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Assessment of Water Quality Variations on Pretreatment and Environmental Impacts of SWRO Desalination

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Table S1: Feed water quality data, reproduced with permission of DESWATER from Loganathan et al. (2019). Readers are referred to the original publication for trace elements data.

Sample	pH	Salinity ppm	T °C	Turbidity NTU	TOC ppm	Cl ⁻ ppm	SO ₄ ²⁻ ppm	Na ⁺ ppm	K ⁺ ppm	Mg ²⁺ ppm	Ca ²⁺ ppm
S 001	8.28	42,210	22	0.23	0.92	23,280	3,371	13,570	45.6	1,683	257.7
S 002	8.11	41,490	22	0.67	0.48	22,910	3,368	13,220	40.6	1,677	265.1
S 003	8.04	41,570	22	0.43	1.41	22,730	3,308	13,400	51.1	1,574	506.2
S 004	8.08	42,330	22	0.23	0.46	23,150	3,629	13,540	45.0	1,696	267.7
S 005	8.25	43,090	22	0.26	1.56	23,530	3,369	13,910	90.9	1,662	519.7
S 006	8.34	41,650	21	0.32	2.04	22,530	3,282	13,840	51.4	1,700	256.2
S 007	8.24	39,170	21	0.53	1.72	21,410	2,947	12,920	24.7	1,617	252.7
S 008	8.34	42,670	19	0.22	1.33	23,670	3,083	13,840	58.8	1,754	261.7
S 009	8.36	43,720	19	0.29	0.52	24,110	3,482	14,040	65.7	1,755	262.9
S 010	8.06	46,540	19	0.36	1.90	25,640	3,793	14,860	98.4	1,868	280.6
S 011	8.3	48,090	20	0.28	0.38	26,020	3,822	15,810	134.3	1,995	303.2
S 012	8.23	44,610	19	0.24	1.43	24,520	3,602	14,350	74.3	1,789	271.3
S 013	8.28	58,330	20	0.19	2.16	31,940	4,606	18,810	236.4	2,358	374.5
S 014	8.13	53,720	21	0.19	3.00	29,460	4,236	17,340	180.3	2,174	331.8
S 015	8.18	43,670	19	0.29	1.11	24,160	3,580	13,850	70.9	1,742	266.1
S 016	8.32	43,300	19	0.18	2.03	23,970	3,438	13,820	65.4	1,737	266.1
S 017	8.21	44,750	20	0.15	1.75	24,270	3,608	14,720	74.3	1,805	277.6
S 018	8.16	53,780	18	0.21	2.52	29,480	4,344	17,240	186.3	2,196	335.6
S 019	8.09	54,490	18	0.21	2.49	30,040	4,296	17,400	190.7	2,216	342.3

Table S2 shows examples for the existing plant normal operation electrical and chemical consumption vs. the simulated plant simulated on the same location using sample number 16.

Item	Example	Existing plant	Simulated plant	Unit
1	Electrical consumption	4.5	4.3	kwh
2	Sodium Hypochlorite (Shock biological disinfection)	11	11	ppm
3	Sulfuric Acid (pH control)	20	22	ppm
4	Ferric Chloride (Coagulation)	3.6	3	ppm
5	Antiscalent (Avoid salt precipitation)	3	1.5	ppm
6	Sodium Bisulphite (Dechlorination)	5.9	6	ppm
7	Sodium Hydroxide (pH increase)	11	12.5	ppm

Table S3 shows the chemicals considered in each pretreatment stage and their origin, as used in the study (either Europe or USA). Table S4 shows comparisons for chemicals that could be sourced from both locations in the database, when at least one of the chemicals under consideration could only come from the USA. In general the impact associated with the geographical source was minor, with the exception of a few impact categories for particular chemicals. The GWP difference was 0 for all assessed chemicals, while MAETP was also minimal, with the exception of hydrogen peroxide which had a 14% reduction if sourced from the USA.

Table S3: Chemicals sources showing priority for Europe as it is closer to Qatar and US was chosen in case there was no other option.

		Europe	USA
Disinfection	Sodium Hypochlorite		•
	Calcium hypochlorite	•	
	Chlorine	•	
	Chlorine dioxide	•	
pH control	Sulfuric acid	•	
	Carbon dioxide	•	
	Hydrochloric acid	•	
Coagulation	Ferric chloride	•	
	Aluminium sulphate	•	
	PACI	•	
Dechlorination	Sodium bisulphite		•
	Sodium sulphite	•	
	Hydrogen peroxide	•	
pH neutralization	Sodium hydroxide	•	
	Calcium oxide	•	
	Sodium carbonate		•

Table S4: Comparison of environmental impact changes at S13 using certain chemicals when sourced from Europe and the USA.

			Europe	USA	% Difference
Disinfection	Chlorine	GWP	2.00E+04	2.00E+04	0
		AP	1.30E+02	1.40E+02	8
		ODP	3.61E-07	9.25E-07	156
		ADP	2.58E-01	2.60E-01	1
		HTP	1.00E+03	6.00E+02	-40
		MAETP	1.32E+06	1.30E+06	-2
Dechlorination	Hydrogen peroxide	GWP	50000	50000	0
		AP	190	200	5
		ODP	4.64117E-06	6.31117E-06	26
		ADP	0.32146	0.32446	1
		HTP	1800	2100	14
		MAETP	2095000	2075000	-1
pH Adjustment	Sodium hydroxide	GWP	40000	40000	0
		AP	190	200	5
		ODP	4.63387E-06	6.91387E-06	33
		ADP	0.44946	0.45946	2
		HTP	1900	2100	10
		MAETP	1925000	1695000	-14
	Calcium hydroxide	GWP	40000	40000	0
		AP	170	170	0
		ODP	4.40603E-06	4.44387E-06	1
		ADP	0.34946	0.34946	0
		HTP	1600	1700	6
		MAETP	1415000	1385000	-2

Table 4 shows the main design output parameters that fed to the LCA model. The recovery ratio used for each model was 45% and in line to the existing plant recovery ratio. No large differences was observed in the number of membrane modules required or their flux was observed.

Table S5: Main design output parameters that fed to the LCA model.

Sample	Electricity kWh	Sodium Hypochlorite Kg	Sulfuric Acid Kg	Ferric Chloride Kg	Antiscalent Kg	Sodium Bisulphite Kg	Sodium Hydroxide Kg
S 001	2,293,315	6,438	13,576	2,337	1,788	3,799	7,082
S 002	2,276,576	6,438	10,832	2,497	1,767	3,799	7,082
S 003	2,264,343	6,438	10,068	2,410	1,751	3,799	7,082
S 004	2,306,192	6,438	10,518	2,337	1,800	3,799	7,082
S 005	2,198,029	6,438	12,480	2,348	1,683	3,799	7,082
S 006	2,295,891	6,438	13,661	2,370	1,788	3,799	7,082
S 007	2,156,824	6,439	12,149	2,447	1,643	3,799	7,082
S 008	2,207,686	6,439	13,194	2,334	1,684	3,799	7,082
S 009	2,225,713	6,439	13,474	2,359	1,697	3,799	7,082
S 010	2,399,547	6,439	10,034	2,385	1,898	3,799	7,082
S 011	2,484,532	6,438	13,101	2,356	1,998	3,799	7,082
S 012	2,206,399	6,439	11,792	2,341	1,684	3,799	7,082
S 013	2,857,952	6,438	13,169	2,323	2,409	3,799	7,082
S 014	2,852,802	6,438	11,274	2,323	2,351	3,799	7,082
S 015	2,164,550	6,439	11,300	2,359	1,833	3,799	7,082
S 016	2,393,753	6,439	13,109	2,319	1,891	3,799	7,082
S 017	2,369,287	6,439	11,809	2,308	1,867	3,799	7,082
S018	2,638,407	6,438	11,104	2,330	2,169	3,799	7,082
S019	2,583,038	6,439	10,306	2,330	2,101	3,799	7,082

Regression analysis was conducted for various water quality parameters and independent predictors of electricity and chemical consumption in the SWRO plant using the generated data from the AqMB model outputs at the 19 different sites. These are summarized below. *Salinity* is total dissolved solids, *T* is temperature, *TOC* is total (dissolved) organic carbon, Ca^{2+} is the calcium ion concentration, *pH* is self explanatory, SO_4^{2-} is the sulfate ion concentration.

Table S6: Model summaries for regression of water quality parameters against electricity

Model	R	R ²	Adjusted R ²	RMSE
0	0.947	0.897	0.884	73106.405
1	0.968	0.937	0.919	60909.561

Note: Null model includes Salinity, T

Table S7: Coefficients and collinearity statistics for model fits of water quality parameters to predict electricity

Model		Unstandardized	Standard Error	Standardized	t	p	95% CI		Collinearity Statistics	
							Lower	Upper	Tolerance	VIF
0	(Intercept)	-265416.517	377359.475		-0.703	0.492	-1.065e +6	534549.833		
	Salinity	41.174	3.587	1.033	11.479	< .001	33.570	48.778	0.796	1.256
	T	37678.478	13557.690	0.250	2.779	0.013	8937.460	66419.496	0.796	1.256
1	(Intercept)	-486782.044	332618.182		-1.463	0.165	-1.200e +6	226613.005		
	Salinity	40.624	3.636	1.019	11.171	< .001	32.825	48.424	0.538	1.860
	T	54069.370	12766.874	0.359	4.235	< .001	26687.148	81451.592	0.623	1.605
	TOC	50781.565	23842.671	0.180	2.130	0.051	-355.878	101919.008	0.628	1.593
	Ca2+	-521.626	210.171	-0.193	-2.482	0.026	-972.398	-70.855	0.741	1.350

Table S8: Partial correlations for the model fits of water quality parameters to predict electricity

Model		Partial	Part
0	Salinity	0.944	0.922
	T	0.571	0.223
1	Salinity	0.948	0.748
	T	0.749	0.283
	TOC	0.495	0.143
	Ca2+	-0.553	-0.166

Table S9: Model summaries for regression of water quality parameters against sulphuric acid consumption

Model	R	R ²	Adjusted R ²	RMSE
0	0.973	0.947	0.944	299.304
1	0.986	0.973	0.969	221.016
2	0.993	0.986	0.983	164.846

Note. Null model includes pH

Table S10: Coefficients and collinearity statistics for model fits of water quality parameters to predict sulphuric acid consumption

Model		Unstandardized	Standard Error	Standardized	t	p	95% CI		Collinearity Statistics	
							Lower	Upper	Tolerance	VIF
0	(Intercept)	-85959.937	5613.211		-15.314	< .001	-97802.776	-74117.097		
	pH	11924.292	683.609	0.973	17.443	< .001	10482.003	13366.581	1.000	1.000
1	(Intercept)	-91279.683	4364.117		-20.916	< .001	-100531.198	-82028.169		
	pH	12218.547	510.419	0.997	23.938	< .001	11136.508	13300.586	0.978	1.022
	T	144.051	36.977	0.162	3.896	0.001	65.663	222.438	0.978	1.022
2	(Intercept)	-98404.794	3779.434		-26.037	< .001	-106460.466	-90349.121		
	pH	12784.883	410.169	1.043	31.170	< .001	11910.630	13659.137	0.843	1.187
	T	198.216	31.206	0.223	6.352	< .001	131.702	264.730	0.764	1.309
	SO42-	0.380	0.102	0.134	3.710	0.002	0.162	0.598	0.721	1.387

Table S11: Partial correlations for the model fits of water quality parameters to predict sulphuric acid consumption

Model		Partial	Part
0	pH	0.973	0.973
1	pH	0.986	0.986
	T	0.698	0.160
2	pH	0.992	0.958
	T	0.854	0.195
	SO42-	0.692	0.114

Table S12: Model summaries for regression of water quality parameters against hypochlorite consumption

Model	R	R ²	Adjusted R ²	RMSE
0	0.640	0.410	0.375	0.302
1	0.826	0.683	0.643	0.228

Note. Null model includes T

Table S13: Coefficients and collinearity statistics for model fits of water quality parameters to predict hypochlorite consumption

Model		Unstandardized	Standard Error	Standardized	t	p	95% CI		Collinearity Statistics	
							Lower	Upper	Tolerance	VIF
0	(Intercept)	6441.351	1.010		6375.386	< .001	6439.220	6443.483		
	T	-0.172	0.050	-0.640	-3.436	0.003	-0.277	-0.066	1.000	1.000
1	(Intercept)	6444.684	1.179		5466.494	< .001	6442.184	6447.183		
	Salinity	-4.157e-5	1.121e-5	-0.585	-3.710	0.002	-6.533e-5	-1.782e-5	0.796	1.256
	T	-0.243	0.042	-0.905	-5.732	< .001	-0.333	-0.153	0.796	1.256

Table S14: Partial correlations for the model fits of water quality parameters to predict hypochlorite consumption

Model		Partial	Part
0	T	-0.640	-0.640
1	Salinity	-0.680	-0.522
	T	-0.820	-0.807

Table S15: Model summaries for regression of water quality parameters against antiscalant consumption

Model	R	R ²	Adjusted R ²	RMSE
0	0.925	0.856	0.848	87.673
1	0.952	0.906	0.894	73.225

Note. Null model includes Mg2+

Table S16: Coefficients and collinearity statistics for model fits of water quality parameters to predict antiscalant consumption

Model		Unstandardized	Standard Error	Standardized	t	p	Collinearity Statistics	
							Tolerance	VIF
0	(Intercept)	222.818	166.439		1.339	0.198		
	Mg2+	0.902	0.090	0.925	10.056	< .001	1.000	1.000
1	(Intercept)	-817.184	385.409		-2.120	0.050		
	T	40.327	13.939	0.256	2.893	0.011	0.756	1.324
	Mg2+	1.025	0.086	1.052	11.897	< .001	0.756	1.324

Table S17: Partial correlations for the model fits of water quality parameters to predict antiscalant consumption

Model		Partial	Part
0	Mg2+	0.925	0.925
1	T	0.586	0.222
	Mg2+	0.948	0.914

Table S18: Model summaries for regression of water quality parameters against ferric chloride consumption

Model	R	R ²	Adjusted R ²	RMSE
1	0.481	0.231	0.186	42.893

Table S19: Coefficients and collinearity statistics for model fits of water quality parameters to predict ferric chloride consumption

Model		Unstandardized	Standard Error	Standardized	t	p
1	(Intercept)	2552.914	86.457		29.528	< .001
	Salinity	-0.004	0.002	-0.481	-2.262	0.037

Table S19: Full table of normalized impacts including all chemical alternatives assessed

Impact Category	S13 Impact Normalized									
	Disinfection				pH Control			Coagulation		
	NaOCl	Ca(ClO) ₂	Cl ₂	ClO ₂	H ₂ SO ₄	CO ₂	HCl	FeCl ₃	Al ₂ (SO ₄) ₃	Al ₂ (OH) ₃ Cl ₃
GWP	20.61	20.50	20.38	20.38	20.61	20.73	20.61	20.61	20.73	20.73
AP	4.24	4.16	4.14	4.14	4.24	4.13	4.11	4.24	4.29	4.25
ODP	1.05E-05	7.21E-07	8.32E-07	8.16E-07	1.05E-05	1.04E-05	1.04E-05	1.05E-05	1.06E-05	1.04E-05
ADP	2.77E-05	1.54E-05	1.60E-05	1.58E-05	2.77E-05	2.77E-05	2.81E-05	2.77E-05	4.01E-05	3.33E-05
HTP	1.63	1.58	1.58	1.58	1.63	1.61	1.61	1.63	2.94	2.49
MAETP	160.20	113.67	113.67	112.14	160.20	153.33	149.52	160.20	1083.25	747.60
Impact Category	S13 Impact Normalized									
	Dechlorination			pH Adjustment (Neutralization)			Electricity (Slovenia database)			
	NaHSO ₃	Na ₂ SO ₃	H ₂ O ₂	NaOH	Ca(OH) ₂	Na ₂ CO ₃	NG	Solar PV	Wind	
GWP	20.61	20.61	20.73	20.61	20.61	20.84	19.47	2.80	0.73	
AP	4.24	4.25	4.24	4.24	4.21	4.43	1.96	1.61	0.42	
ODP	1.05E-05	1.06E-05	1.05E-05	1.05E-05	1.00E-05	1.01E-05	1.06E-05	2.08E-05	1.10E-05	
ADP	2.77E-05	1.07E-04	1.98E-05	2.77E-05	2.15E-05	5.02E-05	3.63E-05	7.34E-04	1.06E-04	
HTP	1.63	1.62	1.62	1.63	1.61	1.63	0.60	8.11	0.70	
MAETP	160.20	152.57	173.17	160.20	118.24	140.37	215.13	5835.84	535.52	

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