Electronic Supplementary Material (ESI) for Energy Advances.

Supporting information

Organized Macro-scale Membrane Size Reduction in Vanadium Redox Flow Batteries: Part 2. Flow-field Informed Membrane Coverage Distribution

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Table S1: 3D VRFB cell model properties, parameters, and nominal operating conditions

Property or Operating Condition	**Value**	**Ref.**
Cell temperature (K)	300	[1]
Electrolyte Bulk diffusion coefficients (m^2/s)[a]		
V^{2+}	2.40×10^{-10}	[1]
V^{3+}	2.40×10^{-10}	[1]
VO^{2+}	3.90×10^{-10}	[1]
VO_2^{+}	3.90×10^{-10}	[1]
H^{+}	9.31×10^{-9}	[1]
SO_4^{2-}	1.07×10^{-9}	[1]
HSO_4^{-}	1.33×10^{-9}	[1]
Electrolyte density (kg/m^3) +ve | -ve	1270 | 1275	[1]
Electrolyte dynamic viscosity (mPa.s) +ve | -ve	3 | 3.3	[1]
Electrode conductivity (S/m)	4538.4	[1]
Electrode porosity	0.92	[1]
Electrode specific area (m^2/m^3)	27062	**
Electrode hydraulic permeability (m^2)	8.00×10^{-11}	[1]
Standard reaction potential (V) +ve | -ve	1.004 | -0.255	[1]
Reaction rate constant (m/s) +ve | -ve	2.24×10^{-8} | 3.00×10^{-8}	**
Reaction anodic transfer coefficient +ve | -ve	0.60 | 0.50	**
Reaction cathodic transfer coefficient +ve | -ve	0.20 | 0.22	**
HSO_4^{-} degree of dissociation constant	0.25	[1]
HSO_4^{-} dissociation reaction rate ($mol/(m^3.s)$)	1.00×10^{4}	[1]
Species concentration at 50 % SOC and 10 mA/cm^2 (M)		
V^{2+}	0.521	
V^{3+}	0.513	
VO^{2+}	0.530	
VO_2^{+}	0.515	
H^{+} +ve | -ve	5.266 | 4.737	
HSO_4^{-} +ve | -ve	3.159 | 2.842	
Membrane thickness (mm)	203	[1]
Membrane porosity	0.28	[1]
Membrane fixed charge concentration (M)	1.99	[1]
Membrane hydraulic permeability (m^2)	1.58×10^{-18}	[1]
Membrane conductivity (S/m)	10	[1]
Current collector thickness (cm)	6	[1]
Current collector conductivity (S/m)	1.00×10^{4}	[1]

[a] – Diffusivity values in electrode and membrane domains were obtained using Bruggeman correction of listed values with porosity of respective domains. ** – Obtained from fitting experimental (dis)charge data of [1].

Table S2: Concentrations of all active and supporting electrolyte species characterizing different SOCs obtained from transient galvanostatic dis(charge) simulation.

j (mA/cm²)	Negative Electrolyte				Positive Electrolyte				SOC (%)
	HSO_4^- (M)	H^+ (M)	V^{2+} (M)	V^{3+} (M)	HSO_4^- (M)	H^+ (M)	VO^{2+} (M)	VO_2^+ (M)	
100	2.669	4.448	0.156	0.884	3.059	5.098	0.884	0.156	15.16
	2.711	4.520	0.271	0.769	3.102	5.170	0.769	0.271	26.24
	2.748	4.580	0.369	0.671	3.139	5.232	0.671	0.369	35.64
	2.778	4.631	0.450	0.590	3.169	5.282	0.591	0.450	43.40
	2.819	4.699	0.559	0.480	3.210	5.351	0.481	0.559	53.93
	2.884	4.807	0.732	0.308	3.275	5.459	0.309	0.732	70.50
	2.907	4.846	0.794	0.245	3.299	5.498	0.247	0.794	76.58
-100	2.907	4.846	0.794	0.245	3.299	5.498	0.247	0.794	76.28
	2.887	4.811	0.736	0.303	3.276	5.459	0.305	0.736	70.61
	2.849	4.747	0.627	0.412	3.233	5.386	0.414	0.626	60.12
	2.829	4.714	0.569	0.469	3.209	5.347	0.473	0.568	54.55
	2.795	4.656	0.470	0.568	3.170	5.281	0.572	0.469	45.02
	2.784	4.638	0.439	0.600	3.157	5.260	0.604	0.438	41.98

SO_4^{2-} concentrations obtained from electroneutrality condition.

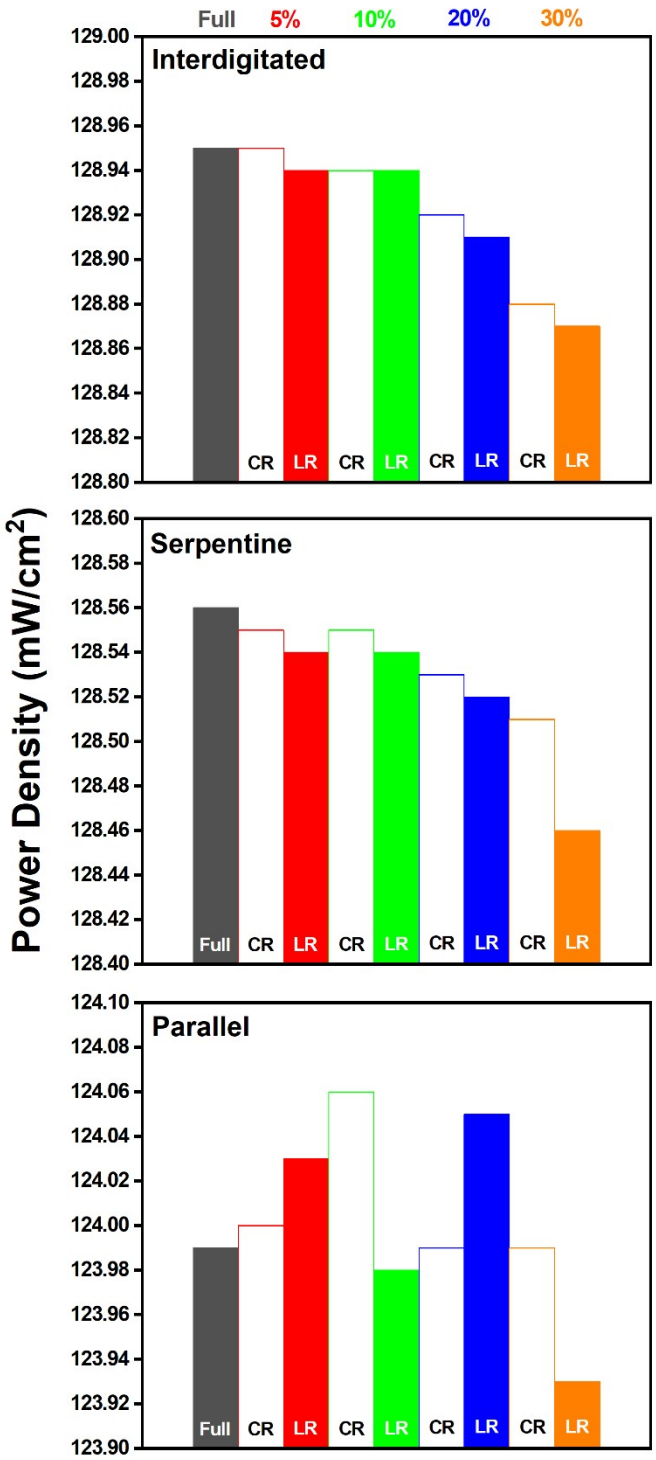

Figure S1: Power density obtained from steady-state discharge polarization simulations of cells adopting interdigitated, parallel, and serpentine flow-fields at 100 mA/cm² current density. Showing full membrane coverage, 5 %, 10 %, 20 %, and 30 % total membrane coverage reduction – adjacent to channel, or land. CR: Channel-adjacent membrane reduction MEA architecture, LR: land-adjacent membrane reduction MEA architecture.

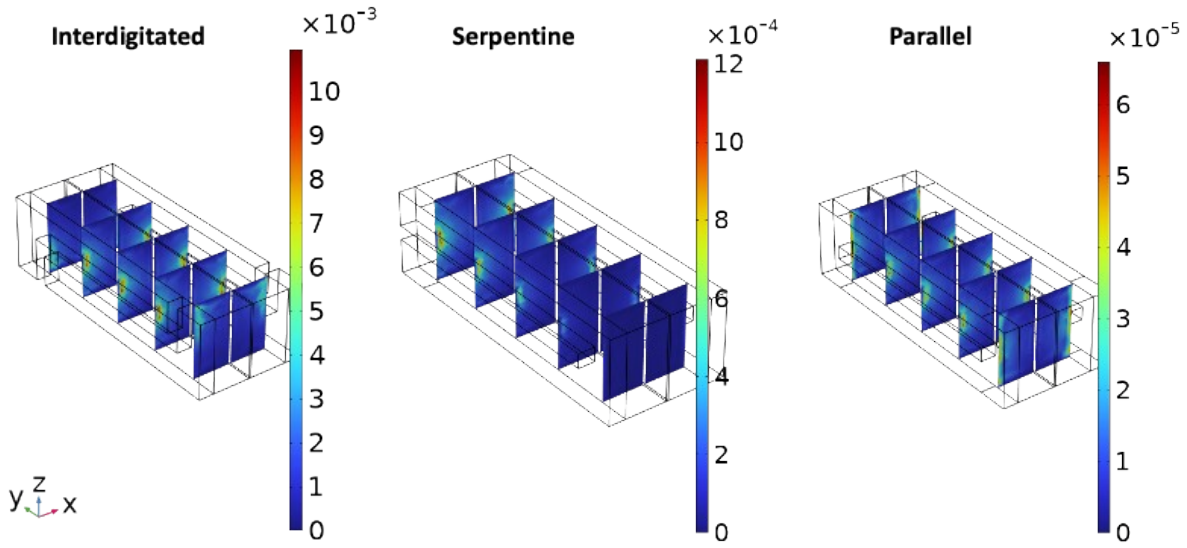

Figure S2: Electrolyte velocity magnitude in the electrodes enforced by the different flow fields at the same nominal flow rate. Negative electrode left and positive right.

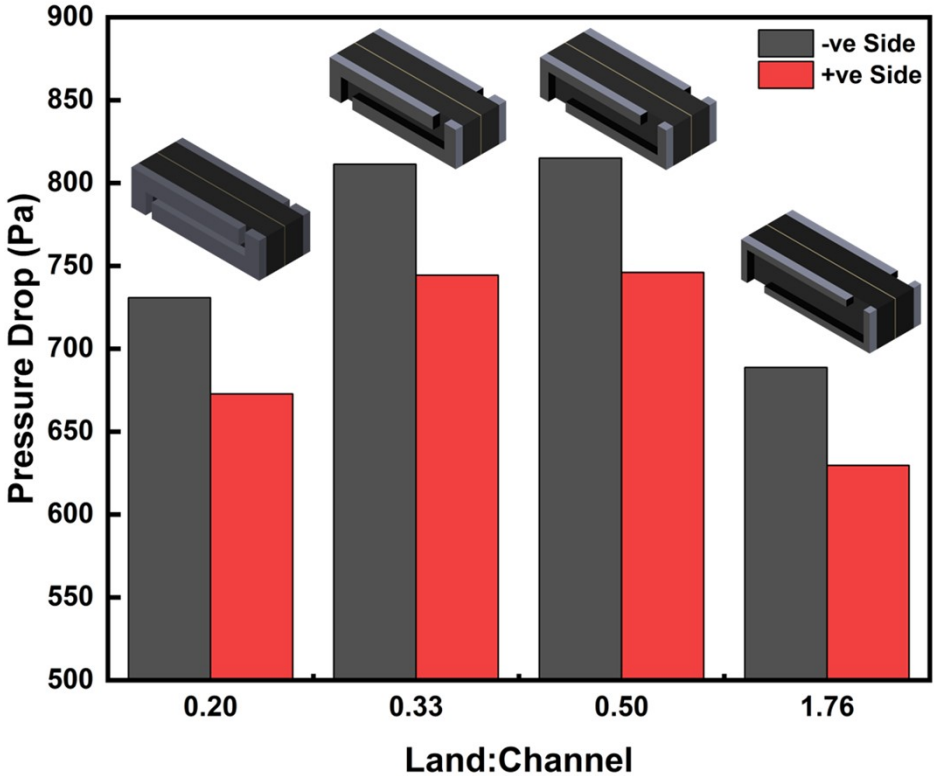

Figure S3: Pressure drop across full membrane coverage interdigitated cell unit with increasing land-to-channel ratios.

References

[1] K. Knehr, E. Agar, C. Dennison, A. Kalidindi, E. Kumbur, A transient vanadium flow battery model incorporating vanadium crossover and water transport through the membrane, Journal of The Electrochemical Society. 159 (2012) A1446–A1459.