# Multiphysics modeling of a novel Non-Aqueous Redox Flow Battery (NAQRFB)


Mirko D'Adamo[1,2] *, Nicolas Daub[3], Juan Manuel Paz[4], Lluís Trilla[2], Jose Saez[1]

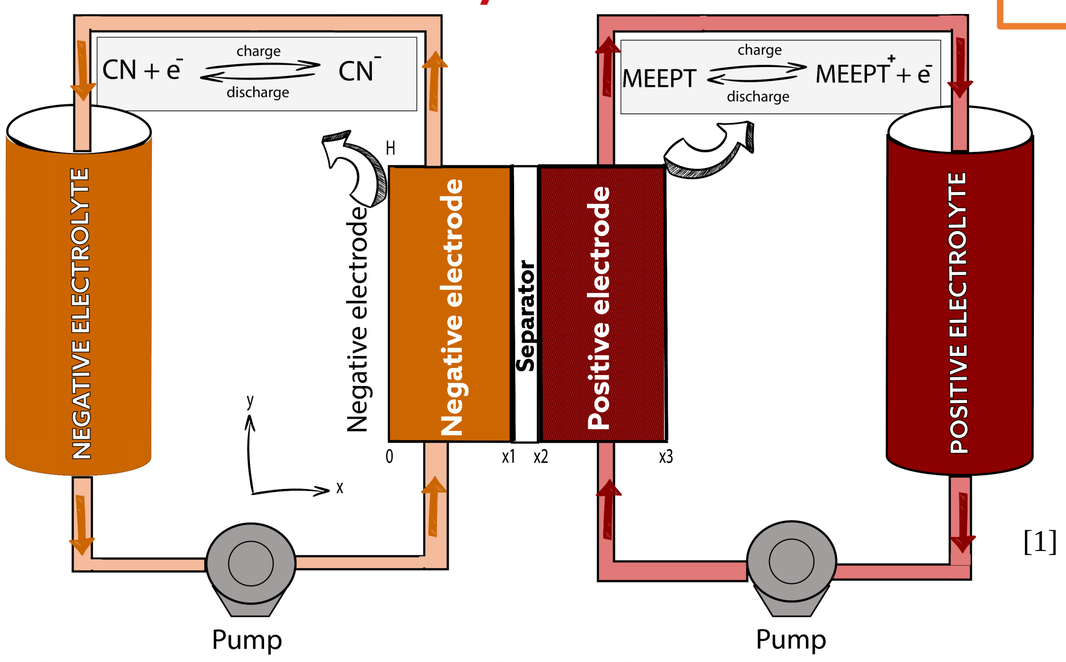
[1]Smart Energy, N Vision Systems And Technologies, Barcelona, Spain

[2]IREC - Fundació Institut de Recerca en Energía de Catalunya, Sant Adrià del Besòs, Spain

[3]Molecular Materials and Nanosystems & Institute for Complex Molecular Systems, University of Technology, Eindhoven, The Netherlands

[4]Department of Chemical Engineering, Universidad de Malaga, Malaga, Spain


## INTRODUCTION




[1]

**N-(2-(2-methoxyethoxy) ethyl)phenothiazine(MEEPT) with a terephthalonitrile derivative**

**Novel NAQRFB Symmetric cell** → **Capacity fading ?** [2]

## OBJECTIVE

**Multiphysics Crossover Modelling** [3]

## METHODOLOGY

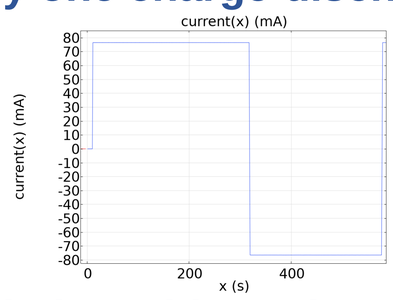
### 1. Defining the physical problem

**Tertiary Current Distribuition**

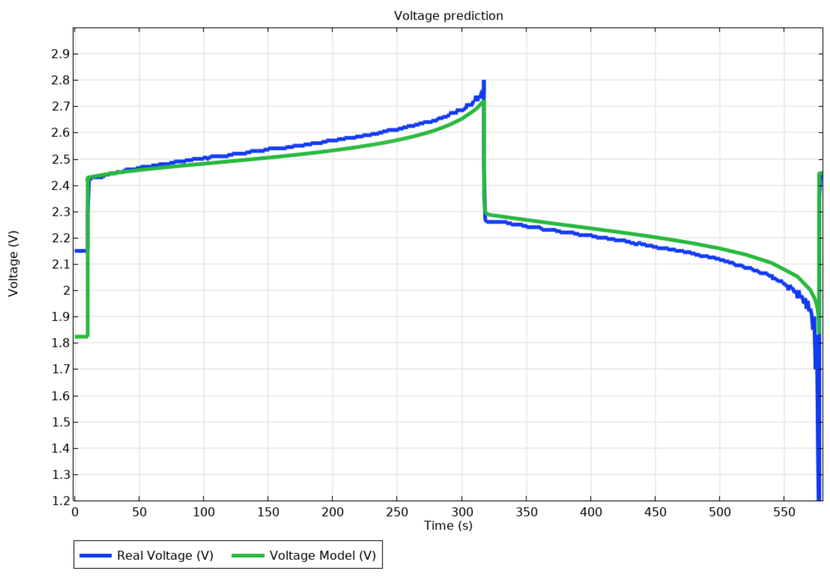
### 2. 2D Physical modelling

COMSOL MULTIPHYSICS®

### 3. Apply one charge-discharge cycle

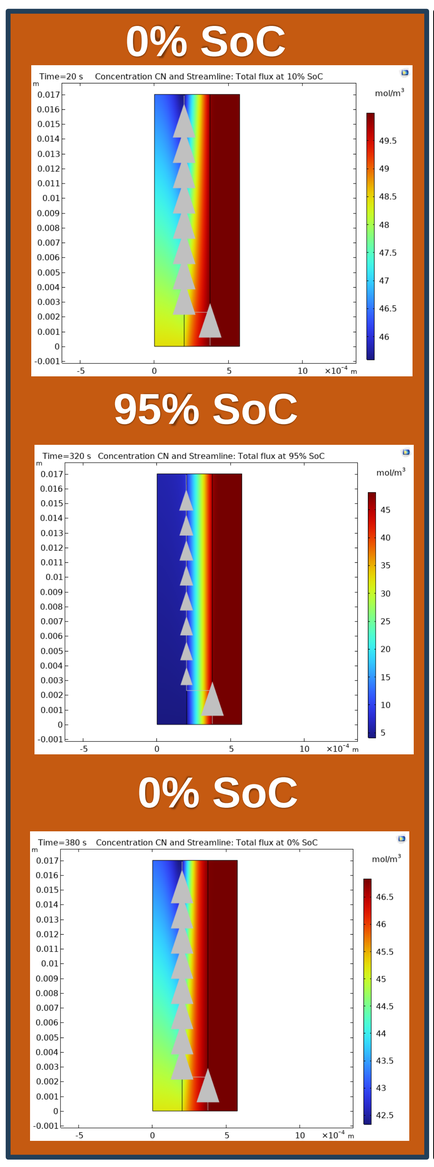



### 4. Validation with Real Data

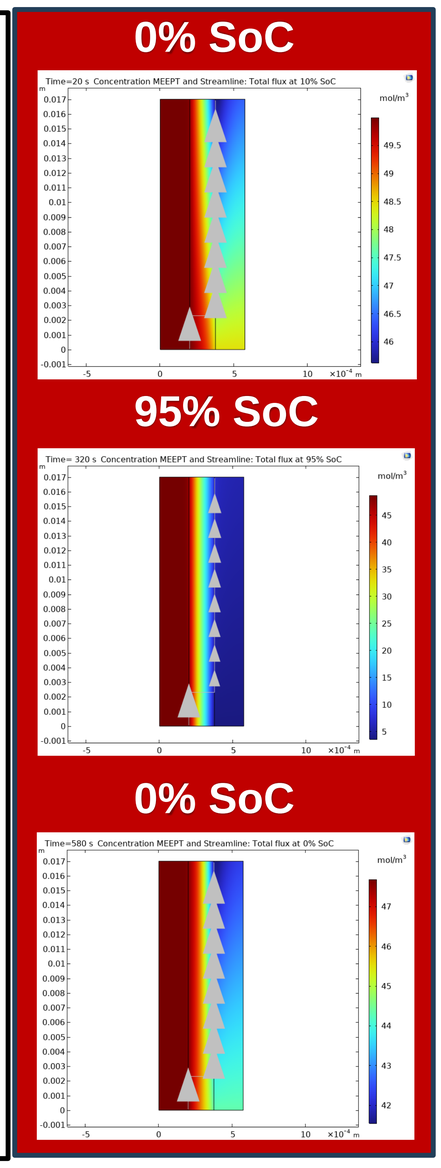



## RESULTS

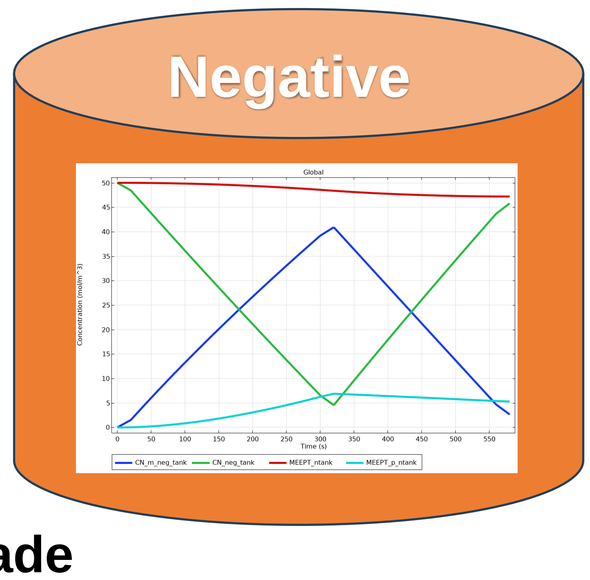
### CN concentrations

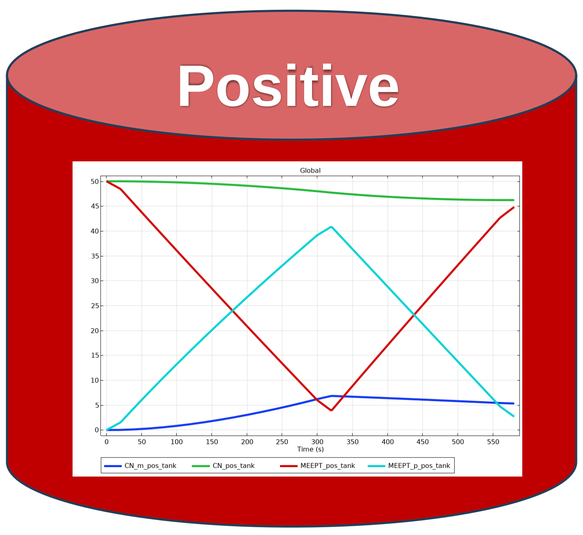



### MEEPT concentrations




### Tanks concentrations over time




## CONCLUSIONS

**2% RMSE Voltage Error**

**Crossover occurs which leads to capacity fade**

## FUTURE WORK

**Optimize current density, flow rate and design**


## ACKNOWLEDGMENTS

- With the support of Pla de Doctorats Industrials de la Secretaria d'Universitats i Recerca del Departament d'Empresa i Coneixement de la Generalitat de Catalunya

DOCTORATS INDUSTRIALS — Generalitat de Catalunya, Departament d'Empresa i Coneixement, Secretaria d'Universitats i Recerca


## REFERENCES


1. J. D. Milshtein et al., "High current density, long duration cycling of soluble organic active species for non-aqueous redox flow batteries," Energy & Environmental Science, vol. 9, no. 11, pp. 3531–3543, Jan. 2016
2. Knehr, K. W. and Kumbur, Open circuit voltage of vanadium redox flow batteries: Discrepancy between models and experiments, E. C., Electrochemistry Communications, 13 (2011) 342
3. Modak, S.V., Shen, W., Singh, S. et al. Understanding capacity fade in organic redox-flow batteries by combining spectroscopy with statistical inference techniques. Nat Commun 14, 3602 (2023).


## ADD ME