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Molar Fluxes and Cell Constants in Redox Flow Batteries – Identifying and Unifying RFB Cell Performance Criteria

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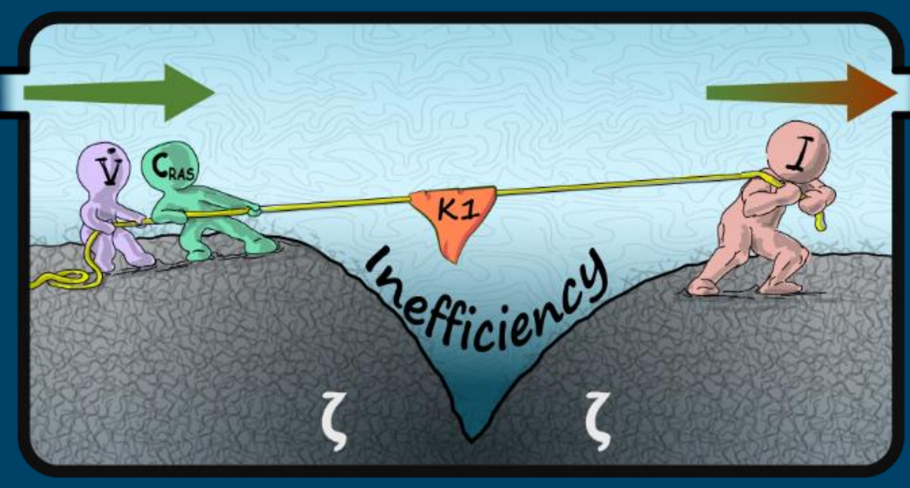


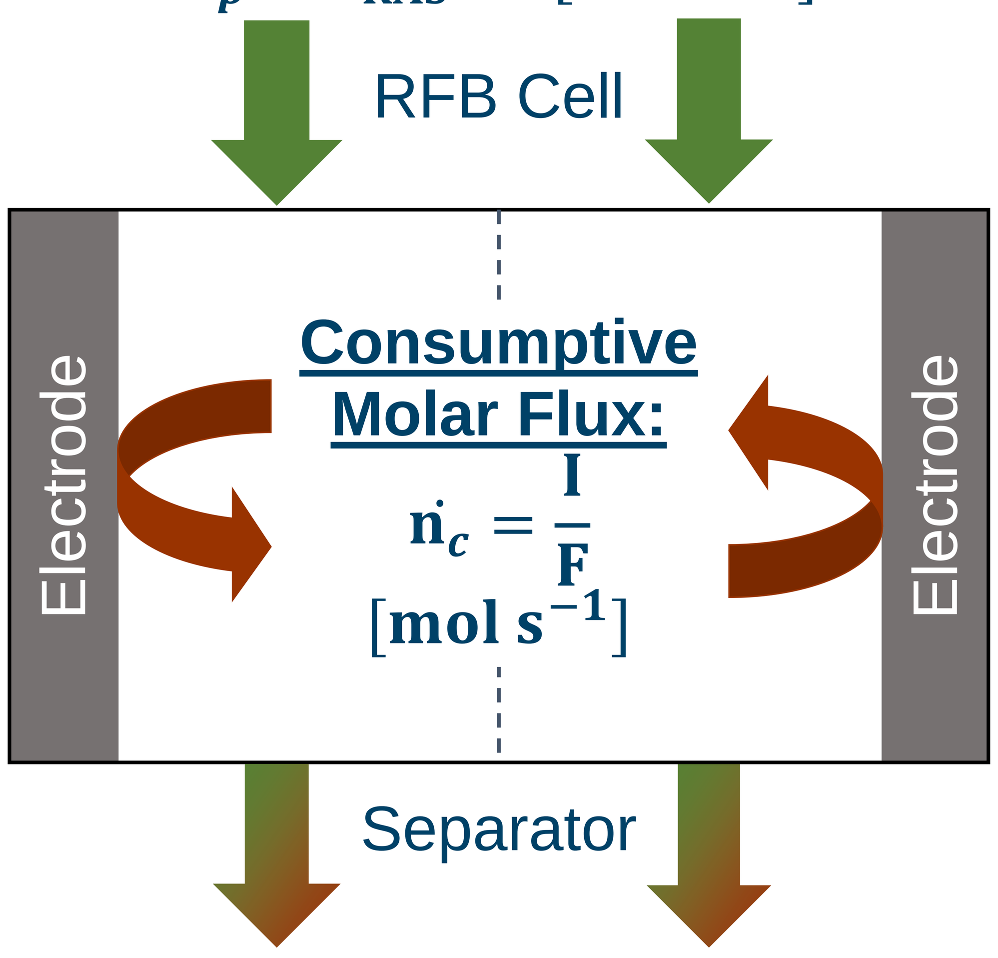
Molar Fluxes

Productive Molar Flux:
$\dot{n}_p = c_{RAS} \cdot \dot{V}\ [\mathrm{mol\ s^{-1}}]$

Efficiency

$K1 = \frac{\dot{n}_p}{\dot{n}_c}$

$K1_{critical} = K1(90\%\ \eta_{min})$



Comparability

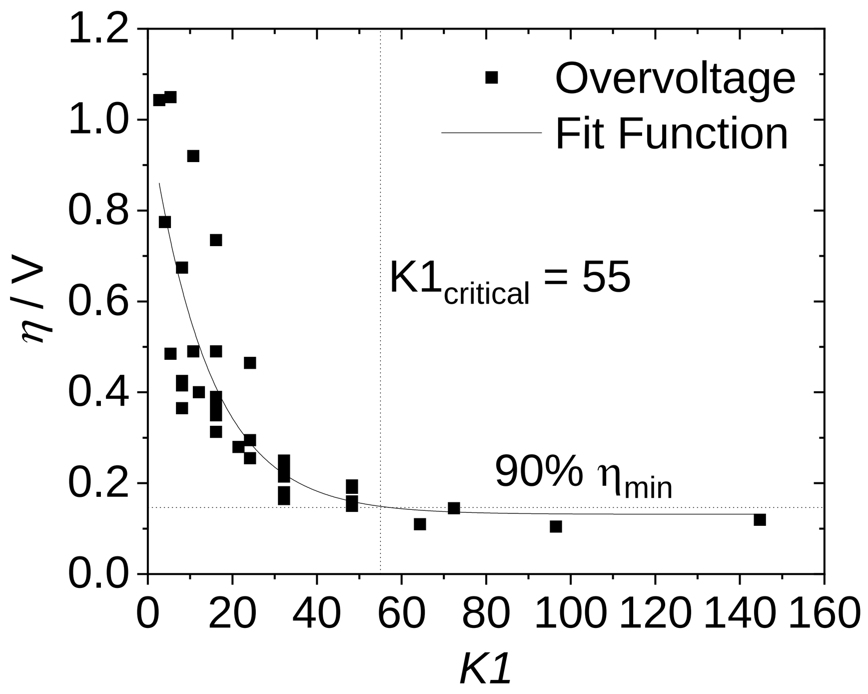
$\zeta\ [\mathrm{cm^{-1}}]$

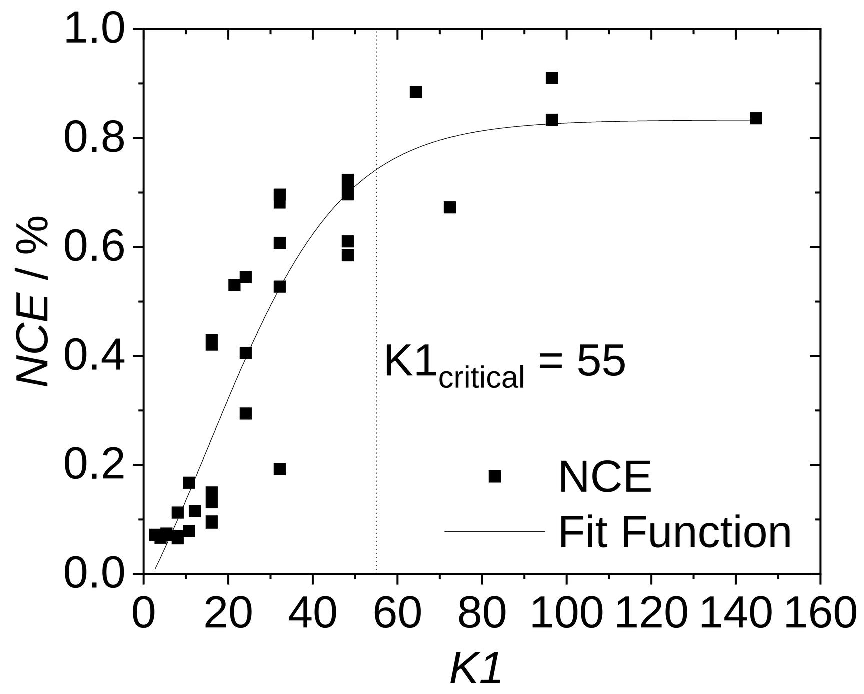
$K2 = \frac{K1_{critical}}{\zeta}\ [\mathrm{cm}]$

RAS	Redox Active Species	-
c_{RAS}	RAS Concentration	mol L^{-1}
$\dot{V}$	Volume Flow Rate	L s^{-1}
I	Current	A
F	Faraday Constant	A s mol^{-1}
$\dot{n}_p$	Productive Molar Flux	mol s^{-1}
$\dot{n}_c$	Consumptive Molar Flux	mol s^{-1}
K1	RFB Operating Constant	-
$K1_{critical}$	Critical Operating Parameters	-
ζ	RFB Cell Constant	cm^{-1}
K2	Comparability Constant	cm
NCE	Normalized Charge Efficiency	%
η (η_{min})	(Minimum) Overvoltage	V

K1 summarizes the operating parameters, $\dot{n}_p$ and $\dot{n}_c$, of an RFB setup to determine the optimal ones by a simple experimental efficiency evaluation using **η** and **NCE**; **K2** and **ζ** allow comparability between different RFB cell configurations by indicating the influence of a RFB configuration on its performance.

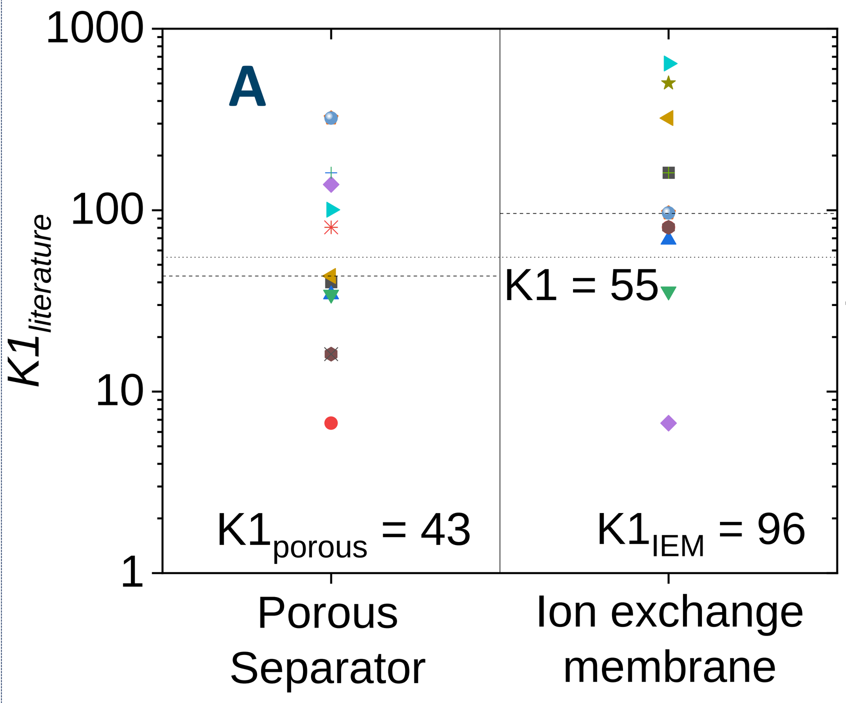
Efficiency Evaluation

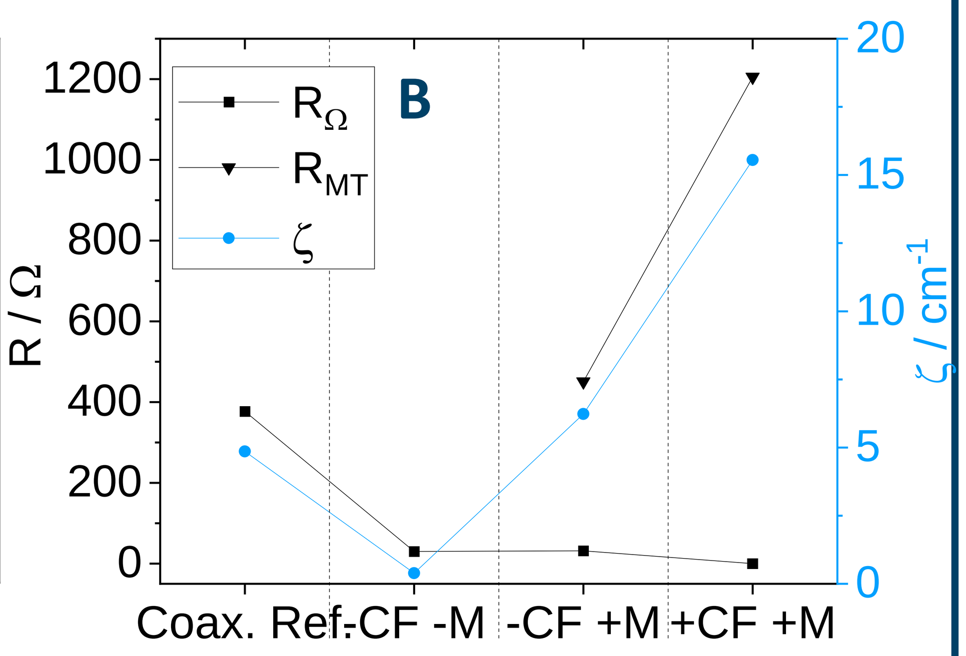




η / V	0.13	Overvoltage (**η**) decreases with higher **K1** until minimum overvoltage (**η_{min}**)
NCE	74%	Normalized charge efficiency (**NCE**) increases with higher **K1** until real limited **NCE**

Application of K1





A Literature K1	$K1_{porous} < K1_{IEM}$	Higher IEM penetration resistance requires larger compensating molar flux
B RFB Cell Constant ζ	ζ = 15.6 cm^{-1} K2 = 3.5 cm	Mass transport through separator as the main limiting factor

Standard Electrolyte

Electrolyte Composition	Operating Parameters	Cell Configuration
$Fc \rightleftarrows FcBF_4$ 0.3 M $TBABF_4$ Acetonitrile	c_{RAS} = 5, 10, 15 mM $\dot{V}$ = 5, 10, 20, 30 mL min^{-1} I = 5, 10, 15 mA	3D-printed RFB Cell[1, 2] Celgard® 2500 Separator

How to use Molar Fluxes?

1. Measure **ζ** according to **ISO 7888** (0.1 M KCl) gradually increasing system complexity
2. Use **K2** ≈ 3.5 cm as first benchmark to estimate **$K1_{critical}$**
3. Screen the cell performance and efficiency at different **K1** around **$K1_{critical}$**
4. Calculate the real **$K1_{critical}$** at 90% of **η_{min}**
5. Recalculate **K2** using real **$K1_{critical}$**

[1] L. Kortekaas, S. Fricke et al., A Digital Blueprint for 3D-Printing Lab-Scale Aqueous and Organic Redox-Flow Batteries, *Batteries & Supercaps* **2023**, e202300045
[2] L. Kortekaas, S. Fricke et al., Building Bridges: Unifying Design and Development Aspects for Advancing Non-Aqueous Redox-Flow Batteries, *Batteries* **2022**, 9, 4

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