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SECTION 1 – CHAPTER 1

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Table 1 Impact on SSR and F-specific bacteriophages of PFA disinfection applied to SEV WWTP discharge (contact time: 10 min).

Date	SSR Spores				F-Specific Bacteriophages			
	Concentration (CFU/100 mL)			Log Removal	Concentration (CFU/100 mL)			Log Removal
	SEV WWTP Discharge	8–12 ppm.min of PFA	20 ppm.min of PFA		SEV WWTP Discharge	8–12 ppm.min of PFA	20 ppm.min of PFA	
Sept 11, 2018	80	7	2	1.06–1.60	33		30	No
Sept 18, 2019*	5200	89	<1	1.77–>3.72	33		<30	>0.04
Jan 30, 2019*	6400	4700		0.13	<30	<30		?
Feb 6, 2019	6400	6500		No	<30	<30		?
Feb 13, 2019	2170	5000		No	<30	<30		?
May 5, 19	1800	1500	675	0.08–0.43				
May 9, 2019	5000	6300	5900	No				
Median	5000	4700	339		<30	<30	<30	

*Days with degraded SEV WWTP operations.

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Table 2 Excitation and emission wavelengths of DOM fluorophores and their interpretation.

Fluorophores (Parlanti <i>et al.</i> , 2000)	Excitation Wavelength (nm)	Emission Wavelength (nm)	Type of Compound
α'	230–260	380–480	Humic-like substances + more recent material
α	330–370	420–480	Humic-like substances
β	310–320	380–420	Recent material + biological components
γ	270–280	300–320	Tyrosine-like
δ	270–280	320–380	Tryptophan-like

Table 3 PFA half-life measured in both SEV WWTP discharge and seine river water in choisy samples spiked with 2.5 ppm of PFA.

Type of Water	Sampling Date	Temperature (°C)	Filtration at 0.45 μm	$t_{1/2}$ (min)
SEV WWTP discharge	Sept 11, 2018	12	Yes	33
		20		17
		25		13
	Oct 16, 2018	20	Yes	29
	Nov 6, 2018		No	29
	Average \pm standard deviation	20	No	33
			–	26 \pm 9
Seine River water in Choisy	Sept 11, 2018	12	Yes	87
		20		53
		25		29

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Table 4 N-nitrosamines monitored in this study and their optimized analytical parameters for detection by gas chromatography coupled with tandem mass spectrometry (GC-MS/MS).

Compound ^a	RT (min) ^b	Parent ion	Product ions (collision energy) ^c
<i>N</i> -nitrosodimethylamine-d6 (NDMA-d6)	6.68	80	50 (10), 46 (20)
<i>N</i> -nitrosodimethylamine (NDMA)	6.70	74	44 (5), 42 (15)
Toluene-d8	6.94	98	70 (15), 98 (10)
<i>N</i> -nitrosomethylethylamine (NMEA)	7.50	88	71 (5), 43 (10)
<i>N</i> -nitrosodiethylamine (NDEA)	8.15	102	85 (5), 44 (10)
<i>N</i> -nitrosodipropylamine-d14 (NDPA-d14)	9.68	144	126 (5), 50 (10)
<i>N</i> -nitrosodipropylamine (NDPA)	9.76	130	113 (5), 43 (10)
<i>N</i> -nitrosopyrrolidine (NPYR)	9.76	100	55 (5), 43 (10)
<i>N</i> -nitrosomorpholine (NMOR)	9.79	116	86 (5), 56 (10)
<i>N</i> -nitrosopiperidine (NPIP)	10.23	114	84 (5), 42 (15)
<i>N</i> -nitrosodibutylamine (NDBA)	11.57	158	99 (10), 141 (5)
<i>N</i> -nitrosodiphenylamine (NDPhA)	15.25	168	167 (20), 166 (25)

^aNDMA-d6 was used as the internal standard for NDMA quantification; NDPA-d14 was used as the internal standard for other N-nitrosamine quantification; Toluene-d8 served as the injection internal standard used to monitor analytical stability and calculate the recovery rate.

^bRT = Retention time.

^cThe first product ion was used for quantification.

Table 5 Formation of AOX and halogenated DBPs from the PFA disinfection of WWTP water at the laboratory scale (various concentrations of PFA, 10-min contact time) or during full-scale disinfection (0.8–2.5 ppm PFA).

Date	Sample ^a	C.t (ppm. min)	AOX (µg/L)	DBPs ^b (µg/L)
<i>Laboratory-scale disinfection trials</i>				
Sept 11, 2018	SEV-TW	–	39.4	n.a ^c
	SEV-TW + 2 ppm PFA	20	48.7	n.a

(Continued)

Table 5 Formation of AOX and halogenated DBPs from the PFA disinfection of WWTP water at the laboratory scale (various concentrations of PFA, 10-min contact time) or during full-scale disinfection (0.8–2.5 ppm PFA) (*Continued*).

Date	Sample ^a	C.t (ppm. min)	AOX (µg/L)	DBPs ^b (µg/L)
Sept 18, 2018	SEV-TW	–	32.0	n.d ^d
	SEV-TW + 2 ppm PFA	20	43.4	n.d
Nov 6, 2018	SEV-TW	–	45.0	n.d
	SEV-TW + 1 ppm PFA	10	40.6	n.d
	SEV-TW + 2 ppm PFA	20	48.9	n.d
	SEV-TW + 30 ppm PFA	300	49.2	DBCM (0.02), BCAN (0.14)
	SEV-TW + 100 ppm PFA	1000	338.7	DCBM (2.35), DBCM (1.39), TBM (0.03), DCAN (8.25), BCAN (1.96), DBAN (0.55), TCAN (0.73), DCP (3.41), TCNM (1.83)
Dec 11, 2018	SEV-TW + 2 mg-N/L of NO ₂ ⁻ + 1 ppm PFA	10	32.6	BCAN (0.15), DBAN (0.10)
	SEC-RW	–	41.7	DBCM (0.34), TBM (0.23)
	SEC-RW + 10 ppm PFA	100	39.5	DBCM (0.43), TBM (0.36), DBAN (0.16)
	SEC-SW	–	42.9	DBCM (0.34), TBM (0.24), DBAN (0.14)
	SEC-SW + 10 ppm PFA	100	39.9	DBCM (0.29), TBM (0.26), DBAN (0.12)
<i>Full-scale disinfection trials</i>				
Sept 26, 2018	SEV-TW	–	31.2	n.d
	SEV-DW (1.2 ppm PFA)	32.1	44.6	n.d
Oct 10, 2018	SEV-TW	–	43.9	n.d
	SEV-DW (0.8 ppm PFA)	28.3	49.9	n.d

(Continued)

Table 5 Formation of AOX and halogenated DBPs from the PFA disinfection of WWTP water at the laboratory scale (various concentrations of PFA, 10-min contact time) or during full-scale disinfection (0.8–2.5 ppm PFA) (*Continued*).

Date	Sample ^a	C.t (ppm. min)	AOX (µg/L)	DBPs ^b (µg/L)
Oct 24, 2018	SEV-TW	–	47.2	BCAN (0.34), DBAN (0.69)
	SEV-DW (2.5 ppm PFA)	74.2	54.8	DCBM (0.07), BCAN (0.43), DBAN (1.1)

^aSEV: Seine Amont Valenton WWTP; SEC: Seine Centre WWTP; TW: treated water; DW: disinfected water at the full-scale; RW: pretreated raw water; SW: settled water; PFA: performic acid.

^bDCBM: dichlorobromomethane; DBCM: dibromochloromethane; TBM: bromoform; DCAN: dichloroacetonitrile; BCAN: bromochloroacetonitrile; DBAN: dibromoacetonitrile; TCAN: trichloroacetonitrile; DCP: dichloropropanone; TCNM: chloropicrin.

^cn.a: not analyzed.

^dn.d: not detected.

Table 6 Concentration of bromide ions in WWTP discharge before and after disinfection with PFA (0.8–2.5 ppm PFA).

Date	C × t (ppm.min)	Bromide ions (µg/L)	
		Before PFA Injection	After PFA Injection
Aug 28, 2018	31.2	100	90
Sept 11, 2018	31.6	120	50
Sept 25, 2018	36.4	250	160
Oct 9, 2018	22.1	170	170
Oct 23, 2018	73.8	170	170

Table 7 N-nitrosamine concentrations in WWTP water disinfected by PFA at the laboratory scale (various concentrations of PFA, 10-min contact time) or during full-scale disinfection (0.8–2.5 ppm PFA).

Date	Sample ^a	C × t (ppm.min)	N-nitrosamines ^b (ng/L)					
			NDMA	NDEA	NDPA	NMOR	NPIP	NDBA
<i>Laboratory-scale disinfection trials</i>								
Sept 11, 2018	SEV-TW	–	30	3.5	2.6	11	1.1	4.3
	SEV-TW + 2 ppm PFA	20	25	1.0	0.2	9.8	0.7	1.7
Sept 18, 2018	SEV-TW	–	31	3.0	1.5	13	2.1	7.7
	SEV-TW + 2 ppm PFA	20	22	2.2	0.3	12	1.2	2.8
Nov 6, 2018	SEV-TW	–	21	1.5	1.5	10	1.1	5.6
	SEV-TW + 1 ppm PFA	10	21	2.1	0.8	14	1.2	2.8
	SEV-TW + 2 ppm PFA	20	24	3.9	0.8	8.8	1.9	2.7
	SEV-TW + 30 ppm PFA	300	24	2.0	0.2	9.1	1.4	2.8
	SEV-TW + 100 ppm PFA	1000	19	2.8	1.9	11	2.1	8.8
Dec 11, 2018	SEV-TW + 2 mg-N/L of NO ₂ [–] + 1 ppm PFA	10	30	4.9	1.0	162	1.2	3.4
	SEC-RW	–	27	19	0.3	7.2	4.5	2.6
	SEC-RW + 10 ppm PFA	100	33	23	0.2	6.4	8.6	2.9
	SEC-SW	–	30	17	0.4	7.4	6.2	1.8
	SEC-SW + 10 ppm PFA	100	28	18	0.6	7.8	12.5	1.9
<i>Full-scale disinfection trials</i>								
Sept 26, 2018	SEV-TW	–	32	14	0.6	11	1.6	6.7
	SEV-DW (1.2 ppm PFA)	32.1	31	11	1.5	14	2.4	19
Oct 10, 2018	SEV-TW	–	31	4.9	1.5	18	3.2	5.2

(Continued)

Table 7 N-nitrosamine concentrations in WWTP water disinfected by PFA at the laboratory scale (various concentrations of PFA, 10-min contact time) or during full-scale disinfection (0.8–2.5 ppm PFA) (*Continued*).

Date	Sample ^a	C × t (ppm.min)	N-nitrosamines ^b (ng/L)					
			NDMA	NDEA	NDPA	NMOR	NPIP	NDBA
Oct 24, 2018	SEV-DW (0.8 ppm PFA)	28.3	31	6.5	0.7	19	3.1	11
	SEV-TW	–	33	3.9	1.8	15	3.2	6.6
	SEV-DW (2.5 ppm PFA)	74.2	33	5.3	0.5	13	1.7	6.7

^aSEV: Seine Amont Valenton WWTP; SEC: Seine Centre WWTP; TW: treated water; DW: disinfected water at full-scale; RW: pretreated raw water; SW: settled water; PFA: performic acid.

^bNDMA: N-nitrosodimethylamine; NDEA: N-nitrosodiethylamine; NDPA: N-nitrosodipropylamine; NMOR: N-nitrosomorpholine; NPIP: N-nitrosopiperidine; NDBA: N-nitrosodibutylamine.

Table 8 Bulk characterization of marker fingerprints obtained from WWTP discharge samples before (SEV-TW) and after PFA disinfection (SEV-DW and SEV-TW + 2 ppm PFA) analyzed by UPLC-IMS-QTOF in positive mode.

	Before PFA SEV-TW ^a		After PFA SEV-DW ^b and SEV-TW + 2 ppm PFA	
	All Markers	Unique Markers	All Markers	Unique Markers
Average RT ^c (min)	8.96	10.26	9.09	11.03
Average <i>m/z</i> ratio	434.4252	505.4057	405.3870	441.2656
Total number of markers	11,608	1799	11,634	2119
Number of markers with intensity >10,000	7369	1792	6222	1303
Total intensity of markers	4.8×10^8	4.5×10^7	4.1×10^8	4.1×10^7
Total intensity of markers with intensity >10,000	4.6×10^8	6.0×10^7	3.8×10^8	5.5×10^7

All values are averaged from six triplicate samples (18 fingerprints). The parameters were calculated from all markers detected in each of the 18 fingerprints, as well as from markers exclusively detected before or after PFA disinfection ('unique markers').

^aSEV-TW: Seine Amont Valenton WWTP treated water.

^bSEV-DW: Seine Amont Valenton WWTP disinfected water at the full scale.

^cRT: retention time.

Table 9 PFA disinfection conditions applied during the 10-week, full-scale trial in 2018.

Weeks	35	36	37	38	39	40	41	42	43	44
Targeted PFA injection dose (ppm)	1	0	1.2	0	1.2	0	0.8	0	2	0
Actual PFA injection dose (ppm)	0.8–1.0	0	0.8–1.2	0	1.2	0	0.8	0	2.1–2.5	0
Hydraulic retention time (min)	22–31	19–56	25–39	25–36	27–38	20–54	22–35	24–37	28–34	23–40
C × t (ppm.min)	17–31	0	16–39	0	32–45	0	18–28	0	60–74	0

Table 10 Sampling conducted and parameters monitored during the 10-week, full-scale trial.

Compound	SEV WWTP Discharge						Seine River		
	Upstream Injection All Weeks			Downstream Injection Weeks with Injection			Upstream and Downstream of WWTP Discharge All Weeks		
	Tu	We	Th	Tu	We	Th	Tu	We	Th
<i>E. coli</i>	3	3	3	3	3	3		1	
Intestinal enterococci	3	3	3	3	3	3		1	
Spores of anaerobic sulfite-reducing microorganisms	1			1					
F-RNA specific bacteriophages	1			1					
TSS	3	3	3	3	3	3		1	
DOC	3	3	3	3	3	3		1	
COD	3	3	3	3	3	3		1	
BOD	3	3	3	3	3	3		1	
TKN	3	3	3	3	3	3		1	
N-NH ₄	3	3	3	3	3	3		1	
N-NO ₂	3	3	3	3	3	3		1	
N-NO ₃	3	3	3	3	3	3		1	
Total phosphorus	3	3	3	3	3	3		1	
P-PO ₄	3	3	3	3	3	3		1	
pH	3	3	3	3	3	3		1	

(Continued)

Table 10 Sampling conducted and parameters monitored during the 10-week, full-scale trial (*Continued*).

Compound	SEV WWTP Discharge						Seine River		
	Upstream Injection All Weeks			Downstream Injection Weeks with Injection			Upstream and Downstream of WWTP Discharge All Weeks		
	Tu	We	Th	Tu	We	Th	Tu	We	Th
Conductivity	3	3	3	3	3	3		1	
Turbidity	3	3	3	3	3	3		1	
Halogenated organic hydrocarbons (AOX)	1			1	0	0			
Bromate	1			1					
Bromide	1			1					
Color								1	
Chloride								1	
Sulfate								1	

Table 11 Analytical methods used for the determination of the monitored parameters.

Analytical Parameter	Applicable Standards	Limit of Quantification	Analytical Uncertainty
Ammonium (NH ₄ ⁺)	NF EN ISO 11732 (August 2005)	0.3 mg N/L	0.3–1.2 = 40%
	NF EN ISO 11732 (August 2005)	0.01 mg NH ₄ /L	>1.2 = 10% 0.010–0.025 = 50% >0.025 = 20%
Halogenated organic hydrocarbons (AOX)	NF EN ISO 9562 (March 2005)	10 µg/L Cl	>10 = 35%
F-RNA specific bacteriophage (F-RNA)	ISO 10705–3/NF EN ISO 10705–1	30 PFU/100 mL	Undetermined
Bromate	ISO 10304–1	5 µg/L	Undetermined
Bromide	Internal method	50 µg/L	Undetermined
Total Kjeldahl nitrogen (TKN)	NF EN 25663 (January 1994)	0.5 mg N/L	0.5–2 = 60%
	or SIAAP internal method		>2 = 15% or 0.5–1.5 = 60% >1.5 = 20%
Dissolved organic carbon (DOC)	NF EN 1484 (July 1997)	0.3 mg C/L (chemical method)	0.3–0.8 = 40%
		or 3 mg/L (thermal method)	>0.8 = 15% or 3–12 = 60% >12 = 15%
Chloride	NF ISO 15923–1 (January 2014)	5 mg Cl/L	5–20 = 40% >20 = 10%
	NF EN ISO 10304–1 (July 2009)	1 mg Cl/L	1–1.5 = 15% >1.5 = 10%
Conductivity	NF EN 27888 (January 1994)	30 mS/m	>30 = 10%
Water color	NF EN ISO 7887	0 mg Pt/L	0–15 = ±4.5 mg Pt/L >15 = 30%

(Continued)

Table 11 Analytical methods used for the determination of the monitored parameters (*Continued*).

Analytical Parameter	Applicable Standards	Limit of Quantification	Analytical Uncertainty
Biochemical oxygen demand (BOD ₅)	NF EN 1899–1 (May 1998) or NF EN 1899–2 (May 1998)	3 mgO ₂ /L or 0.5 mgO ₂ /L	3–4 = 40% >4 = 30% or 0.5–6 = 30%
Chemical oxygen demand (COD)	ISO 15705 (November 2002)	4 mgO ₂ /L	4–6.3 = 55% 6.3–40 = 35% 40–60 = 50% >60 = 25%
<i>E. coli</i> (EC)	NF EN ISO 9308–3 (March 1999)	56 MPN/100 mL 38 MPN/100 mL 15 MPN/100 mL	Undetermined
Intestinal enterococci (IE)	NF EN ISO 7899–1 (March 1999)	56 MPN/100 mL 38 MPN/100 mL 15 MPN/100 mL	Undetermined
Total suspended solids (TSS)	NF EN 872 (June 2005)	2 mg/L	2–6 = 60% >6 = 20%
Nitrate	NF EN ISO 13395 (October 1996)	0.4 mg N/L	0.4–1.4 = 35% >1.4 = 10%
	NF EN ISO 10304–1 (July 2009)	0.5 mg NO ₃ /L	0.5–1.5 = 30% >1.5 = 10%
Nitrite	NF EN ISO 13395 (October 1996)	0.02 mg N/L	0.02–0.09 = 45% >0.09 = 10%
	NF EN ISO 10304–1 (July 2009)	0.01 mg NO ₂ /L	0.01–0.4 = 40% >0.4 = 10%
Orthophosphates (PO ₄ ³⁻)	NF EN ISO 15681–2 (June 2005)	0.1 mg P/L	0.1–0.4 = 40% >0.4 = 10%
	NF EN ISO 15681–2 (June 2005)	0.02 mg PO ₄ /L	0.02–0.08 = 40% >0.08 = 10%

pH	NF EN ISO 10523 (May 2012)	–	10%
Total phosphorus (Pt)	SIAAP internal method	0.3 mg P/L	0.3–1.1 = 55% >1.1 = 15%
Spores of sulfite reducing microorganisms (SSR)	NF EN 26461–2 (July 1993)	200 CFU/100 mL 34 CFU/100 mL 10 CFU/100 mL	Undetermined
Sulfate	SIAAP internal method	10 mg/L	10–25 = 25% >25 = 10%
	NF EN ISO 10304–1 (July 2009)	1 mg/L	1–1.5 = 15% >1.5 = 10%
Turbidity	NF EN ISO 7027–1 (August 2016)	0.5 FNU	>0.5 = 30%

Table 12 Disinfection pilot operation installation: measurement summary and abatement calculation.

In Situ Disinfection	ALERT Pre-Disinfection <i>E. coli</i>/100 mL	Lab Pre-Disinfection MPN/100 mL	ALERT Post-Disinfection <i>E. coli</i>/100 mL	Lab Post-Disinfection MPN/100 mL	ALERT Removal log₁₀	Lab Removal log₁₀
Minimum value	14,574	10,100	4	15		
Maximum value	26,272	21,600	29	61		
Average	21,947	15,917	8	33	3.4	2.7

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Table 13 Conventional wastewater quality parameters measured in SEV WWTP discharge before and after PFA disinfection.

	SEV WWTP Discharge (Average \pm Standard Deviation)	SEV Disinfected Water (Average \pm Standard Deviation)
TSS (mg/L)	5.0 \pm 3.9	5.4 \pm 3.8
DOC (mgC/L)	6.5 \pm 0.5	7.7 \pm 0.6
COD (mgO ₂ /L)	22 \pm 5	24 \pm 5
BOD ₅ (mgO ₂ /L)	1.9 \pm 1.5	2.5 \pm 1.6
TKN (mgN/L)	1.4 \pm 0.6	1.4 \pm 0.5
N-NH ₄ ⁺ (mgN/L)	0.4 \pm 0.2	0.3 \pm 0.2
N-NO ₃ ⁻ (mgN/L)	14.6 \pm 2.1	15.2 \pm 2.1
N-NO ₂ ⁻ (mgN/L)	0.05 \pm 0.04	0.04 \pm 0.03
TP (mgP/L)	0.9 \pm 0.5	0.9 \pm 0.4
P-PO ₄ ³⁻ (mgP/L)	0.6 \pm 0.5	0.6 \pm 0.3
pH	7.07 \pm 0.11	7.26 \pm 0.09
Conductivity (μ S/cm)	1100 \pm 121	1103 \pm 122

Table 14 Effect of PFA applied to SEV WWTP discharge at the industrial scale on *E. coli*, intestinal enterococci, SSR and F-specific RNA phages.

Date	PFA Dose ppm	PFA c × t ppm. min	TSS Mg/L	<i>Escherichia Coli</i>			Intestinal Enterococci		
				Upstream Injection MPN/100 mL	Downstream Injection MPN/100 mL	Log Removal Log	Upstream Injection MPN/100 mL	Downstream Injection MPN/100 mL	Log Removal log
28/08/18	1.0	31.2	3	10,000	76	2.12	1700	<15	≥2.05
11/09/18	1.2	31.6	3	18,600	353	1.72	5030	<15	≥2.53
25/09/18	1.2	36.4	9	51,700	504	2.01	11,500	292	1.60
09/10/18	0.8	22.1	3	15,800	612	1.41	2960	232	1.11
23/10/18	2.2	73.8	3	10,100	46	2.34	4420	<15	≥2.47
Date	PFA Dose ppm	PFA C × t ppm. min	TSS Mg/L	Spore of Sulfite-Reducing Anaerobes			F-Specific RNA Phages		
				Upstream Injection CFU/100 mL	Downstream Injection CFU/100 mL	Log Removal Log	Upstream Injection PFU/100 mL	Downstream Injection PFU/100 mL	Log Removal log
28/08/18	1.0	31.2	3	1170	855	0.14	<30	<30	
11/09/18	1.2	31.6	3	1530	1200	0.11	<30	<30	
25/09/18	1.2	36.4	9	6000	7000	NR	170	<30	≥0.75
09/10/18	0.8	22.1	3	883	2700	NR	<30	<30	
23/10/18	2.2	73.8	3	1650	2000	NR	<30	<30	

NR = Not relevant.

Table 15 Summary of the different variants considered during model construction.

Dataset Used	Explained Variable	Explanatory Variables	Interactions	n
Full dataset	$\ln(\text{EC}_{\text{out}})$	Q, H, T_{plant} , PFA dose, Ct, $\text{pH}_{\text{sampling}}$, T_{sampling} , σ_{sampling} , EC_{in} , $[\text{TSS}]_{\text{in}}$, $[\text{DOC}]_{\text{in}}$, $[\text{COD}]_{\text{in}}$, $[\text{BOD}]_{\text{in}}$, $[\text{TKN}]_{\text{in}}$, $[\text{NH}_4^+]_{\text{in}}$, $[\text{NO}_2^-]_{\text{in}}$, $[\text{NO}_3^-]_{\text{in}}$, $[\text{P}_{\text{tot}}]_{\text{in}}$, $[\text{PO}_4^{3-}]_{\text{in}}$, pH_{lab} , σ_{lab} , turbidity	None Two-way	48
'Online' dataset		Q, H, T_{plant} , PFA dose, Ct, $\text{pH}_{\text{sampling}}$, T_{sampling} , σ_{sampling} , EC_{in} , $[\text{DOC}]_{\text{in}}$, $[\text{NH}_4^+]_{\text{in}}$, pH_{lab} , σ_{lab} , turbidity	None Two-way	

Table 16 Main results from model construction on the full dataset.

ID	Source	Variables Included	p	Maximum VIF Value	R ²	Adj. R ²	MSE	MSE _{val} (LOO)	MSE _{val} (5-fold)
F1	Forward SSE and BIC	Dose, Ct, T _{sampling} , [NH ₄ ⁺]	4	23.1	0.826	0.810	0.704	1.401	1.429
F2	Forward AIC	Dose, Ct, T _{sampling}	3	23	0.793	0.779	0.818	1.726	1.740
F3	Backward SSE, BIC and AIC1	Q, H, T _{plant} , Dose, [DOC], [COD], [BOD], [NH ₄ ⁺]	8	11.6	0.883	0.859	0.511	0.730	0.762
F4	Backward AIC2	Q, H, T _{plant} , pH _{sampling} , Dose, [DOC], [COD], [BOD]	8	11.6	0.885	0.862	0.523	0.807	0.857

Table 17 Main results from model construction using the 'online' dataset.

ID	Source	Variables Included	p	Maximum VIF Value	R ²	Adj. R ²	MSE	MSE _{val} (LOO)	MSE _{val} (5-fold)
S1	All forward procedures	Dose, Ct, T _{sampling} , [NH ₄ ⁺]	4	23.1	0.826	0.810	0.704	1.401	1.429
S2	All backward procedures	Q, H, T _{plant} , Dose, [DOC], [NH ₄ ⁺]	6	10.5	0.847	0.825	0.667	1.023	1.049

Table 18 Main results from model construction on the 'online' dataset with interactions.

ID	Source	Variables Included	P	Maximum VIF Value	R ²	Adj. R ²	MSE	MSE _{val} (LOO)	MSE _{val} (5-fold)
SI1	Forward AIC	Q, H, T _{sampling} , [DOC], Dose*T _{sampling} , Dose*[DOC]	6	147 (10.4)	0.871	0.852	0.548	0.746	0.763
SI2	Backward SSE	Q, T _{sampling} , Dose, [DOC], H*T _{sampling}	5	12.2 (10.6)	0.844	0.825	0.647	1.155	1.177

Table 19 Concentrations of AOX, bromide and bromate in SEV WWTP discharge before and after PFA disinfection.

Date	PFA Dose ppm	PFA C × t ppm. min	TSS Mg/L	A.O.X.			Bromide			Bromate	
				Upstream Injection µgCl/L	Downstream Injection µgCl/L	Variation %	Upstream Injection µgBr/L	Downstream Injection µgBr/L	Variation %	Upstream Injection µgBrO ₃ /L	Downstream Injection µgBrO ₃ /L
28/08/18	1.0	31.2	3	86	110	+28	100	90	-10	<5	<5
11/09/18	1.2	31.6	3	39	48	+23	120	<50	-58	<5	<5
25/09/18	1.2	36.4	9	52	57	+10	250	160	-36	<5	<5
09/10/18	0.8	22.1	3	57	73	+28	170	170	0	<5	<5
23/10/18	2.2	73.8	3	68	96	+41	170	170	0	<5	<5

SECTION 3 – CHAPTER 1

Table 20 Biological panels of general toxicity applied during this project.

Panel	Biological Models	Observed Effects	Number of Tests
General toxicity	Bacterial (two <i>E. coli</i> strains)	Growth (OD)	2
	Yeast – Cryptogams eukaryotes (<i>Saccharomyces cerevisia</i>)	Growth (OD)	2
	Fungal – Ascomycete (<i>Septoria tritici</i>)	Growth (OD)	1

Table 21 Results obtained for the various biological models of general toxicity applied in this project.

		Strong Effect	Moderate Effect	Weak, Yet Significant, Effect	No Significant Effect	Weak, Yet Significant, Effect	Moderate Effect	Strong Effect
Bacterial	AG100A	Below -90%	-30 to -90%	-15 to -30%	-15 to +15%	15-30%	30-90%	Above 90%
	NR698	Below -90%	-60 to -90%	-30 to -60%	-30 to +30%	30-60%	60-90%	Above 90%
Yeast	WT	Below -90%	-60 to -90%	-30 to -60%	-30 to +30%	30-60%	60-90%	Above 90%
	AD1-9	Below -90%	-30 to -90%	-15 to -30%	-15 to +15%	15-30%	30-90%	Above 90%
Fungal	<i>Septoria tritici</i>	Below -95%	-60 to -95%	-30 to -60%	-30 to +30%	30-60%	60-95%	Above 95%

Table 22 Endocrine disruption panels applied in this project.

Panel	Biological Models	Observed Effects
Endocrine disruption	Amphibian xenopus (<i>Xenopus laevis</i>) TH/bZIP	Thyroid activity (effect on development)
	Fish larvae medaka ChgH-GFP (<i>Oryzias latipes</i>)	Estrogenic activity (effect on reproduction)
	Fish larvae medaka SPG-GFP (<i>Oryzias latipes</i>)	Androgenic activity (effect on reproduction)

SECTION 4 – CHAPTER 2

Table 23 Synthesis of the main laboratory and full-scale studies conducted over the period 2005–2018.

Disinfectant	Years	Plants/Matrices	Investigations
PFA	2005/2006, 2011, 2012, 2013–2018	CL-ER-JS-SD	Effectiveness; QI ₁ ; QI ₂ ; ecotoxicity; genotoxicity; decomposition/residuals
PAA	2002, 2006, 2008, 2013, 2017	JS-SD	Effectiveness; QI ₂ ; decomposition/residuals
HYP	2008, 2011, 2012	CL-ER-JS-SD	Effectiveness; decomposition/residuals

Notes: CL = Caorle; ER = Eraclea; JS = Jesolo; SD = San Donà; QI₁ = qualitative impacts in terms of physicochemical parameters, such as pH, total organic carbon, biochemical oxygen demand and formate; QI₂ = Oxidation power and byproducts; PFA = performic acid; PAA = peracetic acid; HYP = chlorine hypochlorite.

Table 24 Methods for chemical and microbiological investigations conducted at both the full and laboratory scales.

Parameter		Method	Description
Fecal indicators	Fecal coliforms	APAT CNR-IRSA Man 29 2003 (7020B, 7030D, 7040C)	MF; mFC agar
	<i>E. coli</i>		MF; chromogenic <i>E. coli</i> agar
	Fecal Enterococci		MF; Slanetz and Bartley/Bile Esculin Azide agar
Quality parameters and impacts	pH	APHA ed. 21st 2005–22nd 2012	Electrometric method
	TOC	(4500-H+B, 5310 C, 5210 D)	Persulfate-Ultraviolet Oxidation Method
	BOD ₅		Respirometric method (WTW)
	TSS – Turbidity	APAT CNR-IRSA Man 29 2003	Gravimetric - Nephelometric
	Ammonium	UNI EN ISO 14911:2001	Ion chromatography
	Nitrite	UNI EN ISO 10304–1:2009	Ion chromatography
	COD	UNI EN ISO 15705:2002	Photometric measurement in sealed tube
Ecotoxicity	Formate	EPA 300.1 1999	Ion chromatography
	Vibrio Fischeri	UNI EN ISO 11348–3B 2001–2009	Microtox test system for determining light emission suppression
	Daphnia Magna Straus	UNI EN ISO 6341:2013	Inhibition of the mobility of Daphnia Magna Straus (cladocera, crustacea)

Notes: MF = Membrane filtration; TOC = total organic carbon; BOD₅ = biochemical oxygen demand; TSS = total suspended solids; COD = chemical oxygen demand.

Table 25 Full-scale experimental operating conditions – average (minimum–maximum).

Disinfection System	Year	WWTP	Flow Rate (m ³ /d)	Disinfectant Dose (mg/L)	Retention Time (min)
PFA-HP prototype	2005–2006	CL	7140 (5400–10,000)	1.1 (0.3–1.8)	24 (10–45)
Pilot	2006		10,900 (3410–20,100)	1.6 (0.9–2.4)	36 (16–59)
PFA	2011	ER	3190 (1790–4970)	1.0 (0.6–1.2)	11 (6–19)
	2013–2018	CL-ER-JS-SD	Typical	0.6 (0.4–1.1)	26 (5–83)
PAA	2006	JS	32,570 (23,620–43,680)	1.4 (0.7–2.5)	27 (13–49)
HYP	2008	CL	10,110 (6860–16,350)	2.6 (1.9–4.7)	24 (12–51)
	2011	JS	24,120 (15,920–34,520)	2.7 (1.9–3.2)	20 (15–30)

Notes: CL = Caorle; ER = Eraclea; JS = Jesolo; SD = San Donà.

Table 26 Median and range of variation of the main chemical-physical parameters of effluents entering the disinfection treatment during the full-scale studies performed from 2005 to 2011.

	pH (unit)	TSS (mg/L)	COD (mg/L)	N-NH ₄ (mg/L)	F. coliforms (Log)	<i>E. coli</i> (Log)	Enterococci (Log)
PFA-HP	7.6 (6.9–8.2)	11.9 (9.0–34)	25 (10–35)	0.57 (0.02–3.7)	4.0 (2.3–5.3)	3.6 (2.0–5.3)	3.4 (2.7–4.5)
PFA	7.7 (7.1–8.3)	9.9 (9.0–17)	26 (14–45)	1.5 (0.02–9)	4.9 (4.4–6.0)	4.6 (3.0–5.6)	3.4 (2.7–4.3)
PAA	7.4 (7.1–8.0)	10 (9.0–11)	34 (14–47)	0.14 (0.14–3.7)	5.2 (4.7–5.3)	4.4 (3.3–5.2)	3.4 (2.7–4.3)
HYP	7.5 (7.3–7.8)	9.0 (9.0–17)	29 (21–48)	1.94 (0.14–10)	5.3 (5.0–6.0)	4.6 (3.6–6.2)	3.5 (2.6–4.6)

Notes: HYP = hypochlorite; PAA = peracetic acid; PFA-HP = Hydroform performic acid solution; PFA = Desinfix performic acid solution; TSS = total suspended solids; COD = chemical oxygen demand; F. coliforms = fecal coliforms.

Table 27 Average and range of variation of bacterial inactivation achieved by PFA, PAA and HYP for each interval of contact time (Kruskal–Wallis test) during the full-scale studies performed from 2005 to 2011.

Time (min)	Disinfectant Type	Doses (mg/L)	Ret. Time (min)	<i>E. coli</i> (log R)	Enterococci (log R)	<i>F. coliform</i> (log R)
≤10	PFA	1.04 ± 0.07	8.32 ± 1.12	2.92 (2.23–3.97)	1.75 (0.65–2.78)	–
>10–20	PFA-HP	1.26 ± 0.54	14.38 ± 2.24	1.05 (0.06–3.28) ^c	0.76 (0.46–2.31) ^b	1.02 (0.30–3.75) ^b
	PFA	0.88 ± 0.22	13.26 ± 2.67	3.3 (2.04–4.19) ^a	1.78 (0.67–3.15) ^a	–
	PAA	1.60 ± 0.38	16.16 ± 1.96	1.92 (1.16–2.61) ^b	0.35 (0.04–0.92) ^c	1.57 (0.84–2.69) ^b
	HYP	2.83 ± 0.70	16.34 ± 2.22	2.71 (0.98–4.05) ^b	1.19 (0.36–3.09) ^{ab}	3.45 (2.11–4.28) ^a
>20–30	PFA-HP	1.16 ± 0.57	22.49 ± 3.25	1.87 (0.32–3.65)	1.42 (0.42–3.26) ^a	1.67 (0.38–3.32)
	PAA	1.94 ± 0.67	25.12 ± 3.32	2.86 (0.16–3.42)	0.28 (0.14–0.71) ^b	–
	HYP	2.45 ± 0.47	25.39 ± 2.89	2.75 (1.21–5.15)	1.48 (0.66–2.23) ^a	–
>30	PFA-HP	1.35 ± 0.60	45.07 ± 10.24	2.52 (0.44–4.29)	1.92 (0.55–3.67) ^a	2.57 (0.62–4.76)
	PAA	1.07 ± 0.20	38.94 ± 6.77	2.45 (1.21–3.37)	0.46 (0.1–1.63) ^b	–
	HYP	2.38 ± 2.46	36.54 ± 7.16	2.51 (1.78–3.13)	1.75 (0.63–3.12) ^a	–

Notes: Ret. Time = retention time; log R = log reduction (CFU/100 mL); PFA-HP=Hyproform performic acid solution; PFA = Desinfix performic acid solution; *F. coliforms* = fecal coliforms; different superscript letters (down columns) mean significant different variations at $p = 0.05$, with values^a > values^b > values^c.

Table 28 Order of effectiveness of the disinfectant against fecal indicators from 2005 to 2011 by the ANCOVA test.

F. coliforms log R (CFU/100 mL)	E. coli log R (CFU/100 mL)	Enterococci log R (CFU/100 mL)
Comparable ($p > 0.05$)	PFA > PAA~PFA-HP > HYP	PFA > PFA-HP > HYP~PAA

Notes: F. coliforms = fecal coliforms; log R = log reduction (CFU/100 mL); PFA-HP = Hydroform performic acid solution; PFA = Desinfix performic acid solution.

Table 29 Disinfection kinetics parameters estimated for the hom and S models, minimum and maximum values (dose range: PFA = 0.5–1.3 mg/L – PAA = 1–3 mg/L).

		<i>E. coli</i>		Enterococci	
		PFA	PAA	PFA	PAA
HOM	n	0.000–0.416	0.000–0.010	0.000–0.401	0.000–1.181
	m	0.000–0.491	0.001–1.141	0.353–0.774	0.225–1.809
	K	2.138–8.928	0.152–8.202	0.305–1.743	0.002–1.212
	R ²	0.969–1.000	0.917–1.000	0.943–0.988	0.922–0.998
S Model	n	0.000–0.139	0.000–0.160	0.001–2.877	0.537–0.598
	m	0.020–8.794	3.059–24.561	0.916–3.524	0.633–4.671
	h	0.006–9.587	5.538–16.251	10.200–30.522	5.500–53.00
	K	6.217–17.571	4.303–8.294	6.011–37.479	2.296–4.457
	R ²	0.984–1.000	0.969–1.000	0.930–0.999	0.943–1.000

Notes: PFA = Desinfix performic acid solution.

Table 30 Percentage of results being in compliance with various levels of microbiological target at disinfection outlet and correspondent disinfection operating conditions (average and range of variation).

WWTP	Disinfectant	Dose (mg/L)	Retention Time (min)		
CL	PFA-HP	1.3 (0.3–2.4)	28 (10–59)		
ER	PFA	1.0 (0.6–1.2)	11 (6–19)		
JS	PAA	1.6 (0.9–2.1)	16 (13–20)		
CL – JS	HYP	2.8 (2.5–3.0)	17 (15–20)		
	CFU/100 mL	<12,000	<2400	<1000	<100
Fecal coliforms	PFA-HP	100%	88%	83%	55%
	PFA	–	–	–	–
	PAA	92%	42%	25%	0%
	HYP	100%	100%	100%	100%
<i>E. coli</i>	CFU/100 mL	<5000	<1000	<100	<10
	PFA-HP	100%	90%	67%	35%
	PFA	100%	100%	76%	31%
	PAA	92%	83%	17%	0%
Enterococci	HYP	100%	93%	59%	14%
	CFU/100 mL	<2000	<400	<100	<10
	PFA-HP	88%	78%	48%	15%
	PFA	100%	90%	69%	10%
	PAA	67%	17%	0%	0%
	HYP	95%	90%	37%	10%

Notes: CL = Caorle; ER = Eraclea; JS = Jesolo; Ret. Time = retention time; PFA-HP = Hydroform performic acid solution; PFA = Desinfix performic acid solution.

Table 31 Bacterial concentrations (average \pm standard deviation) at the disinfection outlet under the disinfectant operating conditions of Table 30.

	<i>E. coli</i> CFU/100 mL	Enterococci CFU/100 mL	F. coliform CFU/100 mL
PFA	62 \pm 81 ^b	169 \pm 153 ^b	454 \pm 429 ^b
PAA	1143 \pm 201 ^a	1757 \pm 375 ^a	5276 \pm 964 ^a
HYP	643 \pm 155 ^a	1311 \pm 310 ^a	2784 \pm 1609 ^{a,b}

Notes: F. coliforms = fecal coliforms; different superscript letters (down columns) mean significant different variations at $p = 0.05$ with values^a > values^b > values^c.

Table 32 Percent of results, recorded between 2013 and 2018, meeting the various *E. coli* targets; percentages are expressed for each contact time interval and the corresponding average applied PFA.

Retention Time (min)	Samples No.	% Samples Respecting the <i>E. coli</i> Limits (CFU/100 mL) (%)				PFA Average Dose mg/L
		<1000	<100	<10	>1000	
≤10	56	96%	48%	0%	4%	0.7
10–20	127	98%	72%	9%	2%	0.6
>20–30	65	100	31	52		0.6
>30–40	33	100	27	48		0.6
>40	77	100	55	6		0.6
Total	358	99	53	18	1%	0.6

Table 33 Qualitative parameter variation at the disinfection inlet from 2013 to 2018; data are reported as average, standard error and (maximum value).

	TSS (mg/L)	COD (mg/L)	N-NH ₄ (mg/L)	N-NO ₂ (mg/L)
Caorle	10 ± 6.4 (36)	19 ± 6.8 (44)	0.58 ± 1.12 (7.0)	0.13 ± 0.13 (0.57)
Eraclea	9.3 ± 4.4 (35)	21 ± 6.4 (54)	1.35 ± 2.18 (17.9)	0.24 ± 0.22 (1.02)
Jesolo	10.0 ± 6.0 (33)	19 ± 7.2 (57)	1.85 ± 1.96 (7.8)	0.12 ± 0.10 (0.67)
San Donà	8.7 ± 3.6 (27)	19 ± 6.4 (45)	0.31 ± 0.57 (4.43)	0.06 ± 0.05 (0.28)

Notes: TSS = total suspended solids; COD = chemical oxygen demand.

Table 34 Comparisons between TOC at the dosage point (T_0) and disinfection outlet (t-student test) for each time interval – average ± standard error (range of variation).

Time Interval (min)	PFA Dose (mg/L)	TOC T_0 (mg/L)	TOC OUT (mg/L)	Probability
<10	1.01 ± 0.18	6.79 ± 0.63 (5.34–8.0)	6.94 ± 0.64 (5.40–7.8)	0.116
10–20	0.87 ± 0.83	6.12 ± 1.05 (4.47–8.95)	6.24 ± 0.97 (4.75–8.90)	0.032
20–30	0.89 ± 0.46	7.19 ± 1.30 (5.20–9.38)	7.17 ± 1.31 (5.60–9.53)	0.084
>30	1.16 ± 0.60	7.37 ± 1.13 (5.52–9.41)	7.57 ± 1.19 (5.28–10.26)	0.001

Notes: TOC = total organic carbon; OUT = disinfection outlet.

Table 35 Comparisons between formate at the dosage point (T_0) and disinfection outlet (Wilcoxon rank test) for each time interval; median and range of variation.

Time Interval (min)	Formate T_0 (mg/L)	Formate OUT (mg/L)	Probability
<10	2.81 (1.62–3.6)	3.10 (1.97–3.6)	0.061
10–20	2.04 (1.35–10.89)	2.0 (0.82–11.08)	0.168
20–30	3.51 (1.15–9.77)	3.08 (1.15–9.92)	0.079
>30	4.04 (1.45–10.31)	3.97 (1.40–10.50)	0.524

Notes: OUT = disinfection outlet.

Table 36 Carbon components associated with PAA and PFA-HP, measured at the laboratory in batch tests by dosing the disinfectant and/or the associated carbon ions in the disinfection mixture.

Disinfectant Type	Doses (mg/L)	Increase for Each mg/L of Active Substance		
		TOC (mg/L)	COD (mg/L O ₂)	BOD ₅ (mg/L O ₂)
PFA-HP	2–50 Formate ion	1.3 ± 0.13	1.8 ± 0.13	0.5 ± 0.21
PAA	1–10 PAA	0.9 ± 0.03	–	1.1 ± 0.18
	2–50 Aceate ion	0.9 ± 0.12	2.0 ± 0.17	1.6 ± 0.29

Notes: PFA-HP = Hydroform performic acid solution.

Table 37 Percentage of cases in which the two peracids respected the microbiological target set at 20% of the guideline or limit values; doses and retention times refer to the conditions under which the target was respected.

Disinfectant	Fecal Indicator	Cases Respecting Target (%)	Doses (mg/L)	Cases at Retention Time <20 min	Cases at Retention Time ≥20 min
PFA	<i>E.coli</i>	99%	0.9	60%	40%
PAA		92%	2.4	30%	62%
PFA	Enterococci	88%	0.8	53%	35%
PAA		48%	2.8	7%	41%