

Supporting Information

Li⁺ separation from multi-ionic mixtures by nanofiltration membranes:
experiments and modeling

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Appendix S1: Details on solving the Differential-algebraic-equation

Setting up eq. (8) for three ion species and the electrostatic potential, it is possible to express the ion concentrations and the electrostatic potential at the collocation points as the following matrix multiplication:

$$[C] = [A] \cdot [\theta] \text{ or } [\theta] = [A]^{-1} \cdot [C] \quad (\text{SE1})$$

The rows of the matrix $[C]$ correspond to the values of the modelled variables at the v collocation points $z_1 - z_v$ whereas the columns are the different modelled variables, namely the different ion species concentrations $c_1 - c_n$ and the electrostatic potential ϕ . Matrix $[A]$ is a Vandermonde-Matrix. The corresponding polynomial coefficients are stored in matrix $[\theta]$, where the rows include the necessary coefficients for the polynomial and the columns represent the different modelled variables.

Equation (SE1) can be transformed for three ion species and the electrostatic potential to:

$$\begin{pmatrix} c_1(z) \\ c_2(z) \\ c_3(z) \\ \phi(z) \end{pmatrix} = [1 \ z \dots z^n] [\theta] \quad (\text{SE2})$$

Thus, substituting eq. (SE1) in eq. (SE2) yields:

$$\begin{pmatrix} c_1(z) \\ c_2(z) \\ c_3(z) \\ \phi(z) \end{pmatrix} = [1 \ z \dots z^n] [A]^{-1} \cdot [C] \quad (\text{SE3})$$

The derivatives at the collocation points of the functions contained in the matrix formulation in eq. (SE3) are evaluated by the following polynomials:

$$\left[\frac{dc_1(z)}{dz} \quad \frac{dc_2(z)}{dz} \quad \frac{dc_3(z)}{dz} \quad \frac{d\phi(z)}{dz} \right] = [D] \cdot [C] \quad (\text{SE4})$$

$$\text{whereby: } [D] = [0 \ 1 \dots n \ z_1^{n-1}] [A]^{-1} \quad (\text{SE5})$$

Equations (SE3) and (SE4) were inserted in the differential-algebraic-equation system from equations (5) and (6). Given that the matrices $[A]$ and $[D]$ are known by the choice of the collocation points, the system was solved algebraically according to eq. (SE3) by resolving the matrix $[C]$.

Appendix S2: Ion rejections in the membrane screening for DL and TS40 membrane

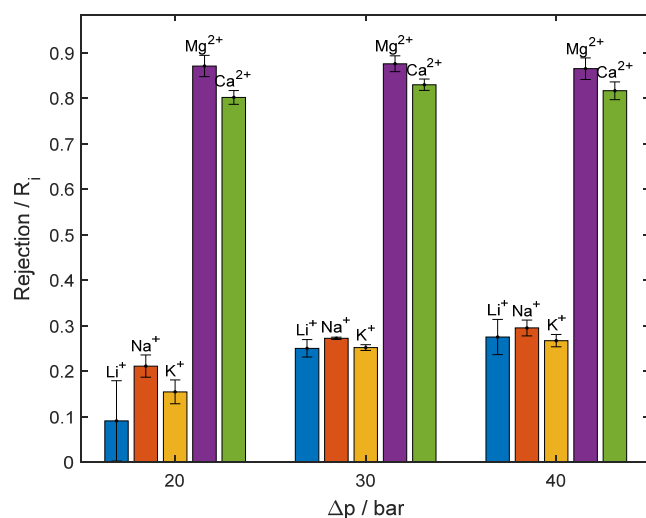


Figure S 1: Experimentally determined ion rejections for DL membrane at different pressure level. Colors denote to the five ion species. Error bars represent standard deviations estimated from four membrane cells. Conditions: Membrane: = DL (Suez), $A_{\text{Mem}} = 17 \text{ cm}^2$, $T = 20^\circ\text{C}$, $\Delta p = 5\text{-}40 \text{ bar}$, $\dot{m}_{\text{feed}} = 75 \text{ kg h}^{-1}$. Feed concentrations according to Table 4 - STS.

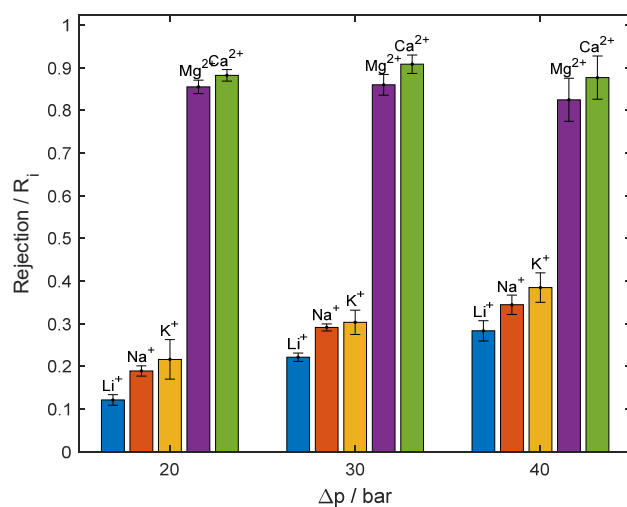


Figure S 2: Experimentally determined ion rejections for TS40 membrane at different pressure level. Colors denote to the five ion species. Error bars represent standard deviations estimated from four membrane cells. Conditions: Membrane: = TS40 (Mann+Hummel), $A_{\text{Mem}} = 17 \text{ cm}^2$, $T = 20^\circ\text{C}$, $\Delta p = 5\text{-}40 \text{ bar}$, $\dot{m}_{\text{feed}} = 75 \text{ kg h}^{-1}$. Feed concentrations according to Table 4 - STS.

Appendix S3 – experimental permeate flows and ion rejections

Table S1: Feed and permeate concentrations in mg kg⁻¹ with STS concentrations (c.f. Table 4) at different transmembrane pressure levels for Cell 1-4. Experiments were performed at a temperature of 20 °C and a feed mass flow rate of 75 kg h⁻¹ and the area of the used membrane TS40 is A = 17 cm².

20 bar

	Li ⁺	Na ⁺	K ⁺	Mg ²⁺	Ca ²⁺
Feed	0.1773	11449.711	701.533	1527.716	505.575
Cell 1	0.1570	9381.763	606.722	295.565	128.919
Cell 2	0.1579	9848.208	643.043	259.740	118.850
Cell 3	0.1556	9148.088	556.855	262.104	121.399
Cell 4	0.1529	9250.688	599.567	271.713	119.33

30 bar

	Li ⁺	Na ⁺	K ⁺	Mg ²⁺	Ca ²⁺
Feed	0.1769	11620.837	713.338	1531.965	510.679
Cell 1	0.1391	8350.893	519.192	303.433	125.116
Cell 2	0.1358	8173.523	508.583	220.221	102.748
Cell 3	0.1393	8350.922	516.072	264.532	114.481
Cell 4	0.1367	8260.972	527.153	259.588	111.840]

40 bar

	Li ⁺	Na ⁺	K ⁺	Mg ²⁺	Ca ²⁺
Feed	0.1790	11041.060	683.600	1448.844	483.871
Cell 1	0.1342	8019.365	481.474	411.142	160.490
Cell 2	0.1278	7641.022	469.245	246.872	106.431
Cell 3	0.1276	7537.242	463.546	292.860	121.196
Cell 4	0.1238	7343.099	463.640	276.618	112.257

Table S2: Feed and permeate concentrations in mg kg⁻¹ with STS concentrations (c.f. Table 4) at different transmembrane pressure levels for Cell 1-4. Experiments were performed at a temperature of 20 °C and a feed mass flow rate of 75 kg h⁻¹ and the area of the used membrane ALNF is A = 17 cm².

20 bar

	Li ⁺	Na ⁺	K ⁺	Mg ²⁺	Ca ²⁺
Feed	0.1370	10908.564	656.557	1400.178	452.036
Cell 1	0.1557	9836.666	639.186	121.240	66.786
Cell 2	0.1439	9770.855	611.300	108.984	60.382
Cell 3	0.1316	9843.756	644.554	113.500	62.848
Cell 4	0.1597	9654.802	633.709	129.567	64.212

30 bar

	Li ⁺	Na ⁺	K ⁺	Mg ²⁺	Ca ²⁺
Feed	0.1542	11428.153	681.779	1427.718	457.619
Cell 1	0.1681	8841.591	570.353	112.157	58.321
Cell 2	0.1291	8684.894	558.848	107.005	58.388
Cell 3	0.1275	8908.654	575.066	115.259	64.055
Cell 4	0.1228	8809.011	565.328	136.361	66.951

40 bar

	Li ⁺	Na ⁺	K ⁺	Mg ²⁺	Ca ²⁺
Feed	0.1515	11281.394	675.701	1399.753	450.009
Cell 1	0.1204	8636.074	554.276	139.109	66.444
Cell 2	0.2442	8250.358	536.853	122.396	62.656
Cell 3	0.1260	8499.544	556.375	123.265	66.929
Cell 4	0.1220	8402.824	548.268	161.570	77.636

Table S3: Feed and permeate concentrations in mg kg⁻¹ with STS concentrations (c.f. Table 4) at different transmembrane pressure levels for Cell 1-4. Experiments were performed at a temperature of 20 °C and a feed mass flow rate of 75 kg h⁻¹ and the area of the used membrane DL is A = 17 cm².

20 bar

	Li ⁺	Na ⁺	K ⁺	Mg ²⁺	Ca ²⁺
Feed	0.1148	8622.447	522.712	1130.107	371.436
Cell 1	0.8066	6490.119	421.555	150.998	75.011
Cell 2	0.1115	6858.466	446.351	124.125	69.154
Cell 3	0.1535	6904.971	449.386	125.871	68.899
Cell 4	0.0972	6951.974	450.398	180.533	80.817

30 bar

	Li ⁺	Na ⁺	K ⁺	Mg ²⁺	Ca ²⁺
Feed	0.1219	8457.240	528.684	1105.307	362.781
Cell 1	0.0883	6124.260	391.486	151.655	69.056
Cell 2	0.0940	6167.809	399.595	119.147	58.523
Cell 3	0.0919	6153.550	396.048	120.847	59.427
Cell 4	0.0913	6167.123	394.753	155.151	66.841

40 bar

	Li ⁺	Na ⁺	K ⁺	Mg ²⁺	Ca ²⁺
Feed	0.1211	8367.517	511.009	1065.245	346.527
Cell 1	0.0865	5740.683	367.300	154.976	66.582
Cell 2	0.0944	5926.281	379.694	123.076	58.789
Cell 3	0.0868	5838.960	369.786	121.492	56.931
Cell 4	0.0834	6086.943	381.152	173.718	71.447

Table S4: Permeate fluxes in g h^{-1} and experimental rejections of the Na^+ and Li^+ ions of the subsystem with Li^+ ions based in SW concentrations (31410 mg kg^{-1} NaCl. 1.28 mg kg^{-1} LiCl in MilliQ water). The experiments were performed at a temperature of 20 °C and a feed mass flow rate of 75 kg h^{-1} and the area of the used membrane NFAL is $A = 17 \text{ cm}^2$.

Subsystem NaCl + LiCl

Permeate flow g h^{-1}	45 bar	40 bar	35 bar	30 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	202.890	171.042	135.882	117.804	95.352	77.832	51.312	38.304	23.142
Cell 2	235.524	203.016	158.856	136.728	112.494	83.970	68.106	47.982	30.084
Cell 3	217.788	189.066	144.822	123.108	101.136	79.260	57.138	41.454	30.510
Cell 4	232.338	186.480	151.830	134.718	97.638	89.604	63.528	32.580	26.712

Rejection of Na^+	45 bar	40 bar	35 bar	30 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.367	0.351	0.280	0.260	0.212	0.191	0.158	0.126	0.094
Cell 2	0.374	0.345	0.267	0.261	0.199	0.202	0.131	0.105	0.086
Cell 3	0.371	0.337	0.282	0.277	0.206	0.221	0.178	0.126	0.083
Cell 4	0.350	0.329	0.270	0.276	0.200	0.201	0.157	0.104	0.073

Rejection of Li^+	45 bar	40 bar	35 bar	30 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.330	0.282	0.261	0.182	0.177	0.176	0.163	0.073	0.081
Cell 2	0.288	0.296	0.255	0.192	0.215	0.165	0.162	0.101	0.063
Cell 3	0.273	0.286	0.263	0.225	0.185	0.165	0.148	0.087	0.046
Cell 4	0.290	0.256	-	0.206	0.161	0.163	0.138	-	0.057

Table S5: Permeate fluxes in g h^{-1} and experimental rejections of the Na^+ and Mg^{2+} ions of the subsystem with Mg^{2+} ions based in SW concentrations (31410 mg kg^{-1} NaCl. 6131 mg kg^{-1} MgCl_2 in MilliQ water). The experiments were performed at a temperature of 20°C and a feed mass flow rate of 75 kg h^{-1} and the area of the used membrane NFAL is $A = 17 \text{ cm}^2$.

Subsystem NaCl + MgCl_2								
Permeate flow g h^{-1}	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	189.624	157.680	127.572	88.098	68.826	54.156	38.112	11.616
Cell 2	171.924	148.362	116.514	73.116	59.826	41.796	31.320	10.152
Cell 3	183.804	152.376	125.166	92.892	73.584	50.772	43.680	13.452
Cell 4	174.732	139.830	113.820	79.524	58.698	42.924	30.060	9.798
Rejection of Na^+	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.385	0.354	0.284	0.199	0.158	0.085	0.065	-0.044
Cell 2	0.389	0.350	0.295	0.200	0.147	0.087	0.060	-0.044
Cell 3	0.367	0.329	0.282	0.185	0.127	0.074	0.026	-0.017
Cell 4	0.369	0.326	0.275	0.190	0.132	0.085	0.039	-0.008
Rejection of Mg^{2+}	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.963	0.963	0.954	0.957	0.950	-	0.908	0.891
Cell 2	0.965	0.966	0.964	0.961	0.956	0.950	0.944	0.894
Cell 3	0.960	0.961	0.955	0.949	0.927	0.906	-	-
Cell 4	0.967	0.965	0.960	0.957	0.948	0.948	0.938	0.895

Table S6: Permeate fluxes in g h^{-1} and experimental rejections of the Na^+ and K^+ ions of the subsystem with K^+ ions based in SW concentrations (31410 mg kg^{-1} NaCl. 1425 mg kg^{-1} KCl in MilliQ water). The experiments were performed at a temperature of 20°C and a feed mass flow rate of 75 kg h^{-1} and the area of the used membrane NFAL is $A = 17 \text{ cm}^2$.

Subsystem NaCl + KCl									
Permeate flow g h^{-1}	45 bar	40 bar	35 bar	30 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	194.826	166.932	146.052	126.006	95.250	81.726	60.468	49.440	29.178
Cell 2	200.418	171.738	154.110	141.480	100.752	92.928	69.144	62.544	33.426
Cell 3	202.440	164.046	145.518	141.066	98.364	82.944	58.764	43.722	30.432
Cell 4	184.980	154.992	137.040	129.006	86.766	79.938	51.042	51.252	23.820
Rejection of Na^+	45 bar	40 bar	35 bar	30 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.289	0.261	0.252	0.259	0.207	0.176	0.141	0.111	0.081
Cell 2	0.293	0.252	0.264	0.252	0.186	0.169	0.155	0.108	0.071
Cell 3	0.300	0.243	0.212	0.245	0.201	0.160	0.145	0.066	0.069
Cell 4	0.294	0.215	0.240	0.245	0.202	0.168	0.166	0.082	0.068
Rejection of K^+	45 bar	40 bar	35 bar	30 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.299	0.246	0.241	0.243	0.176	0.171	0.118	0.067	0.059
Cell 2	0.304	0.247	0.239	0.247	0.163	0.146	0.114	0.064	0.020
Cell 3	0.314	0.236	0.190	0.235	0.181	0.238	0.113	0.041	0.000
Cell 4	0.304	0.207	0.221	0.238	0.183	0.139	0.141	0.047	0.003

Table S7: Permeate fluxes in g h^{-1} and experimental rejections of the Na^+ and Ca^{2+} ions of the subsystem with Ca^{2+} ions based in SW concentrations (31410 mg kg^{-1} NaCl. 1339 mg kg^{-1} CaCl_2 in MilliQ water). The experiments were performed at a temperature of 20°C and a feed mass flow rate of 75 kg h^{-1} and the area of the used membrane NFAL is $A = 17 \text{ cm}^2$.

Subsystem NaCl + CaCl_2

Permeate flow g h^{-1}	45 bar	40 bar	35 bar	30 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	231.186	189.750	163.482	133.146	114.888	80.724	69.594	49.530	27.918
Cell 2	254.328	200.802	179.856	142.716	121.134	85.536	79.644	42.042	30.066
Cell 3	240.468	207.162	172.872	142.842	123.354	78.708	72.606	44.598	21.888
Cell 4	232.062	190.308	164.946	134.598	112.008	79.914	65.088	46.338	28.536
Rejection of Na^+	45 bar	40 bar	35 bar	30 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.393	0.355	0.324	0.271	0.235	0.178	0.217	0.171	0.081
Cell 2	0.378	0.347	0.327	0.259	0.249	0.186	0.218	0.152	0.082
Cell 3	0.370	0.344	0.325	0.248	0.234	0.171	0.181	0.126	0.093
Cell 4	0.368	0.336	0.319	0.210	0.238	0.152	0.193	0.116	0.090
Rejection of Ca^{2+}	45 bar	40 bar	35 bar	30 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.879	0.872	0.867	0.854	0.843	0.821	0.787	0.776	0.694
Cell 2	0.872	0.870	0.874	0.847	0.864	0.838	0.848	0.817	0.765
Cell 3	0.865	0.868	0.863	0.836	0.851	0.826	0.822	0.790	0.763
Cell 4	0.872	0.865	0.869	0.827	0.859	0.827	0.811	0.764	0.738

Table S8: Permeate fluxes in g h^{-1} and experimental rejections of the Na^+ and SO_4^{2-} ions of the subsystem with SO_4^{2-} ions based in SW concentrations (35173 mg kg^{-1} NaCl. 3917 mg kg^{-1} Na_2SO_4 in MilliQ water). The experiments were performed at a temperature of 20°C and a feed mass flow rate of 75 kg h^{-1} and the area of the used membrane NFAL is $A = 17 \text{ cm}^2$.

Subsystem NaCl+Na₂SO₄

Permeate flow g h^{-1}	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	216.000	163.140	139.746	95.766	64.842	44.652	33.012	16.554
Cell 2	247.680	186.600	160.998	114.294	78.990	59.700	25.140	22.422
Cell 3	224.376	168.876	147.204	99.372	65.622	47.670	27.624	14.712
Cell 4	242.580	184.842	159.294	109.464	78.126	53.646	35.916	16.158
Rejection of Cl^-	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.358	0.309	0.277	0.238	0.174	0.117	0.086	0.019
Cell 2	0.344	0.308	0.273	0.242	0.143	0.118	0.084	0.021
Cell 3	0.350	0.295	0.254	0.236	0.147	0.125	0.090	0.015
Cell 4	0.354	0.292	0.275	0.227	0.136	0.098	0.077	0.003
Rejection of SO_4^{2-}	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.976	0.961	0.954	0.963	0.959	0.945	0.944	0.913
Cell 2	0.991	0.995	0.995	0.995	0.976	0.915	0.936	0.974
Cell 3	0.997	0.999	0.998	0.997	0.996	0.995	0.994	0.990
Cell 4	0.995	0.997	0.997	0.993	0.988	0.949	0.987	0.991

Table S9: Permeate fluxes in g h^{-1} and experimental rejections of the ME-SW feed concentrations (c.f. Table 4) The experiments were performed at a temperature of 20 °C and a feed mass flow rate of 75 kg h^{-1} and the area of the used membrane NFAL is $A = 17 \text{ cm}^2$.

MW-Feed									
Permeate flow in g h^{-1}	45 bar	40 bar	35 bar	30 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	165.972	138.498	110.448	80.358	63.816	60.330	37.728	28.074	13.824
Cell 2	172.380	141.384	110.784	84.702	71.730	54.918	38.052	27.702	13.338
Cell 3	164.118	142.158	112.398	85.752	67.464	58.560	35.028	29.754	13.806
Cell 4	156.474	151.170	104.526	77.298	61.572	55.416	36.503	30.180	11.118
Rejection of Na^+	45 bar	40 bar	35 bar	30 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.381	0.333	0.259	0.190	0.133	0.096	0.061	-0.027	-0.071
Cell 2	0.373	0.311	0.265	0.180	0.120	0.099	0.043	-0.014	-0.083
Cell 3	0.341	0.289	0.240	0.161	0.094	0.082	0.029	-0.001	-0.021
Cell 4	0.357	0.297	0.242	0.173	0.121	0.108	0.063	0.004	-0.086
Rejection of Li^+	45 bar	40 bar	35 bar	30 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.221	0.197	0.163	0.076	0.127	-0.019	0.060	0.011	-0.046
Cell 2	0.224	0.180	0.170	-	0.071	0.085	-0.009	0.018	-0.054
Cell 3	0.232	0.147	0.165	0.061	0.034	0.004	0.000	-0.003	0.003
Cell 4	-	0.175	0.124	0.092	0.049	0.064	-0.010	-0.065	-0.029

Rejection of Mg²⁺	45 bar	40 bar	35 bar	30 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.963	0.961	0.955	0.947	0.950	0.944	0.933	0.914	0.851
Cell 2	0.960	0.961	0.959	0.955	0.950	0.947	0.934	0.930	0.886
Cell 3	0.948	0.943	0.942	0.939	0.925	0.928	0.915	0.896	0.882
Cell 4	0.960	0.955	0.958	0.948	0.947	0.942	0.926	0.908	0.880
Rejection of K⁺	45 bar	40 bar	35 bar	30 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.395	0.353	0.262	0.177	0.168	0.117	0.052	-0.001	-0.118
Cell 2	0.360	0.329	0.282	0.211	0.161	0.116	0.030	0.030	-0.090
Cell 3	0.373	0.314	0.257	0.212	0.145	0.105	0.015	-0.053	-0.018
Cell 4	0.377	0.307	0.278	0.181	0.153	0.114	-0.021	-0.084	-0.032
Rejection of Ca²⁺	45 bar	40 bar	35 bar	30 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.876	0.870	0.853	0.838	0.847	0.833	0.804	0.776	0.663
Cell 2	0.871	0.863	0.864	0.855	0.844	0.829	0.803	0.791	0.681
Cell 3	0.864	0.848	0.851	0.839	0.816	0.815	0.787	0.751	0.714
Cell 4	0.871	0.854	0.856	0.835	0.837	0.816	0.792	0.754	0.669

Table S10: Permeate fluxes in g h^{-1} and experimental rejections of the Na^+ and Li^+ ions of the subsystem with Li^+ ions based in ROB concentrations (60881 mg kg^{-1} NaCl. 2.44 mg kg^{-1} LiCl in MilliQ water). The experiments were performed at a temperature of 20°C and a feed mass flow rate of 75 kg h^{-1} and the area of the used membrane NFAL is $A = 17 \text{ cm}^2$.

Subsystem NaCl+LiCl								
Permeate flow in g h^{-1}	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	167.844	146.184	128.856	83.778	67.830	50.730	38.928	20.220
Cell 2	178.734	161.028	144.822	94.278	72.834	51.324	40.968	20.832
Cell 3	165.354	143.640	124.080	79.860	68.376	46.074	35.076	20.748
Cell 4	185.820	146.580	130.872	99.504	64.470	61.740	34.464	19.200
Rejection of Na^+	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.309	0.284	0.268	0.221	0.182	0.145	0.118	0.064
Cell 2	0.302	0.276	0.264	0.222	0.181	0.145	0.120	0.061
Cell 3	0.295	0.269	0.260	0.217	0.175	0.140	0.112	0.062
Cell 4	0.300	0.279	0.269	0.204	0.158	0.124	0.106	0.057
Rejection of Li^+	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.292	0.216	0.163	-	0.133	0.121	0.006	0.041
Cell 2	0.202	0.203	0.209	0.103	0.129	0.114	0.055	-0.038
Cell 3	0.234	0.248	0.233	0.165	0.124	0.093	0.030	-0.062
Cell 4	0.257	0.227	-	0.101	0.122	0.094	-	-0.058

Table S11: Permeate fluxes in g h^{-1} and experimental rejections of the Na^+ and Mg^{2+} ions of the subsystem with Mg^{2+} ions based in ROB concentrations (60881 mg kg^{-1} NaCl. 6131 mg kg^{-1} MgCl_2 in MilliQ water). The experiments were performed at a temperature of 20°C and a feed mass flow rate of 75 kg h^{-1} and the area of the used membrane NFAL is $A = 17 \text{ cm}^2$.

Subsystem NaCl+MgCl_2								
Permeate flow in g h^{-1}	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	98.436	90.468	73.488	52.578	45.108	25.458	19.950	6.912
Cell 2	112.404	98.796	82.644	60.606	44.724	30.108	19.668	7.290
Cell 3	103.590	95.964	80.136	55.440	40.254	28.776	14.484	8.382
Cell 4	114.876	94.554	85.350	57.054	48.012	36.840	22.422	8.010
Rejection of Na^+	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.241	0.213	0.183	0.107	0.088	0.029	-0.031	-0.070
Cell 2	0.253	0.212	0.170	0.110	0.069	0.031	-0.061	-0.072
Cell 3	0.226	0.206	0.175	0.112	0.089	-0.003	-0.042	-0.056
Cell 4	0.230	0.195	0.180	0.118	0.075	-0.027	-0.033	-0.074
Rejection of Mg^{2+}	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.926	0.924	0.933	0.915	0.919	0.895	0.847	0.745
Cell 2	0.953	0.950	0.946	0.931	0.903	0.822	0.827	0.776
Cell 3	0.934	0.933	0.932	0.925	0.920	0.895	0.858	0.779
Cell 4	0.940	0.943	0.937	0.927	0.897	-	0.815	0.727

Table S12: Permeate fluxes in g h^{-1} and experimental rejections of the Na^+ and K^+ ions of the subsystem with K^+ ions based in ROB concentrations (60881 mg kg^{-1} NaCl. 1526 mg kg^{-1} KCl in MilliQ water). The experiments were performed at a temperature of 20°C and a feed mass flow rate of 75 kg h^{-1} and the area of the used membrane NFAL is $A = 17 \text{ cm}^2$.

Subsystem NaCl+KCl								
Permeate flow in g h^{-1}	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	184.098	157.794	125.058	93.024	71.322	53.688	42.978	26.442
Cell 2	148.896	128.934	105.534	77.280	56.580	49.512	36.246	18.006
Cell 3	137.982	113.634	92.778	69.504	56.850	41.964	32.766	16.830
Cell 4	143.844	129.708	73.626	73.626	49.236	41.664	35.328	19.860
Rejections of Na^+	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.182	0.169	0.134	0.123	0.111	0.078	0.071	0.047
Cell 2	0.265	0.236	0.198	0.173	0.141	0.108	0.086	0.059
Cell 3	0.247	0.220	0.187	0.160	0.124	0.103	0.081	0.055
Cell 4	0.246	0.220	0.186	0.162	0.128	0.102	0.083	0.051
Rejections of K^+	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.213	0.195	0.159	0.140	0.127	0.082	0.074	0.047
Cell 2	0.247	0.228	0.194	0.166	0.133	0.099	0.074	0.051
Cell 3	0.242	0.217	0.174	0.143	0.117	0.095	0.070	0.047
Cell 4	0.236	0.212	0.185	0.149	0.123	0.094	0.076	0.043

Table S13: Permeate fluxes in g h^{-1} and experimental rejections of the Na^+ and Ca^{2+} ions of the subsystem with Ca^{2+} ions based in ROB concentrations ($60881 \text{ mg kg}^{-1} \text{ NaCl}$. $2206 \text{ mg kg}^{-1} \text{ CaCl}_2$ in MilliQ water). The experiments were performed at a temperature of 20°C and a feed mass flow rate of 75 kg h^{-1} and the area of the used membrane NFAL is $A = 17 \text{ cm}^2$.

Subsystem NaCl + CaCl_2								
Permeate flow in g h^{-1}	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	140.754	122.970	105.060	74.352	60.582	43.308	30.852	17.004
Cell 2	151.164	129.642	116.970	87.228	59.628	49.200	34.014	18.366
Cell 3	135.126	125.088	104.868	66.396	65.316	40.632	21.690	14.772
Cell 4	159.780	138.246	113.970	84.162	69.510	55.656	34.062	12.540
Rejection of Na^+	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.456	0.418	0.396	0.257	0.205	0.257	0.193	0.107
Cell 2	0.418	0.416	0.314	0.242	0.159	0.236	0.197	0.145
Cell 3	0.461	0.374	0.346	0.238	0.170	0.220	0.150	0.112
Cell 4	0.360	0.370	0.282	0.234	0.216	0.218	0.127	0.155
Rejection of Ca^{2+}	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.920	0.913	0.909	0.874	0.853	0.817	0.802	0.715
Cell 2	0.907	0.913	0.902	0.893	0.860	0.880	0.852	0.802
Cell 3	0.911	0.901	0.895	0.880	0.852	0.857	0.819	0.788
Cell 4	0.898	0.900	0.891	0.887	0.867	0.841	0.787	0.774

Table S14: Permeate fluxes in g h^{-1} and experimental rejections of the Na^+ and SO_4^{2-} ions of the subsystem with SO_4^{2-} ions based in ROB concentrations (66789 mg kg^{-1} NaCl. 7834 mg kg^{-1} CaCl_2 in MilliQ water). The experiments were performed at a temperature of 20 °C and a feed mass flow rate of 75 kg h^{-1} and the area of the used membrane NFAL is $A = 17 \text{ cm}^2$.

Subsystem NaCl + Na_2SO_4								
Permeate flow in g h^{-1}	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	135.876	114.942	96.156	57.438	49.056	35.520	21.978	12.126
Cell 2	150.972	122.844	104.364	63.006	59.370	53.910	27.816	12.318
Cell 3	139.446	113.184	91.674	65.556	48.000	39.024	23.130	10.920
Cell 4	154.590	141.828	111.030	60.906	52.416	39.036	25.308	11.946
Rejection of Cl^-	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.260	0.206	0.188	0.126	0.110	0.070	0.043	0.006
Cell 2	0.255	0.203	0.187	0.124	0.108	0.055	0.033	-0.003
Cell 3	0.254	0.190	0.179	0.118	0.100	0.063	0.036	0.002
Cell 4	0.250	0.193	0.179	0.119	0.095	0.058	0.034	0.001
Rejection of SO_4^{2-}	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.977	0.983	0.976	0.954	0.959	0.965	0.981	0.977
Cell 2	0.990	0.996	0.998	0.992	0.959	0.965	0.935	0.972
Cell 3	0.990	0.994	0.997	0.997	0.996	0.994	0.989	0.986
Cell 4	0.993	0.994	0.993	0.994	0.982	0.965	0.981	0.987

Table S15: Permeate fluxes in g h^{-1} and experimental rejections of the ME-ROB feed concentrations (c.f. Table 4) The experiments were performed at a temperature of 20 °C and a feed mass flow rate of 75 kg h^{-1} and the area of the used membrane NFAL is $A = 17 \text{ cm}^2$

ME-ROB-Feed								
Permeate flow in g h^{-1}	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	93.822	78.030	61.674	40.056	30.444	23.340	16.362	6.648
Cell 2	106.212	90.432	68.058	49.272	36.606	28.746	15.486	7.026
Cell 3	93.654	80.268	58.098	43.848	28.020	22.710	15.972	5.820
Cell 4	111.672	86.334	70.068	45.150	35.778	29.100	13.590	5.922
Rejection of Na^+	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.252	0.206	0.156	0.054	0.013	-0.011	-0.023	-0.058
Cell 2	0.246	0.209	0.161	0.052	0.014	-0.021	-0.036	-0.070
Cell 3	0.242	0.197	0.150	0.045	0.001	-0.017	-0.026	-0.062
Cell 4	0.248	0.198	0.144	0.047	0.005	-0.011	-0.025	-0.049
Rejection of Li^+	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.087	0.043	0.023	-0.047	-0.061	-0.067	-0.066	-0.059
Cell 2	0.012	0.030	0.022	-0.037	-0.062	-0.044	-0.038	-0.043
Cell 3	-	0.017	-0.018	-0.051	-0.048	-0.081	-0.058	-0.056
Cell 4	0.058	0.033	-0.005	-0.038	-0.080	-0.054	-0.065	-0.043
Rejection of Mg^{2+}	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.938	0.934	0.927	0.911	0.880	0.877	0.850	0.773
Cell 2	0.941	0.941	0.938	0.918	0.890	0.825	0.860	0.772
Cell 3	0.940	0.939	0.929	0.913	0.891	0.878	0.864	0.761
Cell 4	0.940	0.942	0.931	0.895	0.853	0.693	0.703	0.698
Rejection of K^+	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar

Cell 1	0.248	0.213	0.167	0.074	0.038	0.011	-0.002	-0.038
Cell 2	0.236	0.216	0.171	0.074	0.035	0.003	-0.015	-0.051
Cell 3	0.231	0.205	0.152	0.068	0.024	0.006	-0.015	-0.044
Cell 4	0.248	0.206	0.157	0.068	0.027	0.004	-0.007	-0.030

Rejection of Ca²⁺	45 bar	40 bar	35 bar	25 bar	20 bar	15 bar	10 bar	5 bar
Cell 1	0.921	0.911	0.892	0.842	0.781	0.751	0.706	0.525
Cell 2	0.926	0.923	0.910	0.854	0.798	0.708	0.707	0.485
Cell 3	0.917	0.912	0.890	0.833	0.781	0.750	0.715	0.480
Cell 4	0.926	0.921	0.899	0.820	0.759	0.586	0.569	0.470

Appendix S4: Circular METcell

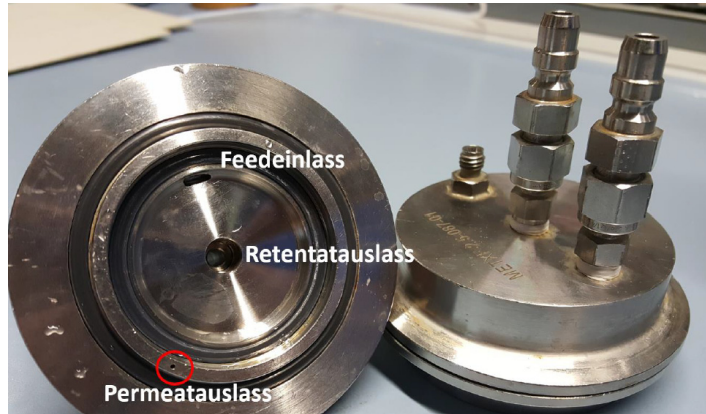


Figure S4: Circular METcell

Appendix S5: Model assumptions and limitations from the SDEM by Yaroshchuk and Bruening [39]

- 1) Salts are assumed to fully dissociate in water without forming ion complexes
- 2) The electroneutrality condition is assumed to hold inside the membrane as well as within the bulk solution.
- 3) Activity coefficients were assumed to be 1.
- 4) Steady-State operation.
- 5) Neglection of convective coupling between the trans-membrane volume and solute flow.
- 5) Ionic permeances are considered composition-independent constants.
- 6) Virtual reference solution: is defined as a bulk electrolyte solution that could be in thermodynamic equilibrium with a given point inside the membrane.

7) The solute transport across the membrane is assumed to be one-dimensional, normal to the area of the active layer.

8) The electric potential is the only way how the transport between charged species is coupled.