Ozonation: Direct and Hydroxyl Radical Destruction of a Micropollutant

Share of target destruction by hydroxyl radicals during ozonation (R_ct concept), half-life and time for a given removal with first-order ozone decay.

Input parameters

Unit system: SI

Parameter	Value	Unit
Target rate constant with HO•, L/(mol·s)	1.4000e+10	
Target rate constant with ozone, L/(mol·s)	10.000	
Ratio [HO•]/[O_3]	1.0000e-08	
Initial dissolved ozone	3.0000	mg/L
Ozone decay rate constant	0.10000	1/min
Target removal	95.000	%

Calculated results

Parameter	Value	Unit
Share of destruction by hydroxyl radicals	93.333	%
Effective rate constant, L/(mol·s)	150.00	
Initial ozone, mol/L	6.2503e-05	
Largest removal possible before the ozone is gone (as ln)	5.6252	
Half-life of the target	1.3150	min
Time for the target removal	7.6047	min

Notes for this case

• [O_3] = [O_3]$_0$e^(−kt) and ln(R_0/R) = ([O_3]$_0$/k)(k_HO•R_ct + k_O_3)(1 − e^(−kt)) for a batch reactor or ideal plug flow. R_ct is typically 10^{-10} to 10^{-7} in natural waters (Elovitz and von Gunten).

Formula and method

$$f_{HO\bullet} = \frac{k_{HO\bullet} R_{ct}}{k_{HO\bullet} R_{ct} + k_{O_3}}, \quad \ln\frac{[R]_0}{[R]} = \frac{[O_3]_0}{k}\left(k_{HO\bullet} R_{ct} + k_{O_3}\right)\left(1 - e^{-kt}\right)$$

$$t_X = -\frac{1}{k}\ln\left[1 + \frac{k\ln(1-X)}{[O_3]_0 (k_{HO\bullet} R_{ct} + k_{O_3})}\right]$$

Variables

$k_{HO\bullet}$	Target rate constant with HO•, L/(mol·s)	-
k_{O_3}	Target rate constant with ozone, L/(mol·s)	-
R_{ct}	Ratio [HO•]/[O_3]	-
$[O_3]_0$	Initial dissolved ozone	kg/m³
k	Ozone decay rate constant	1/s
X	Target removal	-
$f_{HO\bullet}$	Share of destruction by hydroxyl radicals	-
$k_{HO\bullet} R_{ct} + k_{O_3}$	Effective rate constant, L/(mol·s)	-

$\ln(R_0/R)_{max}$	Largest removal possible before the ozone is gone (as ln)	-
$t_{1/2}$	Half-life of the target	s
t_X	Time for the target removal	s

Method and standards

Combined direct ozone and hydroxyl radical oxidation with first-order ozone decay.

Assumptions and limits

- Constant R_ct; batch or plug flow.

Report details

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This calculator online

https://calc.firecad.com/environmental/drinking-water/ozone-aop-target-destruction

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Reopens the calculator with the inputs of this report.