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

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HIGREEW Workshop
Vitoria-Gasteiz 2023

Motivation

- **Modelling for the search for new active materials for redox flow batteries**
- **Huge number of possibilities of organic active materials for redox flow batteries**
- **Develop a framework for virtual evaluation of RFBs across all length scales**
- **Multiscale simulations, measurements & machine learning to assess LCOS**

Anode	E^0,V	Cathode: Mn_2O_3/MnO_2 0.15	$Fe(CN)_6^{4-}/Fe(CN)_6^{3-}$ 0.36	Cu/Cu^+ 0.52	I^-/I_3^- 0.54	Fe^{2+}/Fe^{3+} 0.77	VO^{2+}/VO_2^+ 0.99	$Br^-/BrCl_2^-$ 1.04	$Br^-/Br_2^{\bullet}$ 1.09	NpO_2^{2+}/NpO_2^+ 1.14	I_2/IO_3^- 1.2	O^{2-}/O_2 1.23	$Cr^{3+}/HCrO_4^-$ 1.35	Cl^-/Cl_2 1.36	Pb^{2+}/PbO_2 1.46	Mn^{2+}/Mn^{3+} 1.54	Ce^{3+}/Ce^{4+} 1.72	Co^{2+}/Co^{3+} 1.82
$Al/Al(OH)_4^-$	-2.31											B						
$Zn/Zn(OH)_4^{-2}$	-1.22	B	B															
Zn/Zn^{2+}	-0.76				B	B	B	B	C					B			B	
Fe/Fe^{2+}	-0.45					B												
S_2^{2-}/S	-0.43		B						C			B						
Cr^{2+}/Cr^{3+}	-0.41					C			A				B					
Cd/Cd^{2+}	-0.40					B												
V^{2+}/V^{3+}	-0.26					B	C	B				B				B	B	B
Pb/Pb^{2+}	-0.13														B			
Sn/Sn^{2+}	-0.14								B									
H_2/H^+	0.00					B	B		B					B				
Ti^{3+}/TiO^{2+}	0.04					A		A						A		B		
Cu^+/Cu^{2+}	0.15			B											B			
Np^{3+}/Np^{4+}	0.15									B								
Sn^{2+}/Sn^{4+}	0.15					B			B									
Cu/Cu^{2+}	0.34														B			
I^-/I_2	0.54										A							
Fe^{2+}/Fe^{3+}	0.77															B		

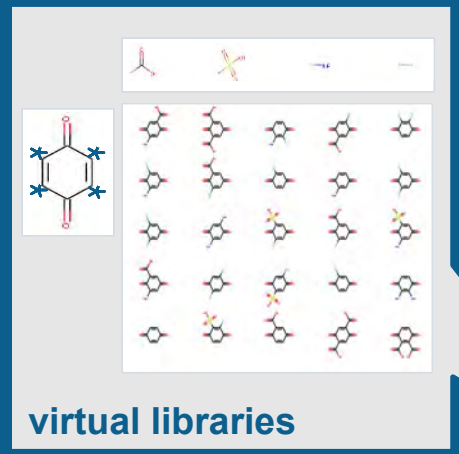
Development of a model-based high-throughput screening method

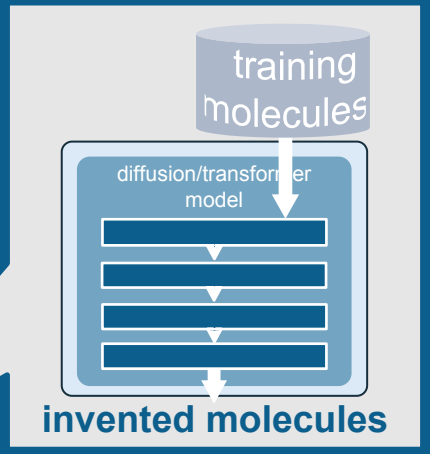
Fraunhofer DTU Danmarks Tekniske Universitet cnrs CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE zhaw KIT Karlsruher Institut für Technologie UNSW SYDNEY

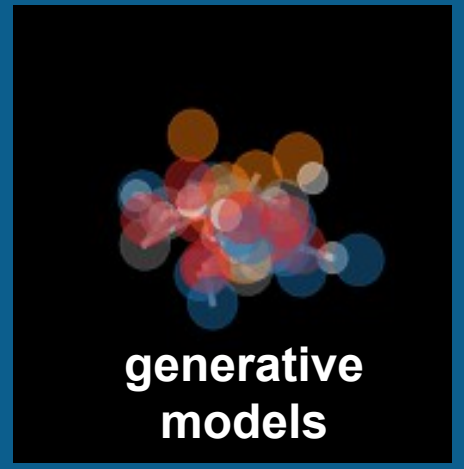
Screening workflow for electroactive molecules

SONAR

candidate space



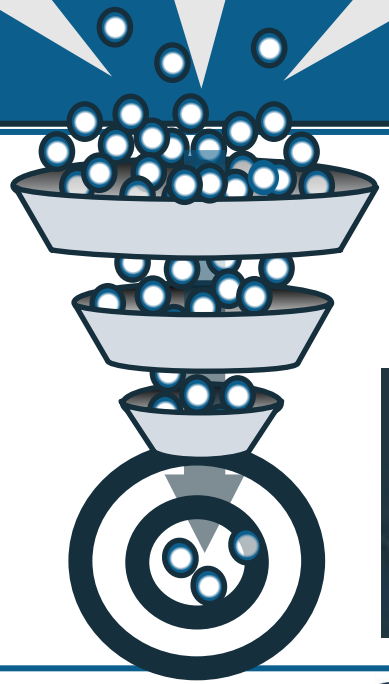




flexible workflow

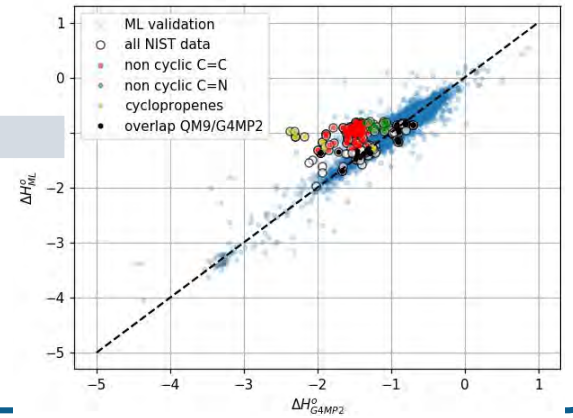
narrow down candidates for further testing based on

- redox potential
- solubility
- synthetic accessibility
- ...
- **OCV**



demo version:
redoxfox.scai.fraunhofer.de

predictive models



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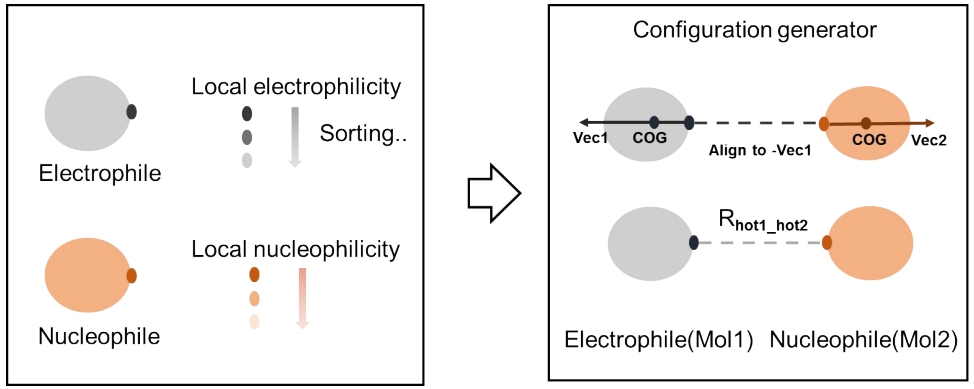
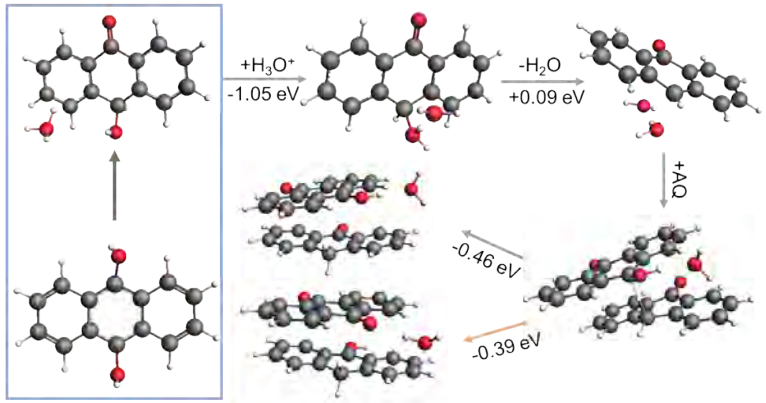
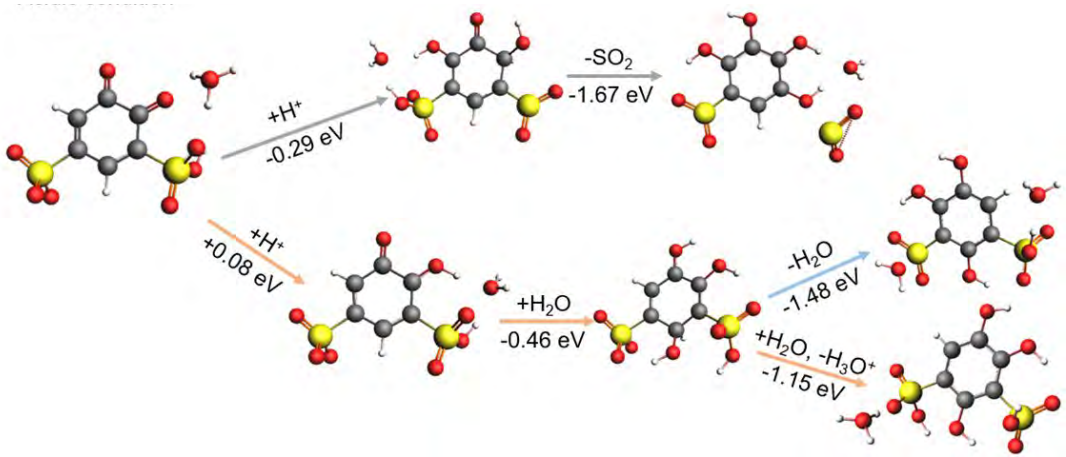
Electronic structure modelling of electroactive molecules



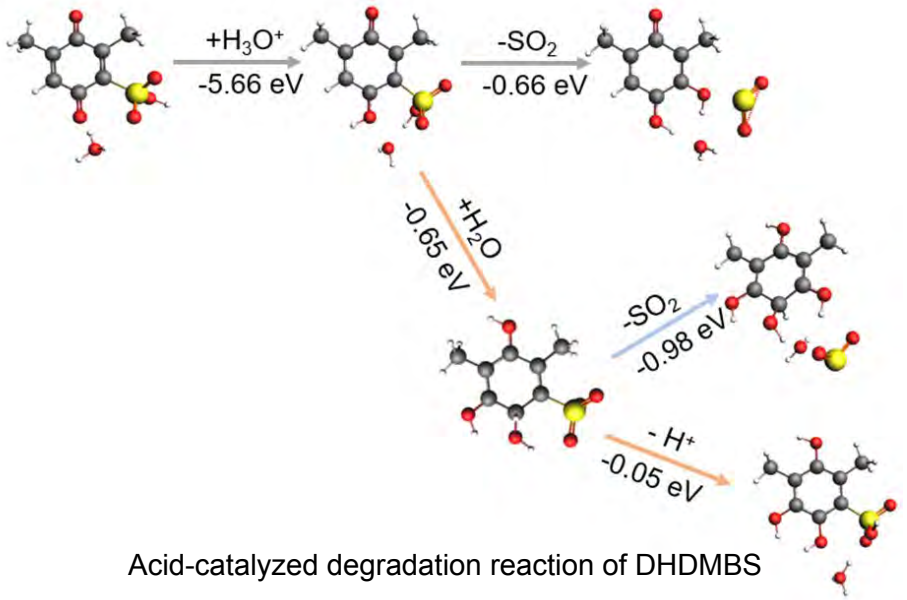
Encounter complexes generated based on electro-/nucleophilicity descriptors



Acid-catalyzed degradation reaction of AHQ



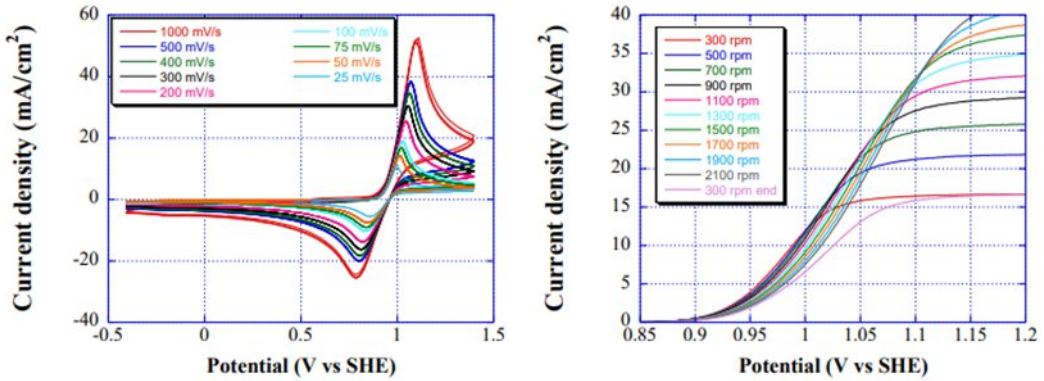
Acid-catalyzed degradation reaction of BQDS



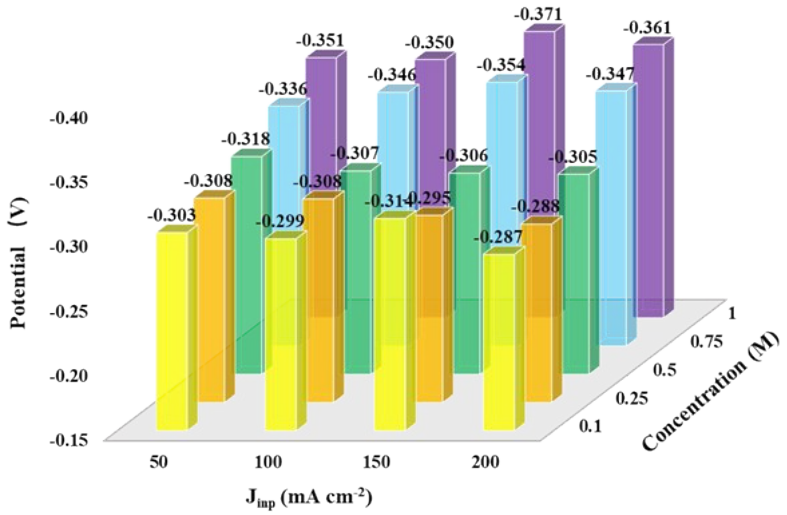
Acid-catalyzed degradation reaction of DHDMBS

Meso-scale modelling of the electrochemical interface

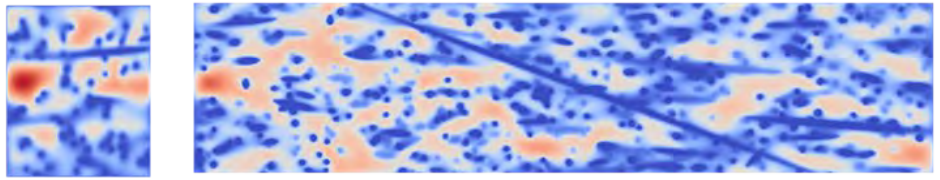
Extraction of kinetic parameters from experiments (TEMPOL)



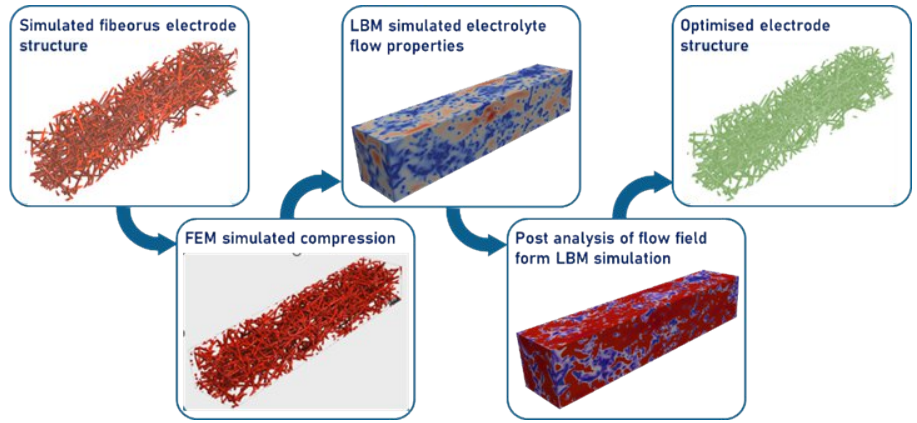
kMC-simulated electrode potentials at steady-state for MV^{+} -> MV^{2+}

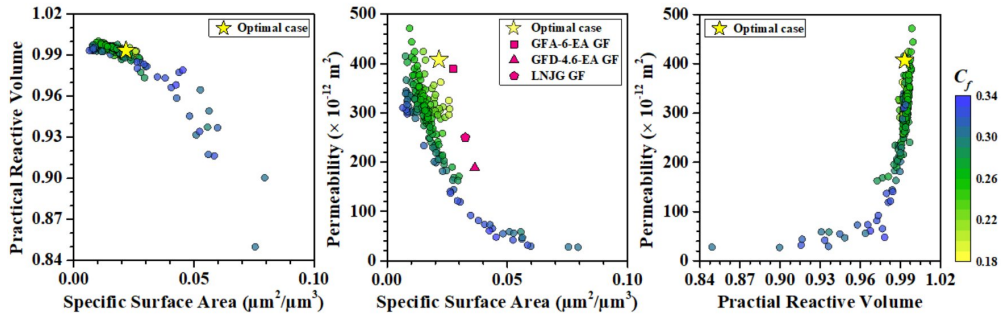


Lattice-Boltzman velocity field simulation



Workflow illustration of LBM based electrode optimisation

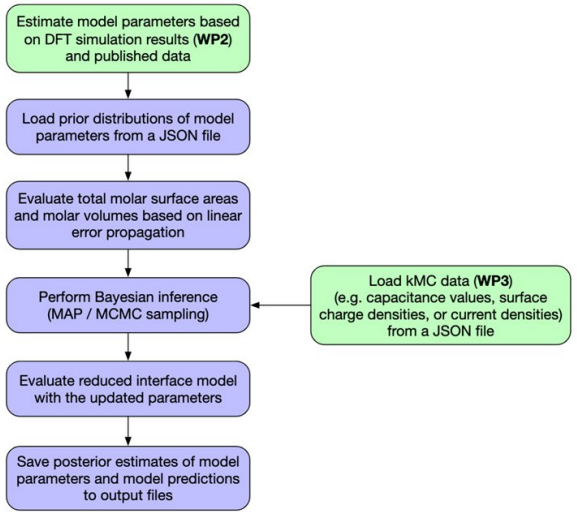


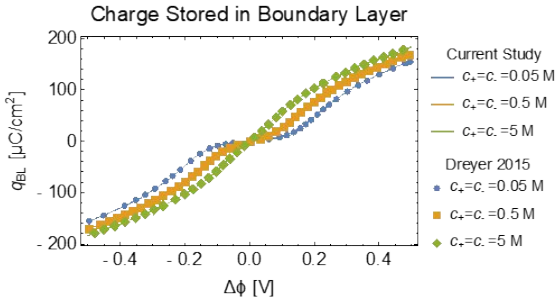


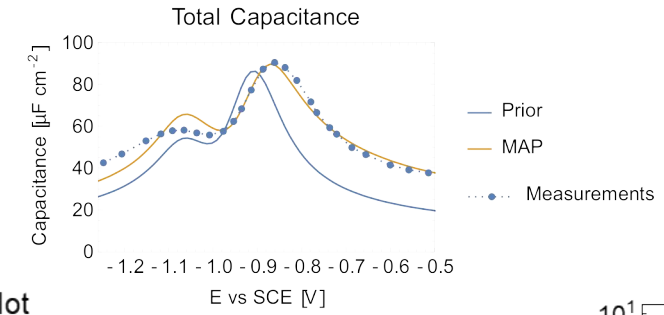
- Bridging the scales: connection of electrochemical double layer properties, porous media flow and continuum modeling of RFBs

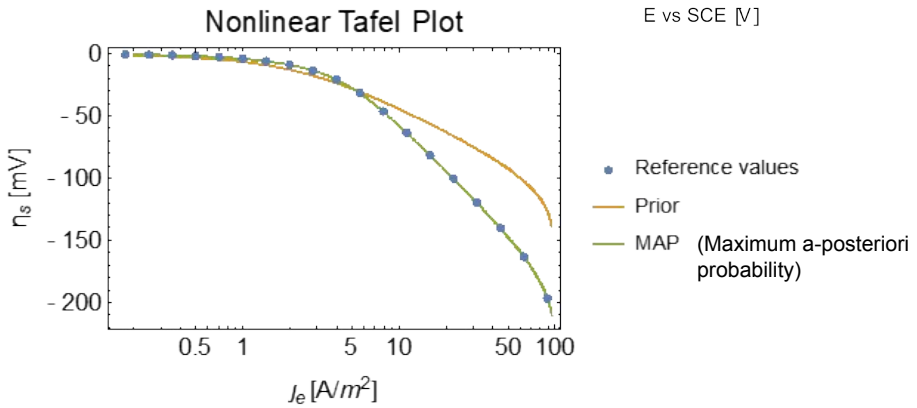
Reduced electrochemical interface model

Workflow of the parameter estimation

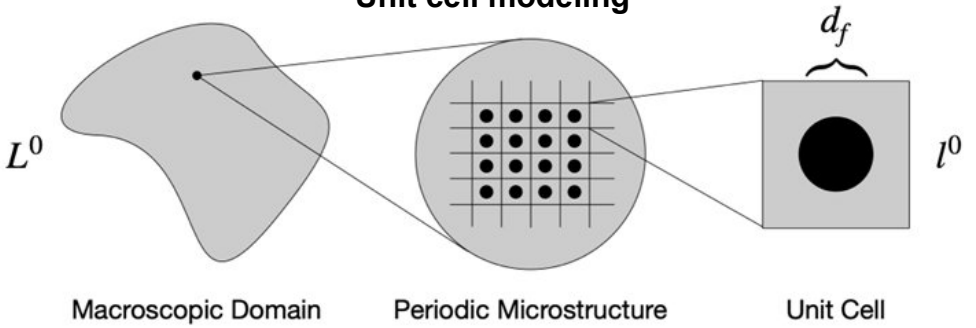


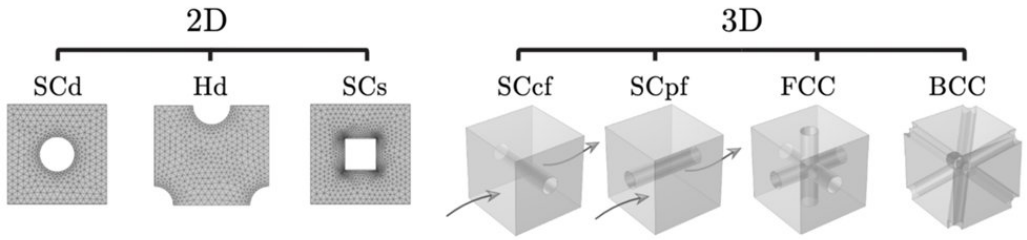


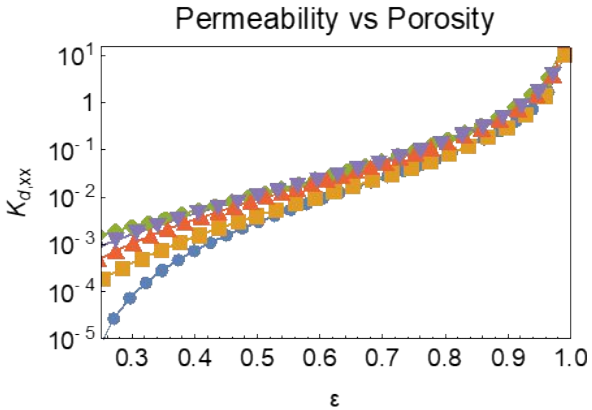


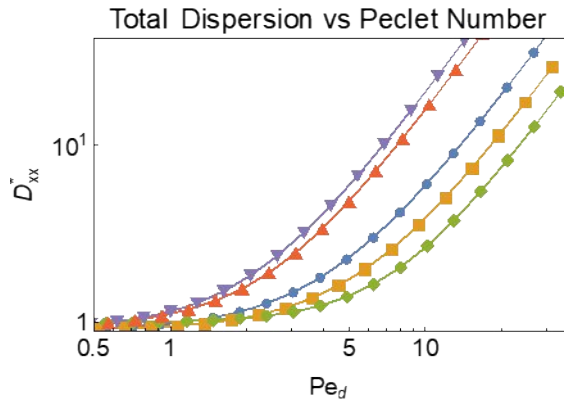


Unit cell modeling





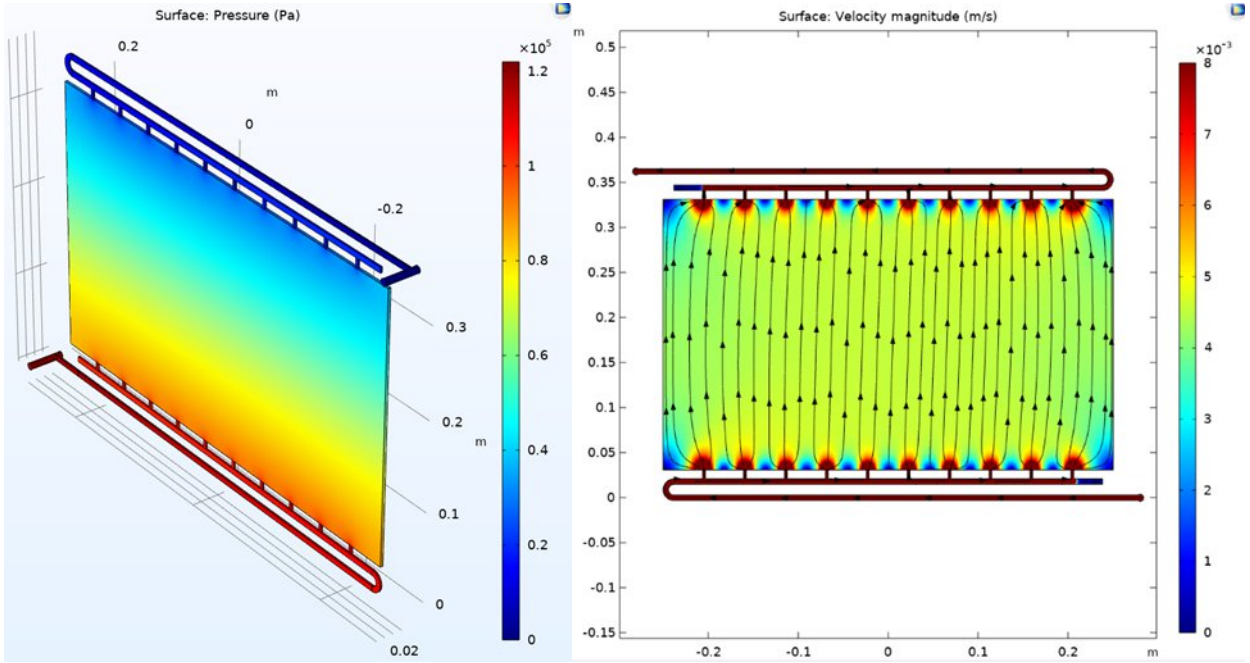




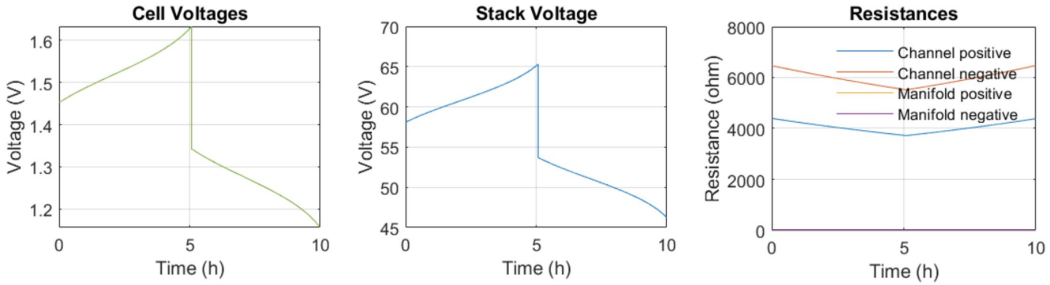
SCd–2D Hd–2D SCpf–3D FCC–3D BCC–3D

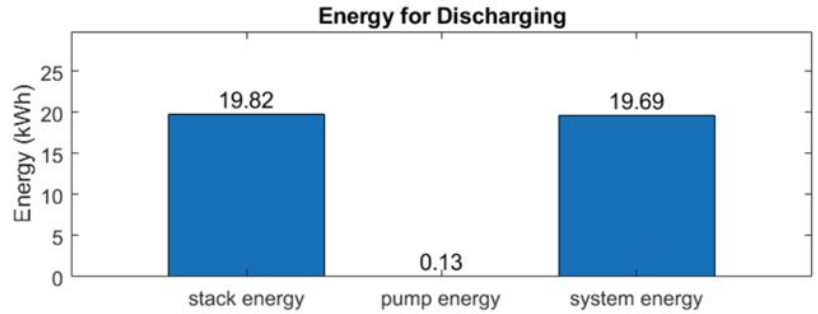
- Stack and system level modelling

Hydraulic simulation MV/TEMPTMA



Hydraulic & electrochemical simulation VRFB





Hydraulic & electrochemical simulation VRFB