# Results of the European Project SONAR with Deeper Insight into Microstructure Simulations of Flow Batteries

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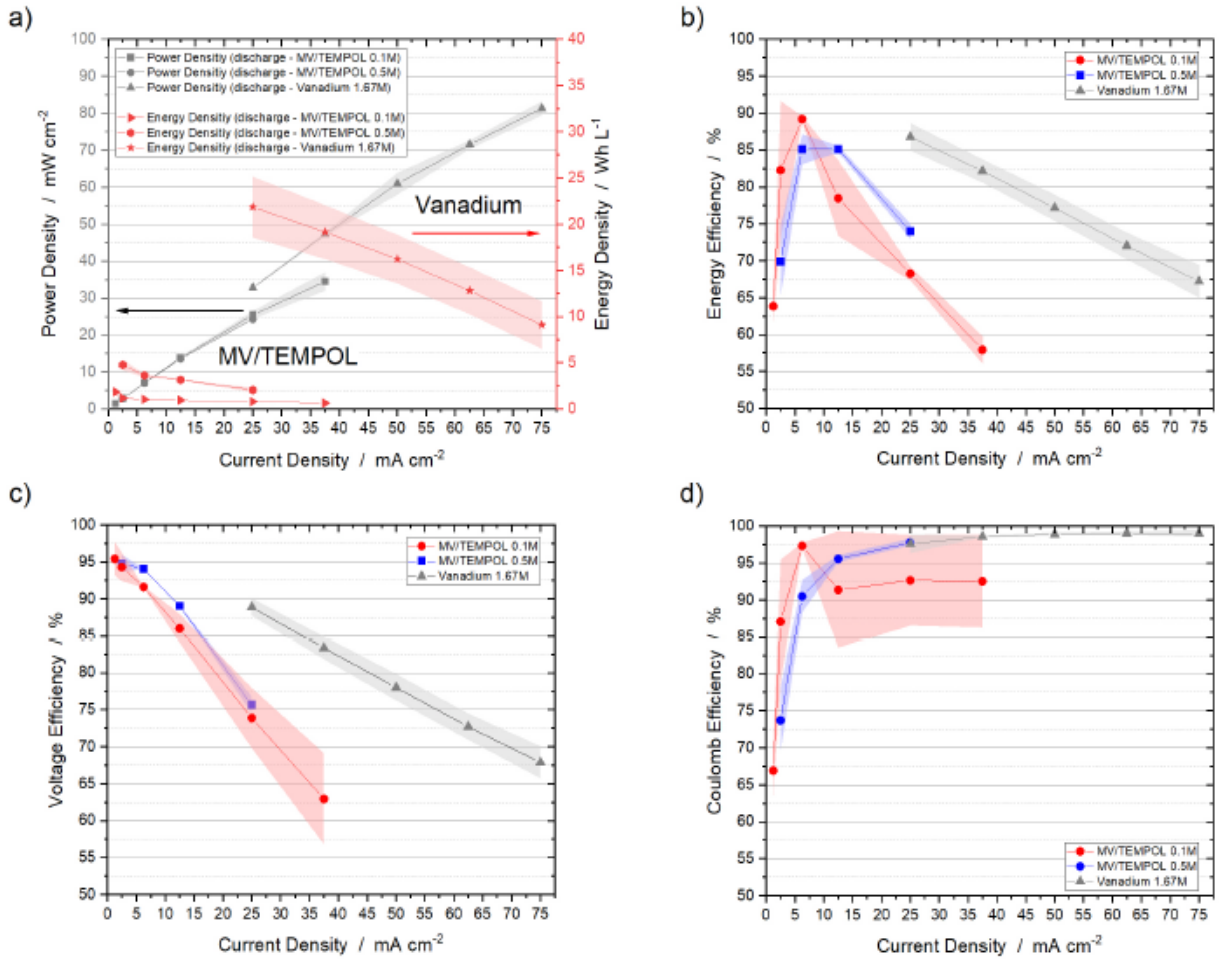
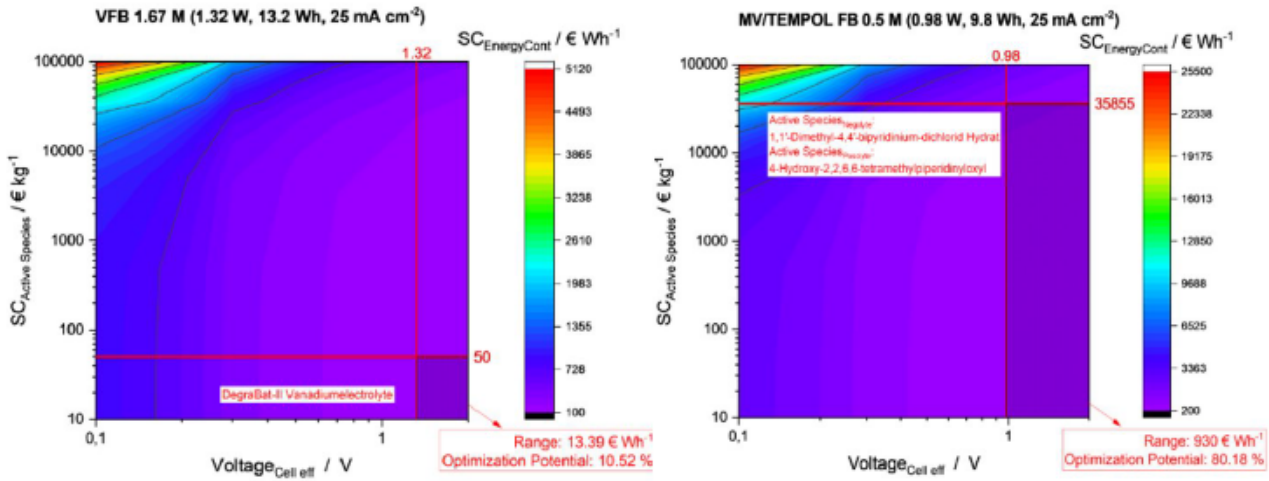
**HIGREEW Workshop**
**Vitoria-Gasteiz 2023**

# Cost analysis of redox flow batteries

## Extraction of data from battery tests




## Optimisation potentials




| Prioritization order of the investigated optimization questions | FlowBattery | | | |
|---|---|---|---|---|
| | VFB 1.67 M | | MV/TEMPOL FB 0.5 M | |
| | Rank | Optimization Potentials | Rank | Optimization Potentials |
| a) $SC_{Membrane} - SRA_{Membrane}$ | 5 | 1.30% | 6 | 1.73% |
| b) $SC_{Electrode} - SRA_{Electrode}$ | 7 | 0.92% | 5 | 3.20% |
| c) $SC_{Carbon\ Paper} - SRA_{Carbon\ Paper}$ | 4 | 3.56% | 7 | 0.54% |
| d) $SC_{Bipolar\ Plate} - SRA_{Bipolar\ Plate}$ | 8 | 0.20% | 8 | 0.03% |
| e) $SC_{Active\ Species} - U_{Cell\ eff}$ | 2 | 10.52% | 1 | 80.18% |
| f) $R_{inner} - CD$ | 6 | 1.20% | 3 | 37.68% |
| g) $U_{Cell\ eff} - CD$ | 3 | 10.44% | 2 | 45.85% |
| h) $Concentration_{Active\ Species} - CD$ | 1 | 61.56% | 4 | 28.61% |

# Microstructure Simulations of Flow Batteries

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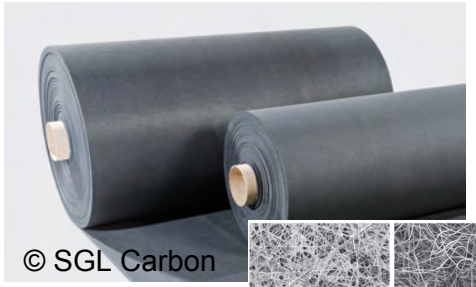
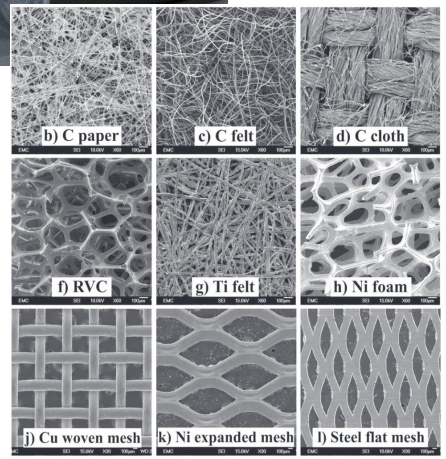
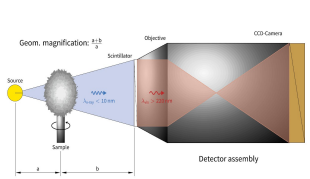
# At first glance: Modelling approach

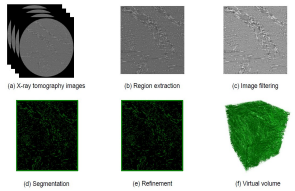


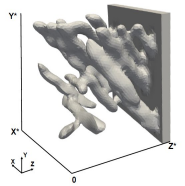
© SGL Carbon

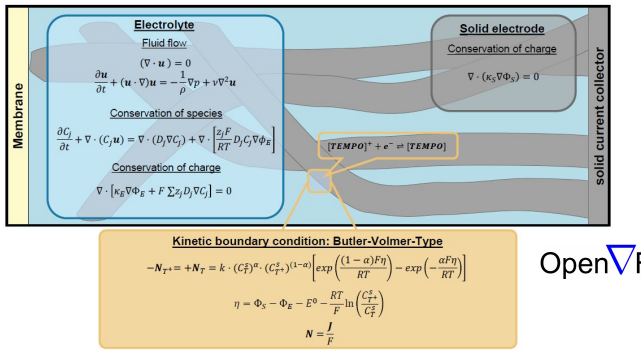



Arenas et al., 2020, DOI:
https://doi.org/10.1149/1945-7111/ab64ba

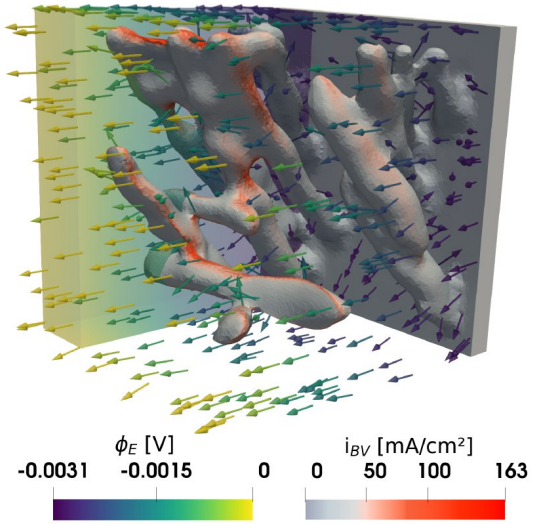


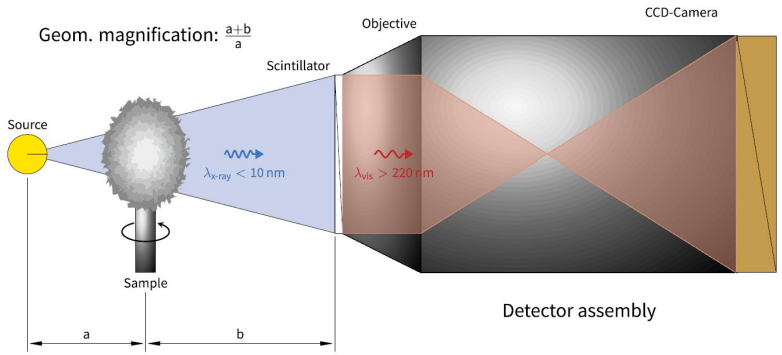



OpenFOAM®

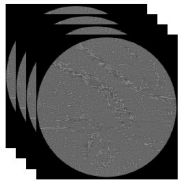


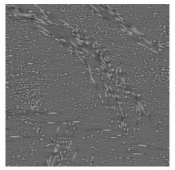

Electrode Material → Reconstruction + Model → Performance Data

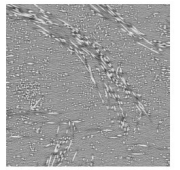
# Microstructure characterization

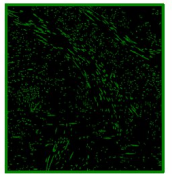


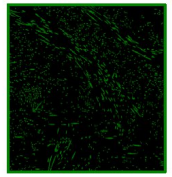

[1] T. Dobler, B. Radel., Crystals 11.6 (2021. doi:10.3390/cryst11060713. url: https://www.mdpi.com/2073-4352/11/6/713


(a) X-ray tomography images

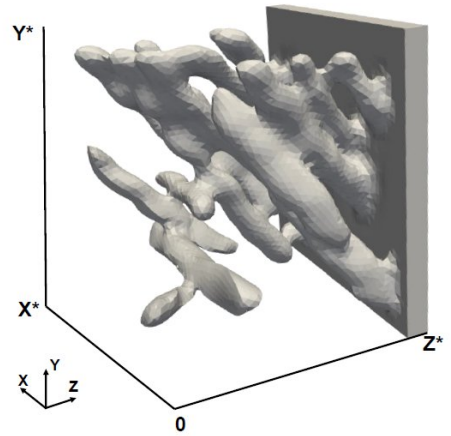

(b) Region extraction


(c) Image filtering


(d) Segmentation

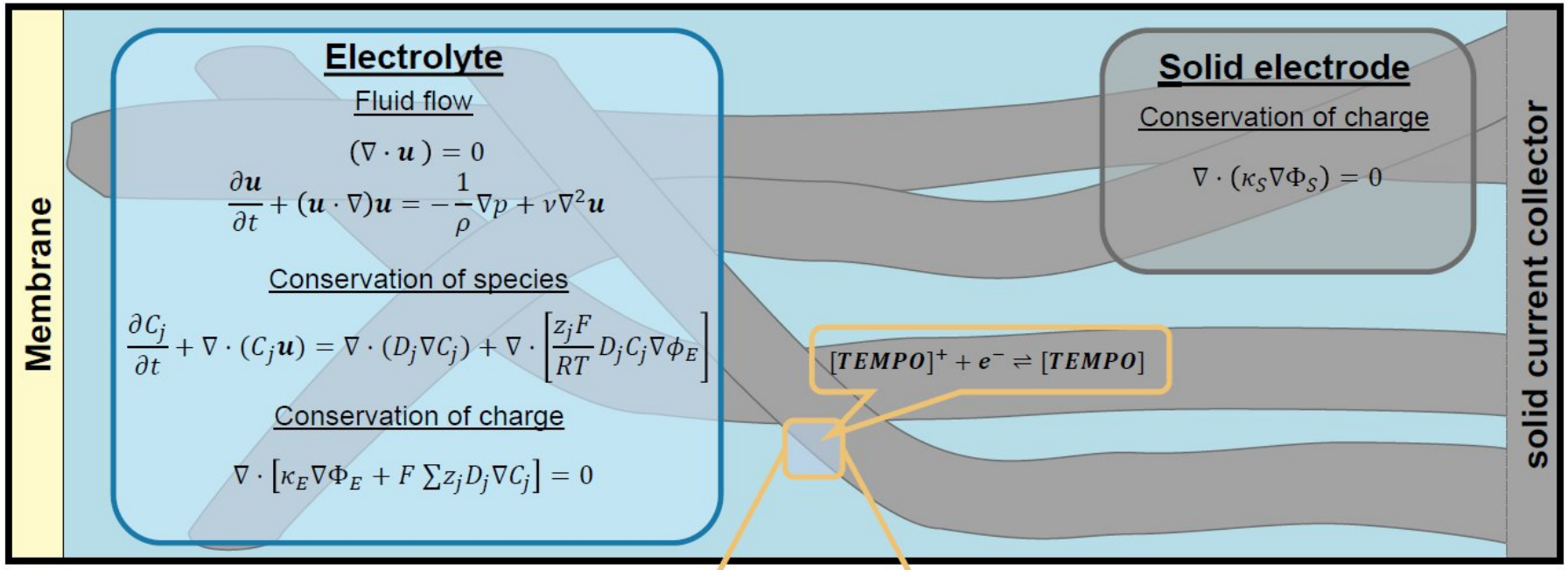

(e) Refinement


(f) Virtual volume




µCT Scans → Image Processing → Digital Twin

# 3D pore-scale resolved continuum model[1]




**Kinetic boundary condition: Butler-Volmer-Type**

$$-\boldsymbol{r}_{T^+} = +\boldsymbol{r}_T = k \cdot (C_T^s)^{\alpha} \cdot (C_{T^+}^s)^{(1-\alpha)} \left[exp\left(\frac{(1-\alpha)F\eta}{RT}\right) - exp\left(-\frac{\alpha F \eta}{RT}\right)\right]$$

$$\eta = \Phi_S - \Phi_E - E^0 - \frac{RT}{F} \ln\left(\frac{C_{T^+}^s}{C_T^s}\right)$$

$$\boldsymbol{r} = \frac{\boldsymbol{i}}{F}$$


[1] Wolf, A., Kespe, S. and Nirschl, H. (2023). „Pore-scale Modeling of Flow Batteries.” In Flow Batteries, John Wiley & Sons (eds C. Roth, J. Noack and M. Skyllas-Kazacos). https://doi.org/10.1002/9783527832767.ch18