

Appendix A: Supplementary data

Nitrate and/or Nitric Acid Formation in the Presence of Different Radical Scavengers during Ozonation of Water Samples; Are Scavengers Effective?

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Table S1. The ANOVA results for linear regression.

		Degree of freedom	Sum of Squares	Mean Square	F Value	Prob>F
UPW	Model	1	99964.58334	99964.58334	535.5287	<0.0001
	Error	4	746.66088	186.66522		
	Total	5	100711.2442			
Tap water	Model	1	112992.773	112992.773	324.6853	<0.0001
	Error	4	1392.02821	348.00705		
	Total	5	114384.8012			
KSW	Model	1	112846.9029	112846.9029	1204.571	<0.0001
	Error	4	374.72901	93.68225		
	Total	5	113221.632			
NaOH	Model	1	110135.5936	110135.5936	1507.166	<0.0001
	Error	4	292.29847	73.07462		
	Total	5	110427.892			
Na ₂ CO ₃	Model	1	88973.4014	88973.4014	437.0518	<0.0001
	Error	4	814.30527	203.57632		
	Total	5	89787.70667			
NaHCO ₃	Model	1	101214.5258	101214.5258	443.0787	<0.0001
	Error	4	913.73851	228.43463		
	Total	5	102128.2643			
H ₃ PO ₄	Model	1	90763.97156	90763.97156	3861.147	<0.0001
	Error	4	94.02799	23.507		
	Total	5	90857.99955			
HCl	Model	1	106700.3374	106700.3374	2708.524	<0.0001
	Error	4	157.57713	39.39428		
	Total	5	106857.9145			
NaCl	Model	1	100803.317	100803.317	2871.253	<0.0001
	Error	4	140.43113	35.10778		
	Total	5	100943.7481			
CaCl ₂	Model	1	85168.1062	85168.1062	717.5339	<0.0001
	Error	4	474.78237	118.69559		
	Total	5	85642.88858			

Table S2. The statistical Welch's test results for nitrate concentrations in the presence of different scavengers at the initial condition.

¹ DF Number	¹ DF Den	F-Value	P-Value
9	9,51712	724,8405	7,15E-13
¹ degree of freedom			

Table S3. Games-Howell Pairwise Comparisons obtained from the One-Way Welch's ANOVA for nitrate concentrations in the presence of different scavengers at the initial condition.

	Mean Diff	SE	T-Value	Prob	Alpha	Sig	LCL	UCL
Tap water - UPW	0.6181	0.03707	16.67442	--	0.05	1	--	--
KSW - UPW	2.39069	0.0231	103.487	0.01678	0.05	1	1.58912	3.19226
KSW - Tap water	1.77259	0.04368	40.58294	0.00706	0.05	1	1.22627	2.31891
NaOH - UPW	0.05172	0.00995	5.19615	0.16692	0.05	0	-0.04674	0.15019
NaOH - Tap water	-0.56638	0.03838	-14.7563	0.09092	0.05	0	-1.52358	0.39082
NaOH - KSW	-2.33897	0.02515	-92.9831	0.00484	0.05	1	-2.76932	-1.90862
Na ₂ CO ₃ - UPW	0.06897	0	--	--	0.05	1	--	--
Na ₂ CO ₃ - Tap water	-0.54914	0.03707	-14.814	--	0.05	1	--	--
Na ₂ CO ₃ - KSW	-2.32173	0.0231	-100.502	0.01727	0.05	1	-3.1233	-1.52015
Na ₂ CO ₃ - NaOH	0.01724	0.00995	1.73205	0.75263	0.05	0	-0.08122	0.11571
NaHCO ₃ - UPW	0.0805	0.0015	53.59335	--	0.05	1	--	--
NaHCO ₃ - Tap water	-0.5376	0.0371	-14.4908	0.1186	0.05	0	-1.81395	0.73874
NaHCO ₃ - KSW	-2.31019	0.02315	-99.7915	0.01687	0.05	1	-3.0961	-1.52428
NaHCO ₃ - NaOH	0.02878	0.01007	2.85864	0.4293	0.05	0	-0.06582	0.12337
NaHCO ₃ - Na ₂ CO ₃	0.01154	0.0015	7.68034	--	0.05	1	--	--
H ₃ PO ₄ - UPW	0.12069	0	--	--	0.05	1	--	--
H ₃ PO ₄ - Tap water	-0.49741	0.03707	-13.4186	--	0.05	1	--	--
H ₃ PO ₄ - KSW	-2.27	0.0231	-98.2626	0.01767	0.05	1	-3.07157	-1.46843
H ₃ PO ₄ - NaOH	0.06897	0.00995	6.9282	0.09861	0.05	0	-0.0295	0.16743
H ₃ PO ₄ - Na ₂ CO ₃	0.05172	0	--	--	0.05	1	--	--
H ₃ PO ₄ - NaHCO ₃	0.04019	0.0015	26.75441	--	0.05	1	--	--
HCl - UPW	1.03448	0	--	--	0.05	1	--	--
HCl - Tap water	0.41638	0.03707	11.23256	--	0.05	1	--	--
HCl - KSW	-1.35621	0.0231	-58.7068	0.02957	0.05	1	-2.15778	-0.55464
HCl - NaOH	0.98276	0.00995	98.7269	5.18E-04	0.05	1	0.88429	1.08122
HCl - Na ₂ CO ₃	0.96552	0	--	--	0.05	1	--	--
HCl - NaHCO ₃	0.95398	0.0015	635.1017	--	0.05	1	--	--
HCl - H ₃ PO ₄	0.91379	0	--	--	0.05	1	--	--
NaCl - UPW	0.86207	0	--	--	0.05	1	--	--
NaCl - Tap water	0.24397	0.03707	6.5814	--	0.05	1	--	--
NaCl - KSW	-1.52862	0.0231	-66.1702	0.02623	0.05	1	-2.3302	-0.72705
NaCl - NaOH	0.81034	0.00995	81.40639	7.62E-04	0.05	1	0.71188	0.90881
NaCl - Na ₂ CO ₃	0.7931	0	--	--	0.05	1	--	--
NaCl - NaHCO ₃	0.78157	0.0015	520.3192	--	0.05	1	--	--
NaCl - H ₃ PO ₄	0.74138	0	--	--	0.05	1	--	--
NaCl - HCl	-0.17241	0	--	--	0.05	1	--	--
CaCl ₂ - UPW	0.58621	0.27586	2.125	--	0.05	1	--	--
CaCl ₂ - Tap water	-0.0319	0.27834	-0.1146	1	0.05	0	-8.85243	8.78864
CaCl ₂ - KSW	-1.80448	0.27683	-6.51844	0.25703	0.05	0	-11.0701	7.46113
CaCl ₂ - NaOH	0.53448	0.27604	1.93624	0.71945	0.05	0	-8.979	10.04797
CaCl ₂ - Na ₂ CO ₃	0.51724	0.27586	1.875	--	0.05	1	--	--
CaCl ₂ - NaHCO ₃	0.5057	0.27587	1.83315	0.74374	0.05	0	-9.06484	10.07624
CaCl ₂ - H ₃ PO ₄	0.46552	0.27586	1.6875	--	0.05	1	--	--
CaCl ₂ - HCl	-0.44828	0.27586	-1.625	--	0.05	1	--	--
CaCl ₂ - NaCl	-0.27586	0.27586	-1	--	0.05	1	--	--

SE: Standard error of the mean

Sig: Significance degree, "1" is significant while "0" is non-significant

LCL: Lower Confidence Limits

UCL: Upper Confidence Limits

Table S4. The statistical Welch's test results for nitrate formations in the presence of different scavengers at the final condition.

¹ DF Number	¹ DF Den	F-Value	P-Value
9	4.5017	17041.72429	1.12999E-10
¹ degree of freedom			

Table S5. Games-Howell Pairwise Comparisons obtained from the One-Way Welch's ANOVA for nitrate formations in the presence of different scavengers at the final condition.

	Mean Diff	SE ¹	T-Value	Prob	Alpha	Sig ²	LCL	UCL
Tap water - UPW	26.79501	14.77413	1.81364	0.72528	0.05	0	-119.262	172.8525
KSW - UPW	14.1676	14.82239	0.95582	0.96912	0.05	0	-130.131	158.4662
KSW - Tap water	-12.6274	1.23758	-10.2033	0.15316	0.05	0	-48.8934	23.63859
NaOH - UPW	16.51277	15.04759	1.09737	0.94461	0.05	0	-120.446	153.4717
NaOH - Tap water	-10.2822	2.87373	-3.57802	0.31055	0.05	0	-38.2908	17.72628
NaOH - KSW	2.34517	3.11236	0.7535	0.99315	0.05	0	-20.9716	25.66192
Na ₂ CO ₃ - UPW	-5.4045	14.78189	-0.36562	0.99994	0.05	0	-151.173	140.3641
Na ₂ CO ₃ - Tap water	-32.1995	0.57664	-55.8403	0.01062	0.05	1	-42.4263	-21.9728
Na ₂ CO ₃ - KSW	-19.5721	1.32702	-14.7489	0.06285	0.05	0	-42.7488	3.60458
Na ₂ CO ₃ - NaOH	-21.9173	2.91336	-7.52301	0.07489	0.05	0	-48.6537	4.81918
NaHCO ₃ - UPW	1070920	1070911	1.00001	0.94467	0.05	0	-3.61E+07	3.82E+07
NaHCO ₃ - Tap water	1070893	1070911	0.99998	0.94467	0.05	0	-3.61E+07	3.82E+07
NaHCO ₃ - KSW	1070906	1070911	0.99999	0.94467	0.05	0	-3.61E+07	3.82E+07
NaHCO ₃ - NaOH	1070903	1070911	0.99999	0.94467	0.05	0	-3.61E+07	3.82E+07
NaHCO ₃ - Na ₂ CO ₃	1070925	1070911	1.00001	0.94467	0.05	0	-3.61E+07	3.82E+07
H ₃ PO ₄ - UPW	-8.32273	14.7724	-0.5634	0.99853	0.05	0	-154.445	137.7994
H ₃ PO ₄ - Tap water	-35.1177	0.22826	-153.851	0.01037	0.05	1	-42.629	-27.6065
H ₃ PO ₄ - KSW	-22.4903	1.21679	-18.4834	0.09354	0.05	0	-64.631	19.65034
H ₃ PO ₄ - NaOH	-24.8355	2.86483	-8.66909	0.06445	0.05	0	-53.1689	3.49793
H ₃ PO ₄ - Na ₂ CO ₃	-2.91824	0.53054	-5.50046	0.30511	0.05	0	-21.146	15.30951
H ₃ PO ₄ - NaHCO ₃	-1070928	1070911	-1.00002	0.94467	0.05	0	-3.82E+07	3.61E+07
HCl - UPW	6.33244	14.7724	0.42867	0.99979	0.05	0	-139.79	152.4545
HCl - Tap water	-20.4626	0.22826	-89.6467	0.01799	0.05	1	-27.9738	-12.9514
HCl - KSW	-7.83516	1.21679	-6.43923	0.26342	0.05	0	-49.9758	34.30552
HCl - NaOH	-10.1803	2.86483	-3.55355	0.31629	0.05	0	-38.5138	18.1531
HCl - Na ₂ CO ₃	11.73694	0.53054	22.12245	0.07769	0.05	0	-6.49081	29.96469
HCl - NaHCO ₃	-1070913	1070911	-1	0.94467	0.05	0	-3.82E+07	3.61E+07
HCl - H ₃ PO ₄	14.65517	0.03271	447.9998	2.06E-05	0.05	1	14.33159	14.97875
NaCl - UPW	8.91865	14.7724	0.60374	0.99768	0.05	0	-137.203	155.0407
NaCl - Tap water	-17.8764	0.22826	-78.3165	0.02065	0.05	1	-25.3876	-10.3652
NaCl - KSW	-5.24895	1.21679	-4.31379	0.38283	0.05	0	-47.3896	36.89172
NaCl - NaOH	-7.59412	2.86483	-2.65081	0.48229	0.05	0	-35.9276	20.73931
NaCl - Na ₂ CO ₃	14.32314	0.53054	26.99709	0.06366	0.05	0	-3.90461	32.55089
NaCl - NaHCO ₃	-1070911	1070911	-1	0.94467	0.05	0	-3.82E+07	3.61E+07
NaCl - H ₃ PO ₄	17.24138	0.03271	527.0585	1.77E-05	0.05	1	16.9178	17.56496
NaCl - HCl	2.58621	0.03271	79.05878	8.08E-04	0.05	1	2.26263	2.90979
CaCl ₂ - UPW	-1.22223	17.91816	-0.06821	1	0.05	0	-121.177	118.7322
CaCl ₂ - Tap water	-28.0172	10.14342	-2.76211	0.55959	0.05	0	-379.056	323.022
CaCl ₂ - KSW	-15.3898	10.21359	-1.5068	0.82447	0.05	0	-344.877	314.0972
CaCl ₂ - NaOH	-17.735	10.53775	-1.683	0.77646	0.05	0	-272.655	237.1847
CaCl ₂ - Na ₂ CO ₃	4.18227	10.15472	0.41185	0.99947	0.05	0	-343.214	351.5784
CaCl ₂ - NaHCO ₃	-1070921	1070911	-1.00001	0.94467	0.05	0	-3.82E+07	3.61E+07
CaCl ₂ - H ₃ PO ₄	7.1005	10.1409	0.70018	0.98762	0.05	0	-344.76	358.9605
CaCl ₂ - HCl	-7.55467	10.1409	-0.74497	0.98334	0.05	0	-359.415	344.3054
CaCl ₂ - NaCl	-10.1409	10.1409	-1	0.94467	0.05	0	-362.001	341.7192

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