

Supporting information for publication

VOLTAMMETRIC DETERMINATION OF DIFFUSION AND PARTITION COEFFICIENTS IN
PLASTICIZED POLYMER MEMBRANES

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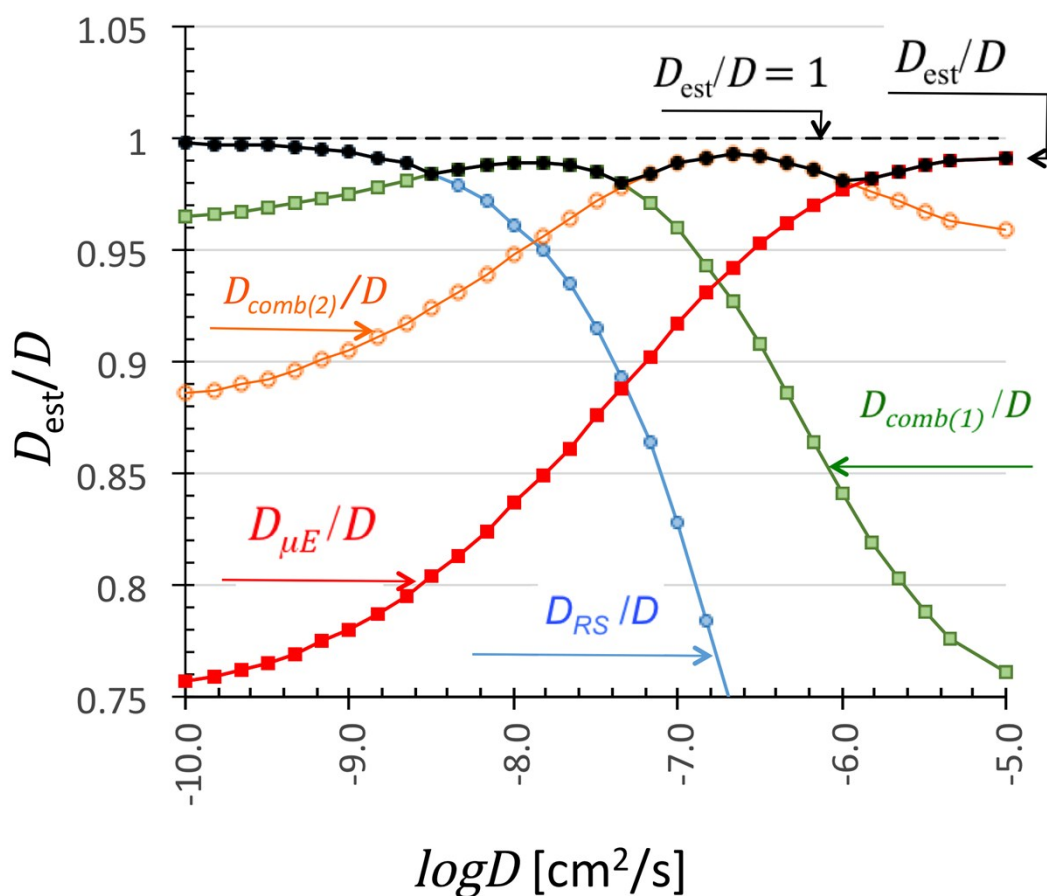
Table-S1. Compilation of diffusion coefficients of ferrocene (D_{Fc}) and ferrocene methanol (D_{FcMeOH}) measured by voltammetry in various solvents in the presence of supporting electrolytes, and calculated by the Stokes-Einstein relationship, or published in the literature. (COV: coefficient of variation, N: number of measurements)

<u>Solvent</u>	Measured			Stokes-Einstein^o			Published
	D (cm ² /s)	N	COV (%)	D (cm ² /s)		slip (%)	
				no-slip	full-slip		
Water	7.5×10^{-6}	19	2	7.4×10^{-6}	1.11×10^{-5}	4	$D_{FcMeOH} 7.6 \times 10^{-6}$ ¹ $D_{FcMeOH} 7 \times 10^{-6}$ ² $D_{FcMeOH} 6.1 \times 10^{-6}$ ³ $D_{FcMeOH} 7.8 \times 10^{-6}$ ⁴
Methanol	1.2×10^{-5}	5	5	1.22×10^{-5}	1.83×10^{-5}	0	
Acetone	2.10×10^{-5}	5	2	2.12×10^{-5}	3.18×10^{-5}	0	$D_{Fc} 2.40 \times 10^{-5}$ = $D_{Fc} 2.76 \times 10^{-5}$ Γ
Acetonitrile	1.97×10^{-5}	6	1	1.78×10^{-5}	2.67×10^{-5}	22	$D_{Fc} 1.74 \times 10^{-5}$ = $D_{Fc} 2.17 \times 10^{-5}$ Γ
DCM	1.76×10^{-5}	9	4	1.59×10^{-5}	2.39×10^{-5}	21	$D_{Fc} 1.12 \times 10^{-5}$ = $D_{Fc} 1.67 \times 10^{-5}$ Γ
THF	1.61×10^{-5}	8	1	1.43×10^{-5}	2.14×10^{-5}	26	
Octanol	1.2×10^{-6}	5	4	9×10^{-7}	1.3×10^{-6}	75	
DOS	5.0×10^{-7}	5	5	4×10^{-7}	6×10^{-7}	65	
oNPOE	6.0×10^{-7}	10	5	5×10^{-7}	7×10^{-7}	65	

^o The calculated values correspond to no-slip (Slip = 0%) and full slip (Slip = 100%) conditions. The data in the column labeled as slip (%) are estimated percent slip values between analyte molecules and the solvent

= 273.15 °K

Γ 298.15 °K



Figure

e S1: Ratios of the estimated diffusion coefficients to the true diffusion coefficient (D_{est}/D) and the largest of the four estimates (\bullet). D_{RS} and $D_{\mu E}$ were determined from the slopes (Eq. 5) and intercepts (Eq.6) of $i_p(i_L)$ vs. $v^{1/2}$ plots constructed from simulated LSVs using D as diffusion coefficient, and $D_{comb(1)}$ and $D_{comb(2)}$ were calculated by Equations 7 and 8 in the main article, respectively. The horizontal dotted line at $D_{est}/D = 1$ represents perfect agreement between the estimated and the true diffusion coefficient.

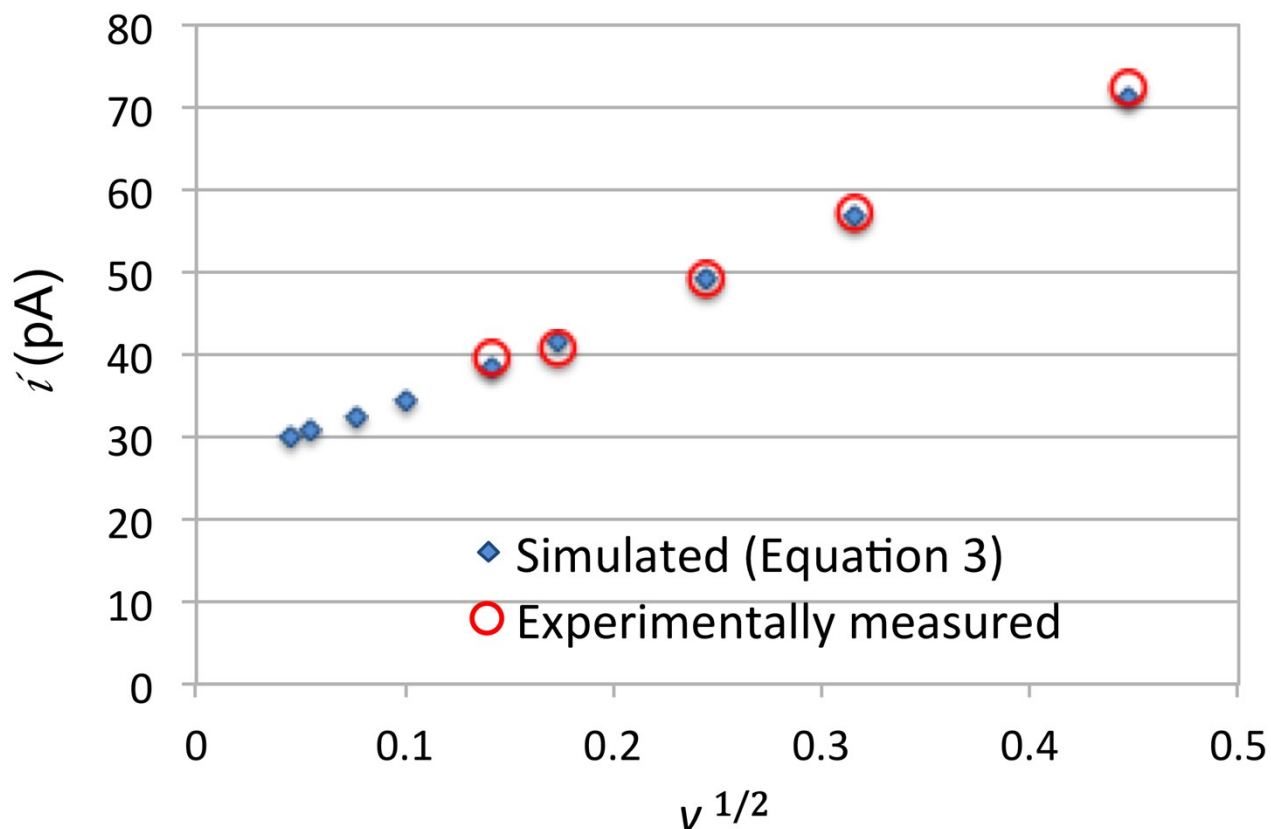


Figure S2: Demonstration of the agreement between $i_p(i_L)$ vs. $v^{1/2}$ plots measured experimentally and constructed from simulated LSVs. The experimental data points were collected by recording CVs of FcCOOH with the PEC in an oNPOE plasticized PVC membrane with 32% PVC content and 2.0 mM FcCOOH concentration.

REFERENCES

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