73	Portland ME	USW00014764	43.6497	-70.3003
28	Duluth	USW00014913	46.8369	-92.2097	74	Raleigh	USW00013722	35.8922	-78.7819
29	Eau Claire	USW00014991	44.8664	-91.4878	75	Rochester NY	USW00014768	43.1167	-77.6767
30	Erie	USW00014860	42.08	-80.1825	76	Roswell	USW00023009	33.3075	-104.5083

#	Name	GHCN ID	Latitude	Longitude	#	Name	GHCN ID	Latitude	Longitude
31	Eureka	USW00024213	40.8097	-124.1603	77	Sacramento	USW00023271	38.5553	-121.4183
32	Evansville	USW00093817	38.0442	-87.5206	78	Salt Lake City	USW00024127	40.7781	-111.9694
33	Fargo	USW00014914	46.9253	-96.8111	79	San Antonio	USW00012921	29.5442	-98.4839
34	Flagstaff	USW00003103	35.1442	-111.6664	80	Sault Ste Marie	USW00014847	46.4794	-84.3572
35	Fort Smith	USW00013964	35.3331	-94.3625	81	Savannah	USW00003822	32.13	-81.21
36	Fresno	USW00093193	36.78	-119.7194	82	Seattle	USW00024233	47.4444	-122.3139
37	Grand Junction	USW00023066	39.1342	-108.54	83	Shreveport	USW00013957	32.4506	-93.8411
38	Grand Rapids	USW00094860	42.8939	-85.5447	84	Sioux Falls	USW00014944	43.5878	-96.7289
39	Green Bay	USW00014898	44.4983	-88.1111	85	Spokane	USW00024157	47.6217	-117.5281
40	Havre	USW00094012	48.5428	-109.7633	86	Springfield IL	USW00093822	39.8447	-89.6839
41	Helena	USW00024144	46.6056	-111.9636	87	Springfield MO	USW00013995	37.2353	-93.4003
42	Houston	USW00012960	29.98	-95.36	88	Tampa	USW00012842	27.9619	-82.5403
43	Huron	USW00014936	44.3981	-98.2231	89	Topeka	USW00013996	39.0725	-95.6261
44	Indianapolis	USW00093819	39.7075	-86.2803	90	Valentine	USW00024032	42.8783	-100.55
45	Jacksonville	USW00013889	30.4844	-81.7019	91	Washington D.C.	USW00013743	38.8483	-77.0342
46	Kansas City	USW00003947	39.2972	-94.7306	92	Williston	USW00094014	48.1739	-103.6367
47	La Crosse	USW00014920	43.8789	-91.2528	93	Winnemucca	USW00024128	40.9017	-117.8081

After preliminary analyses, two cities (Kansas City, MO and Marquette, MI) were removed from the results presented in Figures 4 and 7 in the main text (consequently, 91 cities were included in the analyses), because of the compilation of the records for the two cities. For many of the 93 cities listed in Table S1, the records were compiled from different weather stations (Lai and Dzombak 2021) and the most recent, active weather stations for the cities were relocated to the local airports in the 1940s. The analyses comparing the 1951-1970 and 2001-2020 level are therefore not affected by the station changes. However, the two cities (Kansas City, MO and Marquette, MI) had their stations changed in the 1970s, which leads to a sudden apparent decrease of temperature in the 1970s (because the weather stations were moved to less urban locations), causing the temperature estimates of the 2001-2020 level to be lower than the 1951-1970 level. These two cities were therefore removed from the analysis results presented in the main text to avoid confusion.

A-2. The location-specific temperature projections using the G-ARIMA model

The G-ARIMA model is an integrative technique to provide location-specific temperature and precipitation projections for the studied cities. The G-ARIMA model (Lai and Dzombak 2021) combines the ARIMA model and the results from the GCMs, which are the physics-based climate simulation models that integrate relevant physical processes such as energy balance considerations and atmospheric circulations (Eyring et al. 2016; Taylor et al. 2012). The ARIMA model is a common time series forecasting technique that can be used to produce forecasts based on past observations (Box and Jenkins 1970; Montgomery et al. 2016). The ARIMA model can be directly used to obtain near-term forecasts for the studied cities and the ARIMA-based city-level statistical air temperature forecasts were produced by fitting and forecasting the city-level historical temperature observation series (Lai and Dzombak 2020). While the ARIMA model is a statistical forecasting technique and is consequently limited by a near-term forecasting period (mainly 2-20 years), the G-ARIMA model provides an option of incorporating the GCM-projected climate change signal to the ARIMA model in order to facilitate regional temperature and precipitation projections (Lai and Dzombak 2021). The G-ARIMA model was developed as an alternative approach to acquire regional climate projections relative to the use of downscaled GCM projections (Lai and Dzombak 2021) and provides an alternative option to bring climate model projection results to the regional observation level. Further technical details and performance assessment for the ARIMA and the G-ARIMA models are provided in Lai and Dzombak (2020) and Lai and Dzombak (2021).

The G-ARIMA daily model, similar to the ARIMA daily model developed in Lai and Dzombak (2020), was used to acquire statistical city-level temperature simulations for the projected period 2051-2070. Historical observations up to the end of 2020 were used to fit the G-ARIMA daily

model and 50 sets of daily temperature projections were produced up to 2070. Median values were calculated among the 50 sets of daily temperature simulations for the period 2051-2070 to provide point forecasts (as average projection values) of ambient air temperature for estimating future water temperature in the 91 cities.

A-3. Alternatives for acquiring future air temperature – downscaled GCM projections

Although not applied in this work, it is worth noting that a common approach to obtain regional air temperature projections is to use GCMs and downscaling approaches for translating global projections to regional or city levels. The results of GCMs can be downscaled to regional scale with various downscaling methods, e.g., using the localized constructed analogs method or the LOCA projection (Pierce et al. 2014). The LOCA projections have been recommended for acquiring station-level projections (Kilgore et al. 2019) and have been utilized in the fourth National Climate Assessment report (USGCRP 2017). While it is informative and important to use other regional air temperature projections to assess future air temperature changes (and subsequent water temperature and water quality changes) in addition to the G-ARIMA projections, such work was not carried out, as the focus of this study was to evaluate the general effect of air temperature changes on water temperature and water quality in DWDS (instead of assessing the variations in future air temperature). The G-ARIMA projections were used because they were provided by fitting and projecting the utilized historical city-level observations and consequently better align with the historical observations.

A-4. Interpretation of ambient air temperature observations and projections

The spatial distribution of the estimated water temperature in Figure 4 of the main text and the estimated historical and future changes in water temperature and water quality parameters in

Figures 4 and 7 of the main text generally reflect the results of the air temperature observations and the G-ARIMA projections. As also discussed in the main text, the consistency between air temperature and water temperature is because that the estimated changes (in terms of changes on an annual average basis) in water temperature of DWDS are equal to the changes in air temperature based on the National Renewable Energy Laboratory (NREL) water temperature estimation model. In addition to the discussions presented for the results of estimated changes in water temperature and water quality parameters in Figures 4 and 7 of the main text, some further discussion of the utilized historical observations and G-ARIMA projections (including their limitations) are provided in this section.

Among the 91 assessed cities, some cities, in contrast to many other cities, exhibit relatively stationary or slightly decreasing water temperature and consequent small changes in water quality parameters) between the two historical levels as presented Figures 4 and 7 of the main text. Such results are related to the location-specific historical air temperature changes at the assessed individual cities and possibly limitations of the observation data. As discussed in Lai and Dzombak (2019), although air temperature exhibits overall increases for many cities in the U.S., some cities exhibit relatively stationary or slightly decreasing historical temperature records, e.g., see part (b) of Figure 4 in the main text. As discussed previously, weather station changes for the assessed cities can affect the results as well. Although many cities have changed their local weather stations around 1940s and the results in the analyses conducted here were thus not affected by the station changes, interpretation of the results presented in the Figures 4 and 7 of the main text for specific cities is subject to some limitations and uncertainties. As the goal of these analyses was to provide an overview of changes at different geographical areas and

climate conditions as mentioned in the main text, additional and more detailed analyses are need
to evaluate particular cities.

The G-ARIMA model provided temperature projections based on the compiled city-level
historical observations and GCM-projected trend and is therefore subject to the limitations of the
GCMs as well. Specifically, the G-ARIMA model can provide projections with substantial
uncertainty, as the GCM climate change signal can exhibit a different historical trend from the
city-level historical observations (Lai and Dzombak 2021). While an overview of possible future
projected changes across the different regions and cities are presented in Figures 4 and 7 of the
main text, evaluation of the specific cities is subject to limitations and uncertainties. Further
detailed analyses including the validation using the local water temperature measurements are
needed to evaluate particular locations presented in Figures 4 and 7 of the main text.

Although not assessed and presented in this work, the G-ARIMA projections for the period
2051-2070 would likely trend lower than the climate projections from the GCMs (e.g., the
LOCA projections as described previously). As recent historical observations exhibit a limited
increasing trend during the period 1998-2012 (Flato et al. 2014) and some cities may exhibit a
less increasing or possibly decreasing trend for the recent records, the G-ARIMA model can
adjust and reduce the GCM-projected future trend based on the recent historical trend exhibited
in the city-level observations (Lai and Dzombak 2021). The GCMs, on the other hand, generally
provide higher-than-observed temperature projections for the period 1998-2012 (Flato et al.
2014) and thus the use of these climate model projections are subject to limitations as well. To be
consistent with the use of the city-level observation data, the G-ARIMA projections were used to
provide future air temperature estimation instead of using the downscaled climate model
projections.

Section B. Estimating drinking water temperature

As described and presented in Table 1 of the main text, the NREL model (Hendron and Engebrecht 2010) was utilized in this work to estimate the water temperature in drinking water distribution systems (DWDS). The NREL model of daily water temperature estimation is provided as (Burch and Christensen 2007; Hendron and Engebrecht 2010):

$$T_{mains,day\#} = T_{amb,avg} + \Delta T_{offset} + \Delta T_{main} \cdot sin\left(\frac{2\pi}{365}(day\# - 15 - lag) - \frac{1}{2}\pi\right) \qquad (S1)$$

where $T_{mains,day\#}$ is the daily water temperature estimate (ºC) in the distribution system (note that the original model is in ºF); $T_{amb,avg}$ is the annual average air temperature (ºC) at the location; ΔT_{offset} is an offset value to adjust annual average air temperature (also typically used for soil temperature estimation and given as 6ºF or 3.33ºC in this case by Hendron and Engebrecht 2010); the combination of $T_{amb,avg}$ and ΔT_{offset} can be regarded as an estimate of surface soil temperature; ΔT_{main} is the adjustment of water temperature in the drinking water distribution mains considering buried depths of pipelines; and the sinusoid term in Eq.(S1) is used for generating the observed sinusoid shape of daily temperature which is typically used for estimating soil temperature.

Soil temperature is different at different depths and, as distribution mains have to be buried below frost lines (Rajani et al. 2012), the buried depths of drinking water pipelines are different across different locations. The NREL model utilizes the annual average air temperature at a particular location as a surrogate for the buried depth of the water mains at the location (e.g., the lower the annual average temperature, the colder the climate, and the deeper the buried depth). Thus, the NREL model replaces the soil depth parameter in a typical soil temperature equation with an input of annual average air temperature (Burch and Christensen 2007). The annual

average temperature is compared to a reference temperature of 44 ºF or 6.67 ºC, and thus for the ΔT_{main} and lag terms are calculated as:

$$\Delta T_{main} = [k_1 + k_2(T_{amb,avg}^{hist} - 6.67\ ^\circ C)]\frac{\Delta T_{amb,max}}{2}$$

$$lag = k_3 - k_4(T(F)_{amb,avg}^{hist} - 6.67\ ^\circ C) \qquad\qquad (S2)$$

where $T_{amb,avg}^{hist}$ is the fixed historical annual average temperature of the region (ºC), $\Delta T_{amb,max}$ is annual maximum difference in monthly average temperature (ºC; calculated as the highest monthly average temperature minus the lowest monthly average temperature), and the four coefficients k_1, k_2, k_3, and k_4 are given as 0.4, 0.01, 35, and -1.0, respectively (Burch and Christensen 2007). Because the annual average air temperature is used in the NREL model rather than the buried depths of water mains, and buried depths for an existing system do not change, the long-term historical air temperature records (from the start of record to 2020) were used to estimate the fixed historical annual average temperature values $T_{amb,avg}^{hist}$.

During the calibration of water temperature for the seven locations (see Figure 2 of the main text), the four coefficients k_1, k_2, k_3, and k_4 and ΔT_{offset} values were adjusted using a relatively simple numeric optimization algorithm [the Broyden–Fletcher–Goldfarb–Shanno algorithm (Nocedal and Wright 2006); by minimizing the root mean square errors] to provide better estimation of DWDS water temperature. After calibration, the four coefficients k_1, k_2, k_3, k_4 and ΔT_{offset} values are 0.4, 0.032, 35, -1.7, and 3.4, respectively, for the analyses of the Washington D.C. DWDS. The root mean square errors were calculated as the errors between the monthly or weekly water temperature measurements and the corresponded monthly or weekly average water temperature estimates.

The local weather stations used for the ambient air temperatures to obtain water temperature estimates at the 12 residential sites from Abrams and Shedd (1996) are listed in Table S2. The site IDs are consistent to the original IDs used in Abrams and Shedd (1996).

Table S2. The list of the 12 residential sites with water temperature measurements obtained from Abrams and Shedd (1996) and the corresponding weather stations used for air temperature records to obtain water temperature estimates.

Sites	Locations	Site ID in Abrams and Shedd (1996)	State	GHCN ID	Latitude of the weather station	longitude of the weather station	Weather station
Hartford CT	Hartford	A1	CT	USW00014740	41.9381	-72.6825	HARTFORD BRADLEY INTL AP
Tulsa OK (Site 1)	Tulsa	L1	OK	USW00013968	36.1994	-95.8872	TULSA INTL AP
New Britain CT	New Britain	L2	CT	USW00014740	41.9381	-72.6825	HARTFORD BRADLEY INTL AP
Kennesaw GA	Kennesaw	S1	GA	USC00092485	33.9881	-84.7475	DALLAS 7 NE
Ellettsville IN	Ellettsville	S3	IN	USC00120784	39.1742	-86.5214	BLOOMINGTON INDIANA UNIV
Piedmon OK	Piedmon	S4	OK	USW00013967	35.3889	-97.6006	OKLAHOMA CITY WILL ROGERS AP
Tulsa OK (Site 2)	Tulsa	S5	OK	USW00013968	36.1994	-95.8872	TULSA INTL AP
Broken Arrow OK	Broken Arrow	S6	OK	USW00013968	36.1994	-95.8872	TULSA INTL AP
Tulsa OK (Site 3)	Tulsa	S7	OK	USW00013968	36.1994	-95.8872	TULSA INTL AP
Tulsa OK (Site 4)	Tulsa	S8	OK	USW00013968	36.1994	-95.8872	TULSA INTL AP
Texarkana AR	Texarkana	S9	AR	USW00013977	33.4536	-94.0075	TEXARKANA WEBB FLD
Middletown CT	Middletown	S13	CT	USW00014740	41.9381	-72.6825	HARTFORD BRADLEY INTL AP

Section C. Estimating temperature-related drinking water quality parameters

Estimation of historical and projected changes in the three temperature-related water quality parameters was based on the equations listed in Table 1 of the main text. Additional background information and details about the individual water quality parameters are discussed in this section. It should be noted that the methods for calculating the water quality parameters depend on different studies and both kinetic and empirical predictive models have been used for different parameters. The utilized models in this work for estimating chlorine decay, TTHM formation, and bacterial activity were selected based on their general applicability for multiple locations. Considering that the TTHM estimation model is an empirical predictive model and the estimated parameter coefficients are likely location-specific (in this case for Washington D.C.), the analyses with the 91 cities thus did not include assessment of the TTHM concentrations as also described in the main text.

C-1. Estimating chlorine bulk decay rate

Chlorine decay in DWDS is typically modeled as the addition of bulk decay and decay on the pipe wall, as also described in previous work such as Rossman et al. (1994). A commonly utilized modeling approach for chlorine bulk decay rate is a first-order decay model, while second-order models (Brown et al. 2011) and other work (Fisher et al. 2011) provide alternatives. Chlorine bulk decay rate can be correlated with initial chlorine concentrations, total organic carbon (TOC), and water temperature, and these parameters have been used in the literature (sometimes not all of them were included for a particular study) for the estimation of bulk decay rate (Brown et al. 2011). The temperature effect on bulk decay rate was assessed in this work. While the decay on the pipe wall can be affected by water temperature [with respect to biofilm

activity (Fisher et al. 2017)], such a temperature effect was not explicitly assessed because DWDS-specific information is needed.

A typical expression for a first-order bulk decay model was utilized in this work, involving the use of TOC and water temperature information (Arevalo 2007; Powell et al. 2000). The expression for the bulk decay rate and chlorine residual (the chlorine decay on the wall is not considered in this case) are:

$$C_t = C_0 \cdot e^{-k_b t}$$

$$k_b = F \cdot TOC \cdot e^{-\frac{E}{R(T+273)}} \qquad (S3)$$

where C_t is the chlorine concentration at time t or chlorine residual (mg/L), C_0 is the initial chlorine concentration (mg/L), k_b is the first-order bulk decay rate (in units such as hr^{-1} or day^{-1}), F is a frequency factor, E is the activation energy, R is the ideal gas constant [F and E/R values were estimated as 1.8×10^6 L/mg·hr and 6050°C from a study of different utilities conducted by American Water Works Association (Arevalo 2007; Powell et al. 2000; Vasconcelos et al. 1996)], and T is water temperature (°C).

In addition to the use of Eq.(S3) for assessing chlorine residual when measurements for other parameters are available, the effect of temperature on bulk decay rate in Eq.(S3) follows the Arrhenius equation and the rate of chlorine bulk decay change for two different temperatures can be related [if TOC concentration stays at the same in Eq.(S3)] by:

$$ln \left(\frac{k_{b,T2}}{k_{b,T1}}\right) = \frac{E}{R} \left(\frac{1}{T_1+273} - \frac{1}{T_2+273}\right) \qquad (S4)$$

where $k_{b,T1}$ and $k_{b,T2}$ are bulk decay rates at temperature T_1 and T_2.

For the estimation of chlorine residuals in Washington D.C., Eq.(S3) was used with the available monthly measurements of TOC concentrations. Only bulk decay was considered for estimating the chlorine residuals. The analyses of changes in chlorine bulk decay rates with water temperature estimates for the 91 cities were based on Eq.(S4), in order to assess directly the temperature effect on the chlorine bulk decay rates.

C-2. Estimating TTHM formation

A substantial number of studies have assessed and provided predictive models for disinfection byproduct (DBP) concentrations such as total trihalomethanes (TTHM) (Ged et al. 2015) and research is still on-going for improving the predictive capability of these models. Many empirical predictive regression models have been developed to provide quantitative estimates of TTHM (Brown et al. 2011), although these models are subject to some challenges (Chowdhury et al. 2009). In general, TTHM formation is determined by factors including chlorine dosage, temperature, reaction time (water age) in treatment processes and distribution networks, organic content (typically using surrogate parameters like TOC and ultraviolet absorbance UV_{254}), pH, and bromide concentrations in the water source (Brown et al. 2010). Due to the availability of monthly measurements of water quality parameters from the Washington D.C. Aqueduct (USACE 2019), the following empirical predictive model was utilized for predicting TTHM concentrations in the treated water for the two treatment plants of Washington D.C.:

$$TTHM = k \cdot C_0^a \cdot T^b \cdot TOC^c \cdot pH^d \cdot Br^e \qquad (S5)$$

where C_0 is the chlorine concentration in finished water; T is the temperature of the treated water; TOC, pH, and Br (bromide concentration) are measurements for the water source; and a-e and k are reaction constants determined by model fitting of measurements.

Eq.(S5) was then utilized by fitting the monthly measurements of chlorine concentrations in the treated water, as well as TOC, pH, and bromide concentrations of the water source to predict the TTHM concentrations in the treated water. The values of a to e and k for the analyses of Washington D.C. DWDS are: 0.64, 0.76, 0.85, 1.30, 1.89, and 0.027, respectively. Water temperature observations and water temperature estimates were used to provide a separate prediction, as described in main text.

If other parameters stay the same and reaction constant b is known, it is also possible to derive Eq.(S5) to estimate the effect of temperature on TTHM:

$$ ln\left(\frac{TTHM_{T2}}{TTHM_{T1}}\right) = b \cdot ln\left(\frac{T_2}{T_1}\right) \qquad (S6) $$

The reaction constant b is potentially system specific and varies among reported studies (Brown et al. 2011; Chowdhury et al. 2009). An evaluation of different existing predictive models for TTHM with a common TTHM dataset by Ged et al. (2015) suggested a value of 0.48 for b from one of the most accurate TTHM models. In comparison, the values of b from the fitting of monthly measurements in Washington D.C. with Eq.(S5) were estimated as 0.76, indicating a greater effect from water temperature than the model identified by Ged et al. (2015).

Considering that different parameters such as TOC and the reaction constants are subject to great spatial variation (Brown et al. 2011) and the empirical predictive models of Eq.(S5) and Eq.(S6) with the estimated coefficients may not be applicable for other locations or systems, the effect of water temperature on TTHM formation can also be assessed with an Arrhenius relationship with temperature as suggested by an early study (Kavanaugh et al. 1980). Specifically, Kavanaugh et al. (1980) showed that a 10ºC increase of temperature (within 10-30ºC) doubles the rate of TTHM formation – notably with a similar effect on chlorine bulk decay [if a 10ºC increase in

water temperature leads to a doubling of chlorine decay rate, the E/R value is 5750 ºC for Eq.(S4), which is similar to the 6050ºC utilized]. Therefore, although changes in the rate of TTHM formation were not assessed for the 91 cities, it is expected that the percent changes in the TTHM formation rates will be similar to the percent changes in chlorine bulk decay rate as presented in Figure 7 of the main text.

C-3. Estimating bacterial activity

Both empirical predictive models and mechanistic models are available for describing the bacterial activity, as discussed in the main text and by studies such as Chowdhury (2012). In the empirical predictive models, the correlation coefficients between water temperature and bacterial activity vary in different studies (Chowdhury 2012) and are potentially location specific. These empirical models were thus not utilized for this study.

A commonly utilized expression for describing the temperature effect on bacterial activity in mechanistic models [such as Servais et al. (1995), Dukan et al. (1996), and Digiano and Zhang (2004)] was used. This expression of temperature effect on bacterial activity was proposed in Billen et al. (1992) [based on the Monod equation] and is provided as (assuming no other effect on bacterial activity such as the suppressing effect from chlorine):

$$Act(T) = Act(T_{opt}) \, exp\left(-\left(\frac{T_{opt}-T}{T_{opt}-T_i}\right)^2\right) \qquad (S7)$$

where Act(T) is bacterial activity at temperature T (ºC), T_{opt} is the optimal temperature for the bacteria community, and T_i is a shape parameter. Both T_{opt} and T_i can be estimated with experiments. When both physiological direct response to sudden changes and gradual adaptation

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of a bacteria community to seasonal changes of temperature are considered, a correlation of the two coefficients with water temperature can be utilized (Billen et al. 1992):

$$T_{opt} = 40 - (20 - T)/2$$

$$T_i = 18 - (20 - T)/2 \qquad (S8)$$

Eq.(S7) was consequently utilized to provide estimates of bacterial activity for Washington D.C. and the other 90 cities.

Temperature effects on water quality can be enhanced considering the interactions among different parameters, such as chlorine decay, DBP formation, and bacterial activity. As indicted in Eq. (S5), chlorine dosage and chlorine residual are key parameters for determining the TTHM formation and as well as limiting bacterial activity (Digiano and Zhang 2004). To provide an assessment with consideration of both temperature effects on bacterial activity and chlorine decay, the following expression from the previously mentioned mechanistic models [such as Servais et al. (1995) and Digiano and Zhang (2004)] was utilized to describe the chlorine effect on bacterial activity:

$$Act(C_t) = Act(0) \, exp\left(-\left(\frac{C_t - C_m}{dC}\right)\right); \, for \, C_t > Cl_m \qquad (S9)$$

where $Act(C_t)$ is the bacterial activity under chlorine concentration of C_t at time t, $Act(0)$ is the bacterial activity unsuppressed by chlorine with C_m as a threshold concentration, and dC is a coefficient for describing the decrease of bacterial activity with the increase of chlorine concentration [C_m and dC were given as 0.03 and 0.2 mg/L for suspended bacteria, respectively, or 0.1 and 0.25 for fixed bacteria (Servais et al. 1995)].

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Eq.(S9) was consequently utilized to estimate the bacterial activity considering both changes in water temperature and chlorine residual levels for a hypothetical study location (with a constant water age of 400 hours as an extreme case) in Washington D.C. as presented in the part (d) of Figure 6 in the main text.

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