Appendix A. Supplementary information

Occurrence and factors affecting the formation of trihalomethanes, haloacetonitriles and halonitromethanes in outdoor swimming pools treated with trichloroisocyanuric acid

Fang Yang, Zhaoguang Yang, Haipu Li*, Fangfang Jia, Ying Yang*

College of Chemistry and Chemical Engineering, Central South University, Changsha 410083, PR China

***Correspondence information:**

Names: Haipu Li, Ying Yang

Full postal address: Center for environment and water resources, College of chemistry and chemical engineering, Central South University, No. 932 Lushan Nan Road, Yuelu District, Changsha, 410083, PR China.

Telephone: +86-731-88876961

E-mails: lihaipu@csu.edu.cn, yangy@csu.edu.cn

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Table S1. Occurrence of DBPs in swimming pools in previous studies

Country	Pool type	Disinfection method	Concentrations(μg/L)									Reference
			TCM	BDCM	DBCM	TBM	DCAN	TCAN	BCAN	DBAN	TCNM	
France	indoor	chlorine	nd	nd	4.0(mean)	79.2	nd	-	nd	26.9	-	1
		Ozone/chlorine	95.8-212.8	85.5-141.4	1.5-4.9	38.6-59.2	4.2-8.5	nd	nd	nd	nd-2.1	
China	indoor	chlorine	154.7-333.7	9.9-318.2	2.0-16.8	14.6-60.0	nd-42.3	nd-0.2	nd-8.2	nd	nd	2
		chlorine	46.3-467.3	14.2-255.7	nd-225.8	1.9-133.3	nd-205.5	nd-0.5	nd-88.8	nd-33.6	nd-4.5	
Canada	indoor	chlorine	20.3-320.4	1.3-154.6	<QLM-204.8	<QLM-102.8	2.3-22.4	<QLM-0.12	0.28-29.4	<QLM-30.8	0.02-3.7	3
	Outdoor		69.8(mean)	7.9	1.9	0.6	74.6	1.2	9.2	2.5	4.5	
France	indoor	chlo-rine	nd	nd	3.9	62.5	nd	nd	0.9	16.2	nd	4
	Indoor		nd	nd	5.2	86.7	nd	nd	1.0	27.6	nd	
	indoor		nd	nd	1.6	48.9	nd	nd	0.9	13.1	nd	
Spain	indoor	chlorine	2.4-61.6	3.8-12.9	0.9-4.7	0.2-1.9	3.8-12.2		1.8-4.7	1.1-3.6	-	5
China	Indoor/outdoor	Ozone/chlorine	33.8(THMs, median)					3.2(HANs, median)			nd	6
Spain	indoor	chlorine	8.5-19	9.3-23	6.5-23	3.0-16	-	-	-	-	-	7
		bromine	0.08-0.3	0.22-0.43	2.1-2.5	52-64	-	-	-	-	-	

“nd”: not detected

“-”: not given

“QLM”: quantification limit of the method

Table S2. Details of pool management and operation of swimming pools

NO.	Functional areas	Disinfection type	Disinfectant Dose (kg/day)	Size (m^3)	Visitors per day (Person)	Price (RMB)	Source of pool water	Pool water treatment	Frequency of water replenishment (Day)	Volume of water replenishment (m^3)	Cycle of total water exchange (Day)	Mandatory shower before swimming (Yes/No)
1	Hotel	TCCA	0.9	198	20	100	tap water	Sand filtration	1	-	-	Yes
2	Community	TCAA	–	-	70	30	tap water	Sand filtration	3	-	-	No
3	Hotel	TCAA	2.0	360	40	58	Tank water/Secondary water supply	Sand filtration	7	-	7	Yes
4	Hotel	TCAA	1.5	580	55	68	Tank water/Secondary water supply	Sand filtration	7	200	30	Yes
5	Municipal	TCAA	1.5	1500	200	30	tap water	Sand filtration	1	70	-	Yes
6	Municipal	TCAA	6.0	750	320	30	tap water	Sand filtration	1	300	-	Yes
7	Municipal	TCAA	2.5	510	300	58	tap water	Sand filtration	-	-	90	Yes
8	Municipal	TCAA	3.0	1200	300	35	tap water	Sand filtration	1	50	-	Yes
9	Municipal	TCAA	–	800	600	30	tap water	Sand filtration	15	400	30	Yes
10	School	TCAA	4.0	1200	200	30	tap water	Sand filtration	1	150	-	Yes

NO.	Functional areas	Disinfection type	Disinfectant Dose (kg/day)	Size (m^3)	Visitors per day (Person)	Price (RMB)	Source of pool water	Pool water treatment	Frequency of water replenishment (Day)	Volume of water replenishment (m^3)	Cycle of total water exchange (Day)	Mandatory shower before swimming (Yes/No)
11	School	TCAA	8.0	1800	150	35	tap water	Sand filtration	1	40	-	Yes
12	School	TCAA	6.5	3000	300	30	tap water	Sand filtration	1	500	-	No
13	Water Park	TCAA	5.0	1400	300	135	tap water	Sand filtration	1	100	-	Yes
14	Water Park	TCAA	15.0	3000	1200	80	tap water	Sand filtration	1	1000	-	Yes
15	Health club	TCAA	1.5	750	100	50	tap water	Sand filtration	-	-	7	Yes
16	Health club	TCAA	1.0	300	100	30	tap water	Sand filtration	-	-	30	Yes
17	Community	TCAA	–	860	20	30	tap water	Sand filtration	2	200	-	Yes
18	Community	TCAA	2.0	200	40	35	tap water	Sand filtration	-	-	-	Yes
19	Community	TCAA	8.0	1000	200	30	tap water	Sand filtration	-	-	-	Yes
20	Community	TCAA	1.0	400	20	30	tap water	Sand filtration	-	-	-	Yes
21	Community	TCAA	–	260	200	20	tap water	Sand filtration	1	60	-	No
22	Community	TCAA	3.0	1000	150	30	tap water	Sand filtration	1	200	-	Yes

NO.	Functional areas	Disinfection type	Disinfectant Dose (kg/day)	Size (m^3)	Visitors per day (Person)	Price (RMB)	Source of pool water	Pool water treatment	Frequency of water replenishment (Day)	Volume of water replenishment (m^3)	Cycle of total water exchange (Day)	Mandatory shower before swimming (Yes/No)
23	Community	TCAA	3.0	600	100	40	tap water	Sand filtration	1	50	-	No
24	Community	TCAA	1.0	400	150	35	tap water	Sand filtration	1	50	-	Yes
25	Community	TCAA	2.0	400	100	25	tap water	Sand filtration	1	50	-	Yes
26	Community	TCAA	–	900	150	25	tap water	Sand filtration	-	-	7	Yes
27	Community	TCAA	2.5	500	65	30	tap water	Sand filtration	2	150	-	No
28	Community	TCAA	2.0	670	55	25	tap water	Sand filtration	1	70	-	No
29	Community	TCAA	2.5	680	150	30	tap water	Sand filtration	7	250	30	Yes
30	Community	TCAA	5.0	2700	200	25	tap water	Sand filtration	1	80	-	No
31	Community	TCAA	3.0	1100	300	35	tap water	Sand filtration	15	500	60	Yes
32	Community	TCAA	2.0	750	150	30	tap water	Sand filtration	1	75	-	Yes
33	Community	TCAA	1.5	500	60	25	tap water	Sand filtration	3	250	15	Yes
34	Community	TCAA	2.0	200	80	25	tap water	Sand filtration	3	70	15	No

NO.	Functional areas	Disinfection type	Disinfectant Dose (kg/day)	Size (m^3)	Visitors per day (Person)	Price (RMB)	Source of pool water	Pool water treatment	Frequency of water replenishment (Day)	Volume of water replenishment (m^3)	Cycle of total water exchange (Day)	Mandatory shower before swimming (Yes/No)
35	Community	TCAA	3.0	600	90	25	tap water	Sand filtration	3	300	-	Yes

“TCAA”: Trichloroisocyanuric acid

“-”: not given

“Cycle of total water exchange”: the time taken for changing a volume of water equivalent to the volume of the entire pool

Table S3. Linear range, linearity, recovery, relative standard deviation (RSD) and the method detection limits (MDL) of all analysed DBPs

DBPs	Linear range (μg/L)	Linearity (r^2)	Recovery (%)	RSD (%)	MDL (μg/L)
TCM	0.32 - 64	0.9998	96.3	1.1	0.15
TBM	0.32 - 64	0.9910	97.8	4.5	0.12
DCBM	0.32 - 64	0.9920	97.1	1.3	0.14
DBCM	0.32 - 64	0.9911	97.0	1.2	0.12
TCAN	0.32 - 64	0.9924	98.8	1.6	0.12
DCAN	0.32 - 64	0.9920	98.0	1.6	0.09
DBAN	0.32 - 64	0.9931	94.6	2.8	0.09
BCAN	0.32 - 64	0.9946	100.7	2.6	0.15
TCNM	0.32 - 64	0.9939	100.3	2.3	0.08

Table S4. Water parameters of the swimming pools

NO.	Functional areas	Temperature (°C)	FRC (mg/L)	pH	UV_{254} (cm^{-1})	TOC (mg/L)	Urea (mg/L)	TN (mg/L)
1	Hotel	32	1.4	7.4	0.013	2.0	7.0	18
2	Community	34	nd	6.9	0.033	27	16	-
3	Hotel	33	nd	7.5	0.014	2.4	1.4	2.5
4	Hotel	33	0.25	7.2	0.025	9.9	3.7	-
5	Municipal	34	0.31	7.5	0.016	23	6.6	26
6	Municipal	34	0.02	7.8	0.014	3.7	2.1	4.4
7	Municipal	33	0.43	7.8	0.074	16	10	-
8	Municipal	32	1.4	7.7	0.013	20	5.0	22
9	Municipal	35	0.24	6.5	-	17	-	-
10	School	35	1.5	6.9	0.021	12	0.17	-
11	School	34	0.01	7.5	0.012	6.2	9.8	12
12	School	34	1.7	6.8	0.056	14	nd	17
13	Water Park	34	0.12	7.2	0.034	11	12	13
14	Water Park	34	0.03	7.1	0.012	5.9	5.2	-
15	Health club	32	0.04	6.8	0.013	39	11.4	35
16	Health club	32	0.76	6.9	0.017	8.8	2.3	-
17	Community	36	nd	7.3	0.012	12	4.0	15
18	Community	34	0.65	7.8	0.013	21	7.6	23
19	Community	34	0.05	6.7	0.014	8.5	6.0	12
20	Community	34	nd	7.6	0.012	8.8	5.5	-
21	Community	34	0.04	8.3	0.014	23	nd	2.6
22	Community	33	2.2	7.3	0.013	15	0.94	18
23	Community	35	0.77	7.7	0.012	16	2.5	17
24	Community	33	0.06	7.9	0.017	2.9	nd	2.6
25	Community	31	0.33	6.9	0.020	8.9	nd	9.2

NO.	Functional areas	Temperature (°C)	FRC (mg/L)	pH	UV_{254} (cm^{-1})	TOC (mg/L)	Urea (mg/L)	TN (mg/L)
26	Community	34	0.40	7.3	0.012	7.8	2.0	
27	Community	34	0.40	7.2	0.012	6.2	0.66	7.6
28	Community	34	0.04	7.0	0.040	18	6.4	18
29	Community	33	0.03	8.1	0.036	11	17	16
30	Community	34	0.93	6.7	0.040	24	5.2	27
31	Community	34	0.14	7.7	0.012	5.7	1.8	7.7
32	Community	33	0.04	7.5	0.014	10	8.6	-
33	Community	33	0.05	6.9	0.015	8.3	7.0	-
34	Community	33	1.9	6.4	0.013	20	4.2	-
35	Community	33	0.03	6.7	0.011	18	10	-

"-": not measured

nd: not detected

Table S5. Pearson correlations between DBPs and water parameters

	THMs	HANs	TCNM	FRC	UV_{254}	pH	TOC	TN	Urea
THMs	1	0.555**	0.761**	0.447**	0.561**	−0.116	0.270	0.254	0.011
HANs		1	0.765**	0.529**	0.217	−0.701**	0.279	0.211	-0.111
TCNM			1	0.484**	0.303	−0.387*	0.332	0.340	-0.070
FRC				1	0.107	-0.153	0.161	0.342	-0.344*
UV_{254}					1	-0.055	0.207	0.203	0.275
pH						1	-0.133	-0.174	0.097
TOC							1	0.768**	0.351*
TN								1	0.508*
Urea									1

*p < 0.05; **p < 0.01

Table S6. Octanol-water partition coefficient (K_{ow}), Molecular weight and K_p of DBPs

DBPs	K_{ow} (unitless)	Molecular weight (g/mol)	K_p (cm/h)
TCM	93	119.4	8.90E-03
BDCM	126	163.8	5.92E-03
DBCM	127	208.3	3.18E-03
TBM	128	252.8	1.71E-03

***Dermal permeability coefficient can be calculated by the following formula[8].**

Log K_p = -2.72 + (0.71 × log K_{ow}) - 0.0061 × MW

K_p: Permeability coefficient (cm/hr)

K_{ow}: Octanol-water partition coefficient

MW = Molecular weight (g/mol)

Table S7. Slope factor (SF) of DBPs[9]

DBPs	$SF_{ingestion}$ $(mg/Kg/d)^{-1}$	SF_{dermal} $(mg/Kg/d)^{-1}$
TCM	6.10E-03	3.05E-02
BDCM	6.20E-02	6.33E-02
DBCM	8.40E-02	1.40E-01
TBM	7.90E-03	1.32E-02

Table S8. Human body information for swimmers[2]

Swimmer	Body weight (kg)	Skin surface area (m^2)	Swimming frequency (event/year)	Exposure duration (years)	Ingestion rate (L/h)	Event duration (h/event)
Non-Athletic						
Adult male	66.2	1.75	120	30	0.025	1
Adult female	57.3	1.57	120	30	0.025	1
Child (11-14)	43.2	1.33	120	4	0.05	1
Athletic						
Adult male	66.2	1.75	238	22	0.0125	1
Adult female	57.3	1.57	238	22	0.0125	1
Child (11-14)	43.2	1.33	189	4	0.025	1

Table S9. Cancer risk assessment of DBPs from the average concentrations

Group	Exposure routes	cancer risk				
		TCM	TBM	DCBM	DBCM	Total
Non-Athletic male	Ingestion	7.49E-09	2.88E-10	2.84E-09	1.92E-09	
	Dermal	2.33E-07	5.78E-10	1.20E-08	7.14E-09	
	Total	2.41E-07	8.66E-10	1.49E-08	9.07E-09	2.65E-07
Non-Athletic female	Ingestion	8.65E-09	3.33E-10	3.28E-09	2.22E-09	
	Dermal	2.42E-07	5.99E-10	1.25E-08	7.40E-09	
	Total	2.50E-07	9.32E-10	1.57E-08	9.63E-09	2.77E-07
Non-Athletic Child	Ingestion	4.00E-09	1.54E-10	1.52E-09	1.03E-09	
	Dermal	2.77E-09	4.45E-11	2.55E-09	1.63E-09	
	Total	6.77E-09	1.99E-10	4.06E-09	2.66E-09	1.37E-08
Athletic male	Ingestion	7.66E-09	2.95E-10	2.91E-09	1.97E-09	
	Dermal	4.77E-07	1.18E-09	2.46E-08	1.46E-08	
	Total	4.85E-07	1.48E-09	2.75E-08	1.66E-08	5.31E-07
Athletic female	Ingestion	8.86E-09	3.41E-10	3.36E-09	2.27E-09	
	Dermal	4.95E-07	1.23E-09	2.55E-08	1.52E-08	
	Total	5.04E-07	1.57E-09	2.89E-08	1.74E-08	5.52E-07
Athletic Child	Ingestion	2.16E-08	8.31E-10	8.19E-09	5.55E-09	
	Dermal	7.24E-08	1.79E-10	3.73E-09	2.22E-09	
	Total	9.40E-08	1.01E-09	1.19E-08	7.76E-09	1.15E-07

Table S10. Cancer risk assessment of DBPs from the highest concentrations pool (pool 30#)

Group	Exposure routes	cancer risk				
		TCM	TBM	DCBM	DBCM	Total
Non-Athletic male	Ingestion	2.29E-08	8.28E-10		1.53E-09	
	Dermal	7.13E-07	1.66E-09		5.70E-09	
	Total	7.36E-07	2.49E-09		7.23E-09	7.46E-07
Non-Athletic female	Ingestion	2.65E-08	9.57E-10		1.77E-09	
	Dermal	7.39E-07	1.72E-09		5.91E-09	
	Total	7.66E-07	2.68E-09		7.68E-09	7.76E-07
Non-Athletic Child	Ingestion	1.22E-08	4.43E-10		8.20E-10	
	Dermal	2.77E-09	4.45E-11		1.63E-09	
	Total	1.50E-08	4.87E-10		2.45E-09	1.79E-08
Athletic male	Ingestion	2.34E-08	8.48E-10		1.57E-09	
	Dermal	1.46E-06	3.4E-09		1.17E-08	
	Total	1.48E-06	4.25E-09		1.32E-08	1.50E-06
Athletic female	Ingestion	2.71E-08	9.80E-10		1.81E-09	
	Dermal	1.51E-06	3.52E-09		1.21E-08	
	Total	1.54E-06	4.50E-09		1.39E-08	1.56E-06
Athletic Child	Ingestion	6.60E-08	2.39E-09		4.42E-09	
	Dermal	2.21E-07	5.16E-10		1.77E-09	
	Total	2.87E-07	2.90E-09		6.19E-09	2.96E-07

Table S11. Cancer risk assessment of DBPs from the lowest concentrations pool (pool 1#)

Group	Exposure routes	Cancer risk				
		TCM	TBM	DCBM	DBCM	Total
Non-Athletic male	Ingestion	1.21E-09				
	Dermal	3.77E-08				
	Total	3.89E-08				3.89E-08
Non-Athletic female	Ingestion	1.40E-09				
	Dermal	3.91E-08				
	Total	4.05E-08				4.05E-08
Non-Athletic child	Ingestion	6.47E-10				
	Dermal	2.77E-09				
	Total	3.42E-09				3.42E-09
Athletic male	Ingestion	1.24E-09				
	Dermal	7.72E-08				
	Total	7.85E-08				7.85E-08
Athletic female	Ingestion	1.43E-09				
	Dermal	8.00E-08				
	Total	8.15E-08				8.15E-08
Athletic child	Ingestion	3.49E-09				
	Dermal	1.17E-08				
	Total	1.52E-08				1.52E-08

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