Supplementary Information

Manuscript title:

Modeling the response of control-released ion-selective electrode and employing it for the study of permanganate oxidation kinetics

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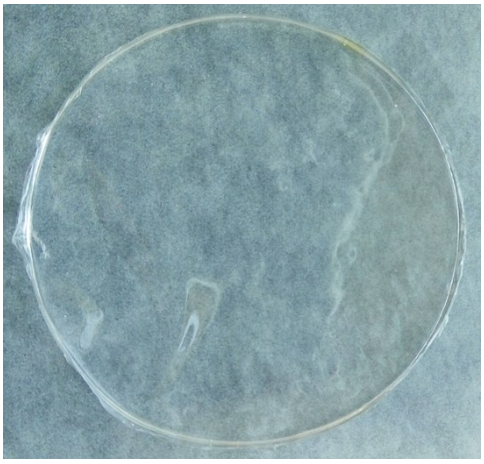

Fig. S1 A sample photograph of the polymeric membrane obtained in this work.

Table S1 Experimental second-order rate constants (k) and computational energy barriers (ΔG^{++}) for the different permanganate oxidation reactions in water.

Bond	Name	T (°C)	k ($M^{-1}s^{-1}$) [a]	k_A ($M^{-1}s^{-1}$) [b]	lnk_A	ΔG^{++} (kcal mol^{-1})
C=C	PCE	25	4.58×10^{-2} 4.11×10^{-2}	4.35×10^{-2}	–3.13	32.86
	TCE	25	7.80×10^{-1} 6.70×10^{-1} 4.60×10^{-1}	6.30×10^{-1}	–0.46	29.56
	trans-DCE	25	3.90×10^{1}	3.90×10^{1}	3.66	26.45
C–H	Ethanol	20 30	1.67×10^{-3} 4.03×10^{-3}	2.85×10^{-3} [c]	–5.86	33.08
	Toluene	25	8.32×10^{-4}	8.32×10^{-4}	–7.09	34.23
O–H	H_2O_2	25	3.70×10^{2}	3.70×10^{2}	5.91	24.51

[a] k values were obtained from the reference "R. H. Waldemer and P. G. Tratnyek, *Environ. Sci. Technol.*, 2006, **40**, 1055-1061".

[b] k_A represents the average k value at 25 °C

[c] k_A value for ethanol was obtained by averaging the k values at 20 and 30 °C

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The following section gives the Cartesian coordinates of optimized structures, including MnO_4^-, H_2O_2, RC, TS, PC, PC(T); and PCE, TCE, *trans*-DCE, Ethanol, Toluene with the corresponding transition states TS_{PCE}, TS_{TCE}, $TS_{trans\text{-}DCE}$, $TS_{Ethanol}$, $TS_{Toluene}$.

MnO_4^-	Cartesian coordinates		
Atom	x	y	z
Mn	0	0	0
O	0.921033	0.921033	0.921033
O	-0.921033	-0.921033	0.921033
O	-0.921033	0.921033	-0.921033
O	0.921033	-0.921033	-0.921033

H_2O_2	Cartesian coordinates		
Atom	x	y	z
O	0	0.726713	-0.065629
H	0.752828	0.918397	0.525032
O	0	-0.726713	-0.065629
H	-0.752828	-0.918397	0.525032

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RC	Cartesian coordinates		
Atom	x	y	z
Mn	-0.990431	0.018519	0.001978
O	-2.107364	-1.014849	-0.4616
O	-0.62249	-0.239476	1.52699
O	0.327889	-0.17669	-0.899739
O	-1.534472	1.503346	-0.171643
O	2.839471	-0.727242	0.05855
H	1.929703	-0.517307	-0.276656
O	3.510929	0.54972	-0.122803
H	3.51937	0.895854	0.789157

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TS	Cartesian coordinates		
Atom	x	y	z
Mn	0.860233	0.041848	-0.022495
O	2.031111	-1.008108	-0.19787
O	-0.245847	-0.099961	-1.166713
O	1.329217	1.542338	0.156595
O	-0.155432	-0.419452	1.28896
O	-2.222755	-0.700202	-0.109
H	-1.08648	-0.579165	0.827271
O	-2.898064	0.526952	0.09648
H	-3.125193	0.800421	-0.812515

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PC	Cartesian coordinates		
Atom	x	y	z
Mn	0.818982	0.069557	-0.041886
O	1.097451	1.623104	-0.139702
O	1.889945	-1.026707	-0.439156
O	-0.724669	-0.290776	-0.943323
O	0.176548	-0.316505	1.601372
H	-0.746397	-0.609286	1.493962
O	-1.869674	-0.693546	-0.177083
O	-2.643115	0.485538	0.129795
H	-3.140047	0.621479	-0.70201

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PC(T)	Cartesian coordinates		
Atom	x	y	z
Mn	-0.717099	-0.103718	0.038683
O	-0.49887	-1.147001	1.238449
O	-1.833688	-0.557086	-1.041029
O	0.78213	0.03396	-1.008299
O	-1.035365	1.586605	0.545731
H	-0.297989	1.925126	1.086238
O	1.8105	0.640141	-0.238889
O	2.649466	-0.398144	0.304335
H	3.232075	-0.599975	-0.455715

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PCE	Cartesian coordinates		
Atom	x	y	z
C	0	0	0.673389
C	0	0	-0.673389
Cl	0	1.461128	-1.603618
Cl	0	-1.461128	-1.603618
Cl	0	-1.461128	1.603618
Cl	0	1.461128	1.603618

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TS_{PCE}	Cartesian coordinates		
Atom	x	y	z
C	1.093204	-0.697976	0.008897
C	1.093202	0.697976	-0.00888
Cl	1.439767	1.595937	1.445544
Cl	1.464675	1.562951	-1.477512
Cl	1.439893	-1.595938	-1.445496
Cl	1.464558	-1.562946	1.477562
O	-0.964505	1.237467	-0.040481
Mn	-2.013	0	-0.000031
O	-2.881994	0.044746	1.333689
O	-2.882073	-0.044752	-1.333699
O	-0.964505	-1.237468	0.040366

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TCE	Cartesian coordinates		
Atom	x	y	z
C	-1.045831	-0.391041	0
H	-2.062129	-0.019232	0
C	0	0.441219	0
Cl	-0.257319	2.164845	0
Cl	1.657233	-0.062624	0
Cl	-0.909496	-2.1188	0

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TS_{TCE}	Cartesian coordinates		
Atom	x	y	z
C	-1.075301	0.618275	-0.942409
H	-1.007267	0.453931	-2.007194
C	-1.330149	-0.435214	-0.087824
Cl	-1.452645	-2.028745	-0.805275
Cl	-2.161364	-0.246748	1.429816
Cl	-1.441713	2.259891	-0.500814
O	1.026331	0.780694	-1.049634
Mn	1.827322	-0.02436	0.116885
O	2.821337	-1.094122	-0.520789
O	2.530662	0.997123	1.118353
O	0.584691	-0.768451	0.847458

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trans-DCE	Cartesian coordinates		
Atom	x	y	z
C	0	0.66612	0.968443
H	0	1.220914	1.899558
C	0	-0.66612	0.968443
H	0	-1.220914	1.899558
Cl	0	-1.668376	-0.453542
Cl	0	1.668376	-0.453542

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$TS_{trans\text{-}DCE}$	Cartesian coordinates		
Atom	x	y	z
C	-1.300865	0.687634	-0.869109
H	-1.087778	1.223632	-1.78292
C	-1.300865	-0.687635	-0.869108
H	-1.087777	-1.223634	-1.782918
Cl	-2.164902	-1.63644	0.312839
Cl	-2.164899	1.636441	0.312839
O	0.66725	-1.246713	-0.282988
Mn	1.650805	0	0.074771
O	2.001709	0.000004	1.632072
O	2.929092	-0.000005	-0.879922
O	0.667253	1.246714	-0.282995

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Ethanol	Cartesian coordinates		
Atom	x	y	z
O	1.247729	-0.257846	-0.112281
C	0.074461	0.558862	0.047635
C	-1.219107	-0.244333	-0.02115
H	0.133933	1.114263	0.994191
H	0.122343	1.284734	-0.769594
H	-2.08497	0.423778	0.067645
H	-1.294107	-0.782448	-0.973082
H	-1.274167	-0.975268	0.795626
H	1.283012	-0.889464	0.624551

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$TS_{Ethanol}$	Cartesian coordinates		
Atom	x	y	z
O	-2.595042	-1.310033	-0.002355
C	-2.17817	-0.051784	0.385237
C	-2.941595	1.12524	-0.18118
H	-2.042531	-0.046247	1.458859
H	-0.957681	0.147063	-0.32382
H	-2.479838	2.063795	0.141105
H	-2.966893	1.111456	-1.277313
H	-3.978112	1.106461	0.188985
H	-2.830851	-1.31008	-0.947276
Mn	1.25352	0.015371	-0.015241
O	-0.060946	0.271886	-1.050187
O	0.312054	-0.209306	1.307876
O	2.033037	-1.325188	-0.396127
O	2.14046	1.335457	0.130312

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Toluene	Cartesian coordinates		
Atom	x	y	z
C	0.917023	0.000008	-0.012143
C	0.195387	1.204567	-0.009372
C	0.195397	-1.204563	-0.009373
C	2.429493	0.000005	0.009524
C	-1.203421	1.207763	0.002156
C	-1.203406	-1.20777	0.002157
C	-1.909469	-0.000005	0.008795
H	0.734527	2.149894	-0.018253
H	0.734546	-2.149885	-0.018254
H	2.836936	-0.887296	-0.487235
H	2.836921	0.887821	-0.486319
H	2.80882	-0.000536	1.040461
H	-1.740641	2.153207	0.00217
H	-1.74062	-2.153218	0.002171
H	-2.996515	-0.000013	0.014798

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$TS_{Toluene}$	Cartesian coordinates		
Atom	x	y	z
C	1.922673	-0.012462	0.653572
C	2.550234	1.208608	0.304103
C	2.560886	-1.218783	0.273495
C	0.651325	-0.026464	1.36171
C	3.767069	1.220726	-0.374948
C	3.777885	-1.20317	-0.405139
C	4.388019	0.015833	-0.733795
H	2.073313	2.146263	0.580451
H	2.092184	-2.167266	0.525959
H	0.38641	-0.945646	1.87747
H	0.378887	0.87822	1.897922
H	-0.227764	-0.027902	0.160707
H	4.236018	2.168945	-0.62532
H	4.255248	-2.140628	-0.679001
H	5.336801	0.026711	-1.263471
Mn	-2.460574	0.003546	-0.18555
O	-2.04994	0.015395	1.389173
O	-0.868021	-0.030401	-0.764194
O	-3.234258	-1.337582	-0.566257
O	-3.188444	1.360955	-0.597466

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