Bromide and its associated brominated disinfection byproducts: occurrence, toxicity and control strategies

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Supporting Information

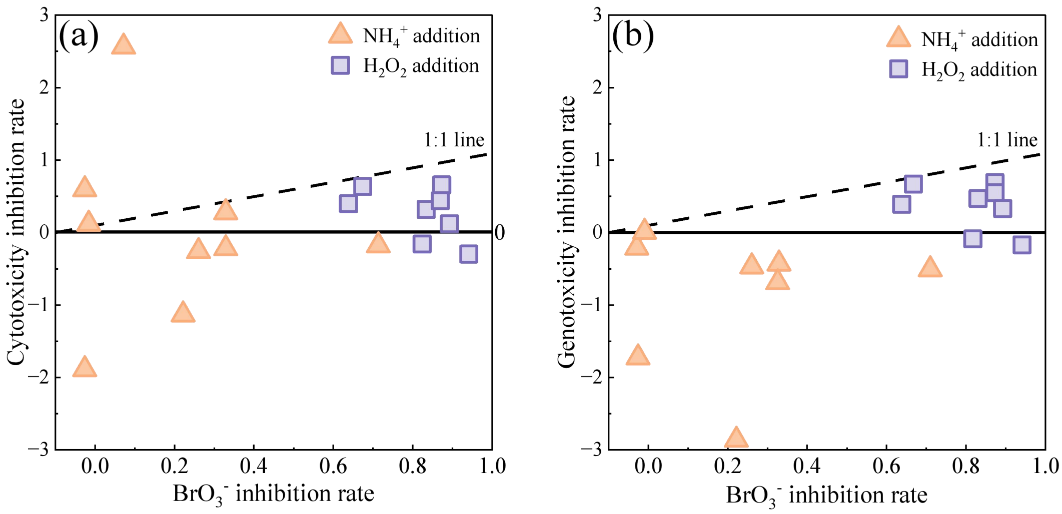

Fig. S1 The relationship between bromate inhibition rate and toxicity inhibition rate with the NH_4^+ or H_2O_2 addition: (a) Cytotoxicity; (b) Genotoxicity (Data collected from Wu et al., 2020) (copyright: ACS Publications).

Table S1 Comparison of three disinfectants: chlorine, ozone and PMS/PDS.

Disinfector	Redox potential	Disinfection target	Typical disinfection byproducts
Chlorine	HOCl (1.49 V) Cl·（2.40 V）(Zhang et al., 2023)	phenolic compound, harmful microbe (Westerhoff et al., 2004; Zhu and Zhang, 2016)	halogenated disinfection byproducts (Park et al., 2016)
Ozone	O_3（2.07 V）(Zhang et al., 2023)	chlorine-resistant protozoa, electron-rich functional compounds, pathogens, micro-pollutants (Mao et al., 2018; Yang et al., 2019)	aldehydes compounds (formaldehyde, acetaldehyde, glyoxal, methylglyoxal, and tri chloroacetaldehyde) (Park et al., 2016)
PMS/PDS	SO_4· (2.5-3.1 V) OH·（1.8-2.7 V）SO_4 ·（2.80 V）(Zhang et al., 2005; Zhang et al., 2023)	micropollutants, electron-rich compound (Koudjonou and LeBel, 2006; Zhou et al., 2022)	

Table S2 **Formation of bromate and Br-DBPs during the chlorine-based disinfection process.**

No.	Reaction	*k*	Reference
R1	$Br\ \ + HOCl \rightarrow HOBr + Cl$	$1.55\text{-}1.68\times10^{3}$ $M^{\ 1}\cdot s^{\ 1}$	(Farkas et al., 1949; Kumar and Margerum, 1987; Bousher et al., 1989)
R2	$ClO\ \ + Br\ \ \rightarrow BrO\ \ + Cl$	$9\times10^{\ 4}M^{\ 1}\cdot s^{\ 1}$	
R3	$NH_2Cl + Br\ \ \rightarrow NH_2Br + Cl$	$1.4\times10^{\ 2}M^{\ 1}\cdot s^{\ 1}$	(Zhu and Zhang, 2016)
	$NH_2Br{+}H_2O \rightarrow HOBr{+}NH_3$	$1.5\times10^{\ 3}M^{\ 1}\cdot s^{\ 1}$	
R4	$HOBr/BrO\ \ + HOCl \rightarrow BrO_2$		(Yang et al., 2019)
R5	$Cl\cdot + HOBr/BrO\ \ \rightarrow Cl\ \ + BrO\cdot$		(Yang et al., 2019)
R6	$BrO\ \ + OH\cdot \rightarrow BrO\cdot$	$4.5\times10^{9}M^{\ 1}\cdot s^{\ 1}$	(Buxton et al., 1988)
R7	$HBrO\cdot + OH\cdot \rightarrow BrO\cdot$	$2.0\times10^{9}M^{\ 1}\cdot s^{\ 1}$	(Buxton et al., 1988)
R8	$Br\ \ + OH\cdot \rightarrow Br\cdot$	$1.1\times10^{10}M^{\ 1}\cdot s^{\ 1}$	(Zehavi and Rabani, 1972; Neta et al., 1988)
R9	$Br\cdot + Br\ \ \rightarrow Br_2\cdot$	$10^{10}M^{\ 1}\cdot s^{\ 1}$	(Legube et al., 2004)
R10	$Br_2\cdot + BrO\ \ \rightarrow BrO\cdot + 2Br$	$8.0\times10^{7}M^{\ 1}\cdot s^{\ 1}$	(Legube et al., 2004)
R11	$2BrO\cdot + H_2O \rightarrow BrO_2\ \ + BrO\ \ + 2H^{+}$	$4.9\times10^{9}M^{\ 1}\cdot s^{\ 1}$	(Legube et al., 2004)
R12	$OH\cdot + BrO_2\ \ \rightarrow BrO_2\cdot$	$1.9\times10^{9}M^{\ 1}\cdot s^{\ 1}$	(Yang et al., 2019)
	$BrO_2\cdot + OH\cdot \rightarrow H^{+} + BrO_3$	$2.0\times10^{9}M^{\ 1}\cdot s^{\ 1}$	
R13	$HOBr/BrO\ \ + DOM \rightarrow Br\text{-}DBP_s$		(Langsa et al., 2017)

Table S3 Formation of bromate and Br-DBPs during the ozonation.

No.	Reactions	*k*	References
R1	$O_3 + Br \rightarrow BrO + O_2$	$160\ M^{1}\cdot s^{1}$	(Legube et al., 2004)
R2	$O_3 + BrO \rightarrow BrO_2 + O_2$	$100\ M^{1}\cdot s^{1}$	(Legube et al., 2004)
R3	$O_3 + BrO_2 \rightarrow BrO_3 + O_2$	$>10^5\ M^{1}\cdot s^{1}$	(Legube et al., 2004)
R4	$Br + OH\cdot \rightarrow Br\cdot$	$1.1\times10^{10}\ M^{1}\cdot s^{1}$	(Zehavi and Rabani, 1972; Neta et al., 1988)
R5	$Br\cdot + Br \rightarrow Br_2\cdot$	$10^{10}\ M^{1}\cdot s$	(Legube et al., 2004)
R6	$Br_2\cdot + BrO \rightarrow BrO\cdot + 2Br$	$8.0\times10^7\ M^{1}\cdot s^{1}$	(Legube et al., 2004)
R7	$Br\cdot + O_3 \rightarrow BrO\cdot$	$>10^5\ M^{1}\cdot s^{1}$	(Wu et al., 2020)
R8	$2BrO\cdot + H_2O \rightarrow BrO_2 + BrO + 2H^+$	$4.9\times10^9\ M^{1}\cdot s^{1}$	(Legube et al., 2004)
R9	$BrO + OH\cdot \rightarrow BrO\cdot$	$4.5\times10^9\ M^{1}\cdot s^{1}$	(Buxton et al., 1988)
R10	$HBrO + OH\cdot \rightarrow BrO\cdot$	$2.0\times10^9\ M^{1}\cdot s^{1}$	(Buxton et al., 1988)
R11	$OH\cdot + BrO_2 \rightarrow BrO_2\cdot$ $BrO_2\cdot + OH\cdot \rightarrow H^+ + BrO_3$	$1.9\times10^9\ M^{1}\cdot s^{1}$ $2.0\times10^9\ M^{1}\cdot s^{1}$	(Yang et al., 2019)
R12	$HOBr/BrO + DOM \rightarrow Br\text{-}DBP_s$		(Langsa et al., 2017)

Table S4 Formation of bromate and Br-DBPs during the persulfate-based disinfection process.

No.	Reaction	*k*	Reference
R1	$HSO_5\ + Br\ \rightarrow HOBr + SO_4^{2}$	$0.7\ M^{\ 1}\cdot s^{\ 1}$	(Lente et al., 2009)
R2	$SO_5^{2}\ + Br\ \rightarrow BrO\ + SO_4^{2}$	$0.17\ M^{\ 1}\cdot s^{\ 1}$	(Lente et al., 2009)

Disinfector	Bromide concentration (μg/L)					
	500	1000	1812	2000	5000	10000

R3	$SO_4\cdot\ + Br\ \rightarrow Br\cdot + SO_4^{2}$	$3.5\times10^{9}\ M^{\ 1}\cdot s^{\ 1}$	(Zehavi and Rabani, 1972; Neta et al., 1988)
R4	$Br\ + OH\cdot \rightarrow Br\cdot$	$1.1\times10^{10}\ M^{\ 1}\cdot s^{\ 1}$	(Zehavi and Rabani, 1972; Neta et al., 1988)
R5	$Br\cdot + Br \rightarrow Br_2\cdot$	$10^{10}\ M^{\ 1}\cdot s^{\ 1}$	(Kläning and Wolff, 1985)
R6	$Br_2\cdot + BrO\ \rightarrow BrO\cdot + 2Br$	$8\times10^{7}\ M^{\ 1}\cdot s^{\ 1}$	(Legube et al., 2004)
R8	$2BrO\cdot + H_2O \rightarrow BrO_2\ + BrO\ + 2H^{+}$	$4.9\times10^{9}\ M^{\ 1}\cdot s^{\ 1}$	(Legube et al., 2004)
R9	$BrO\ + OH\cdot \rightarrow BrO\cdot$	$4.5\times10^{9}\ M^{\ 1}\cdot s^{\ 1}$	(Buxton et al., 1988)
R10	$HBrO\ + OH\cdot \rightarrow BrO\cdot$	$2\times10^{9}\ M^{\ 1}\cdot s^{\ 1}$	(Buxton et al., 1988)
R11	$OH\cdot + BrO_2\ \rightarrow BrO_2\cdot$ $BrO_2\cdot + OH\cdot \rightarrow H^{+} + BrO_3$	$1.9\times10^{9}\ M^{\ 1}\cdot s^{\ 1}$ $2.0\times10^{9}\ M^{\ 1}\cdot s^{\ 1}$	(Yang et al., 2019)
R12	$BrO_2\ + SO_4\cdot\ \rightarrow BrO_3$		(Yang et al., 2019)
R13	$HOBr/BrO\ + DOM \rightarrow Br\text{-}DBP_s$		(Langsa et al., 2017)

Table S5 The increase in cytotoxicity induced by the presence of bromide relative to that in bromide-free water.

O_3	1.36	1.64	/	3.06	/	/
NaClO or Cl_2	1.16	/	/	1.60	1.89	2.12
NH_2Cl	1.43	/	/	/	3.62	3.64
PMS	/	1.69	1.93	/	/	/
UV/PMS	/	1.88	1.97	2.70	/	/

Disinfector	Bromide concentration (μg/L)				
	100	200	1000	1812	2000

Table S6 The increase in genotoxicity induced by the presence of bromide relative to that in bromide-free water.

O_3	1.21	1.52	4.72	/	/
NaClO or Cl_2	2.93	2.49	3.49	/	1.93
NH_2Cl	/	/	/	/	/
PMS	/	/	2.20	2.25	/
UV/PMS	/	/	1.59	1.82	3.64

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