



UNIVERSITÀ
DEGLI STUDI
DI PALERMO


Dipartimento di Ingegneria Chimica,
Gestionale, Informatica, Meccanica (DICGIM)

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Reverse Electrodialysis process with seawater and concentrated brines: a COMSOL model for equipment design

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Outline

1. Introduction

- Reverse Electrodialysis process
- Modelling goals

2. Model development

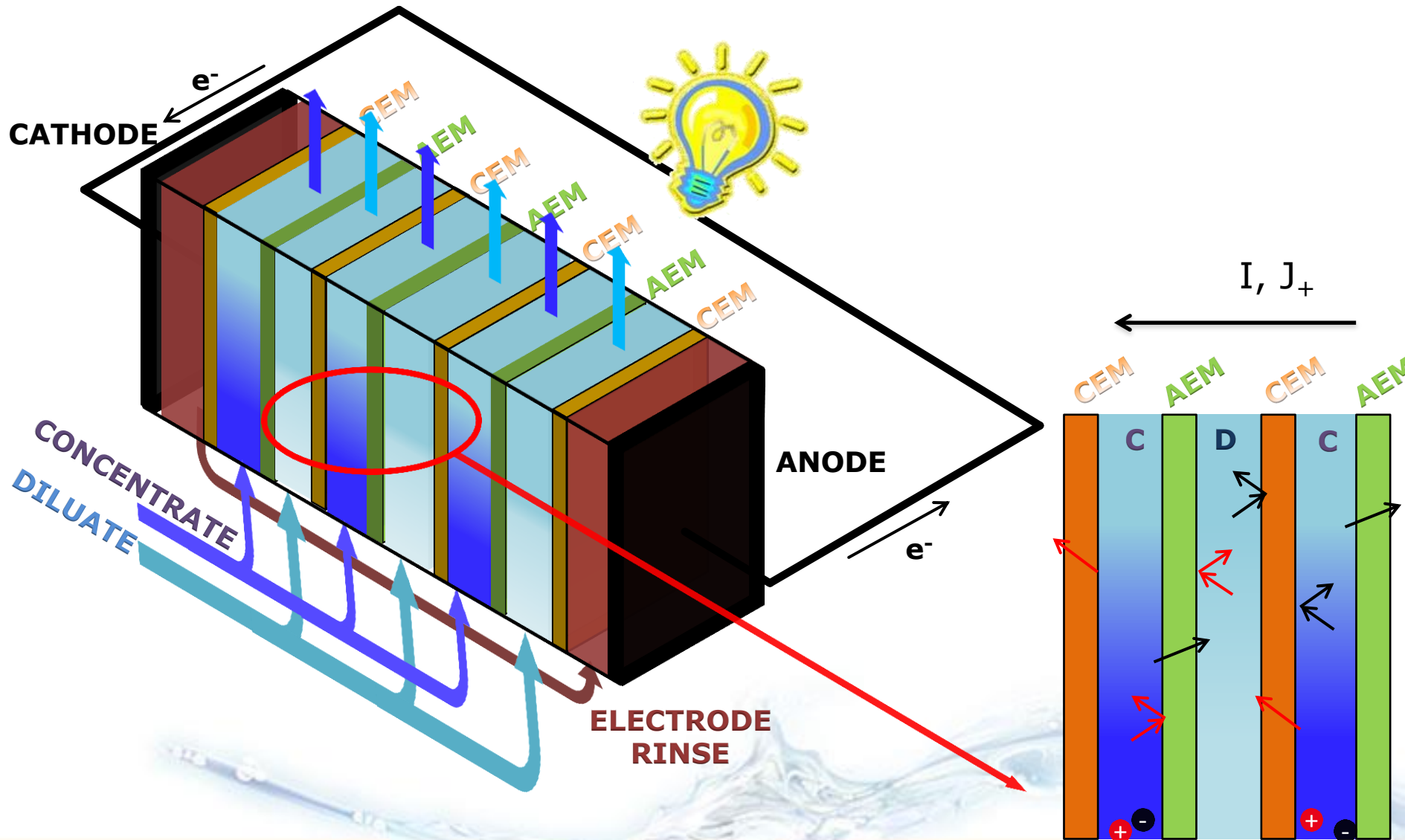
- System definition
- Governing equations
- Model calibration

3. Results

- Concentration profiles inside channels
- Electric potential through the stack
- Salt fluxes through membranes

4. Conclusions

Reverse Electrodialysis Technology



Modelling goals

Investigated physics

COMSOL Multiphysics®

ELECTRICAL	MECHANICAL	FLUID	CHEMICAL	MULTIPURPOSE	INTERFACING	
AC/DC Module	Heat Transfer Module	CFD Module	Chemical Reaction Engineering Module	Optimization Module	LiveLink™ for MATLAB®	LiveLink™ for Excel®
RF Module	Structural Mechanics Module	Microfluidics Module	Batteries & Fuel Cells Module	Material Library	CAD Import Module	ECAD Import Module
Wave Optics Module	Nonlinear Structural Materials Module	Subsurface Flow Module	Electrodeposition Module	Particle Tracing Module	LiveLink™ for SolidWorks®	LiveLink™ for SpaceClaim®
MEMS Module	Geomechanics Module	Pipe Module				LiveLink™ to CAD®
Plasma Module	Fatigue Module	Molecular Dynamics Module				LiveLink™ for ANSYS®
Semiconductor Module	Multibody Dynamics Module					Import from TIA® V5
	Acoustics Module					

- ✓ Mass transport through membranes
- ✓ Transport of electrolytes
- ✓ Electrochemical reaction
- ✓ Fluid dynamics

System definition and model assumptions

Model assumptions:

- **Empty channels**
- **NaCl** aqueous solutions
- **Negligible solvent flux** through membranes
- Adopting **Nernst-Planck** equation
- **Activity coefficients** equal to unity
- Adopting **Einstein** relation for ion diffusion coefficient

Governing equations

- Laminar flow for Newtonian fluid:

$$\nabla \mathbf{u} = 0 \quad \rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \nabla \mathbf{u} = -\nabla P + \mu \nabla^2 \mathbf{u} + \mathbf{F}$$

- Transport equation through solutions (*Nernst-Planck* model):

$$N_i = -D_i \nabla c_i - z_i u_{m,i} F c_i \nabla \Phi_l + u c_i$$

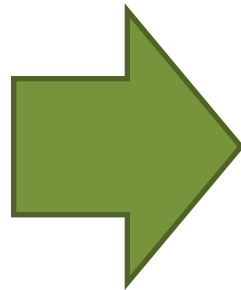
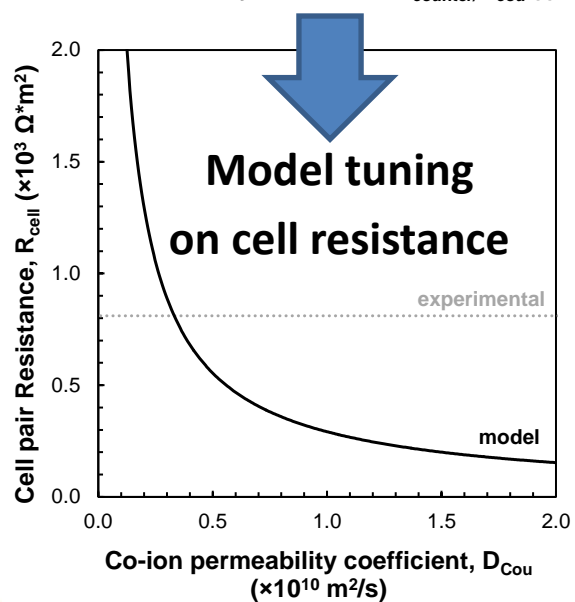
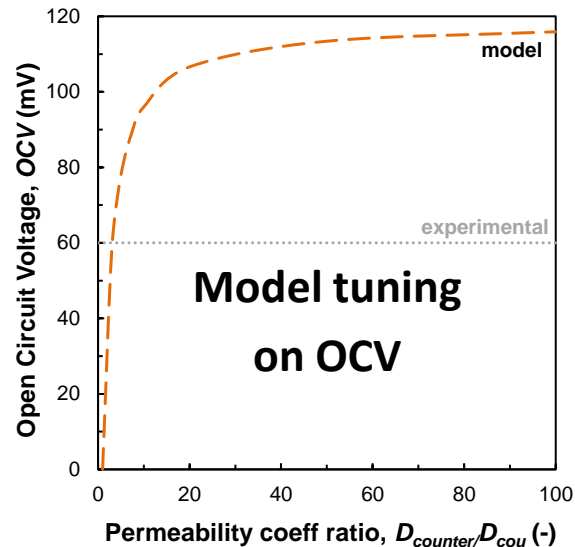
$$i_l = F \sum_i z_i (-D_i \nabla c_i - z_i u_{m,i} F c_i \nabla \Phi_l) \quad \sum_i z_i c_i = 0$$

- Electrode kinetics (*Butler-Volmer* theory):

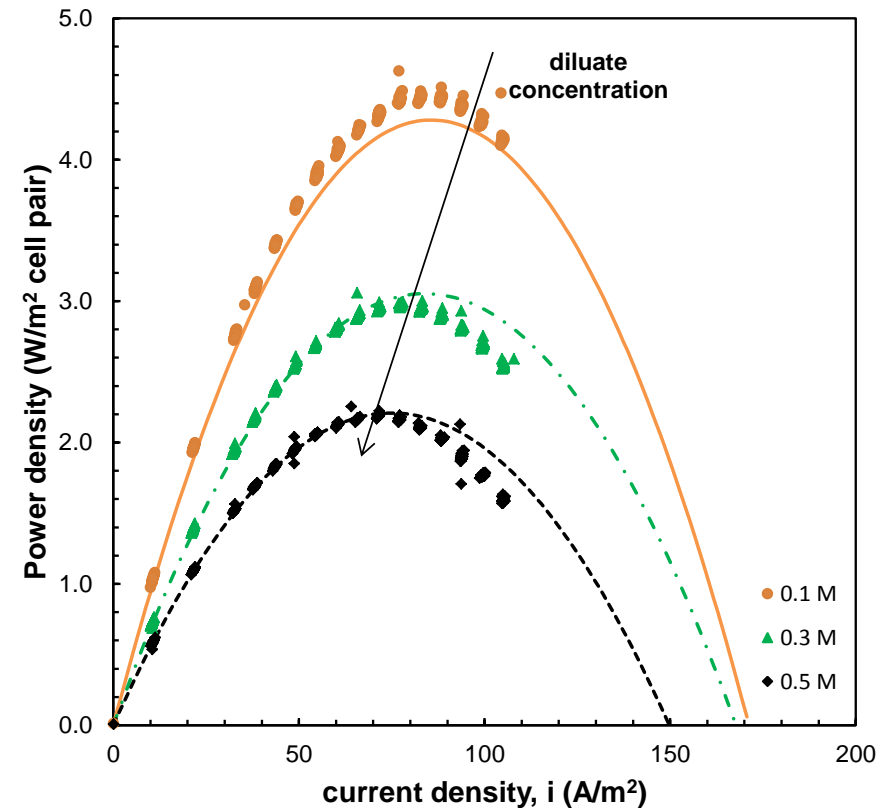
$$i = i_0 \left[\exp\left(\frac{\alpha_a F \eta}{RT}\right) - \exp\left(\frac{-\alpha_c F \eta}{RT}\right) \right]$$

$$\nabla \cdot i_l = F \sum_i z_i R_{i,src} Q_l$$

Model tuning/validation

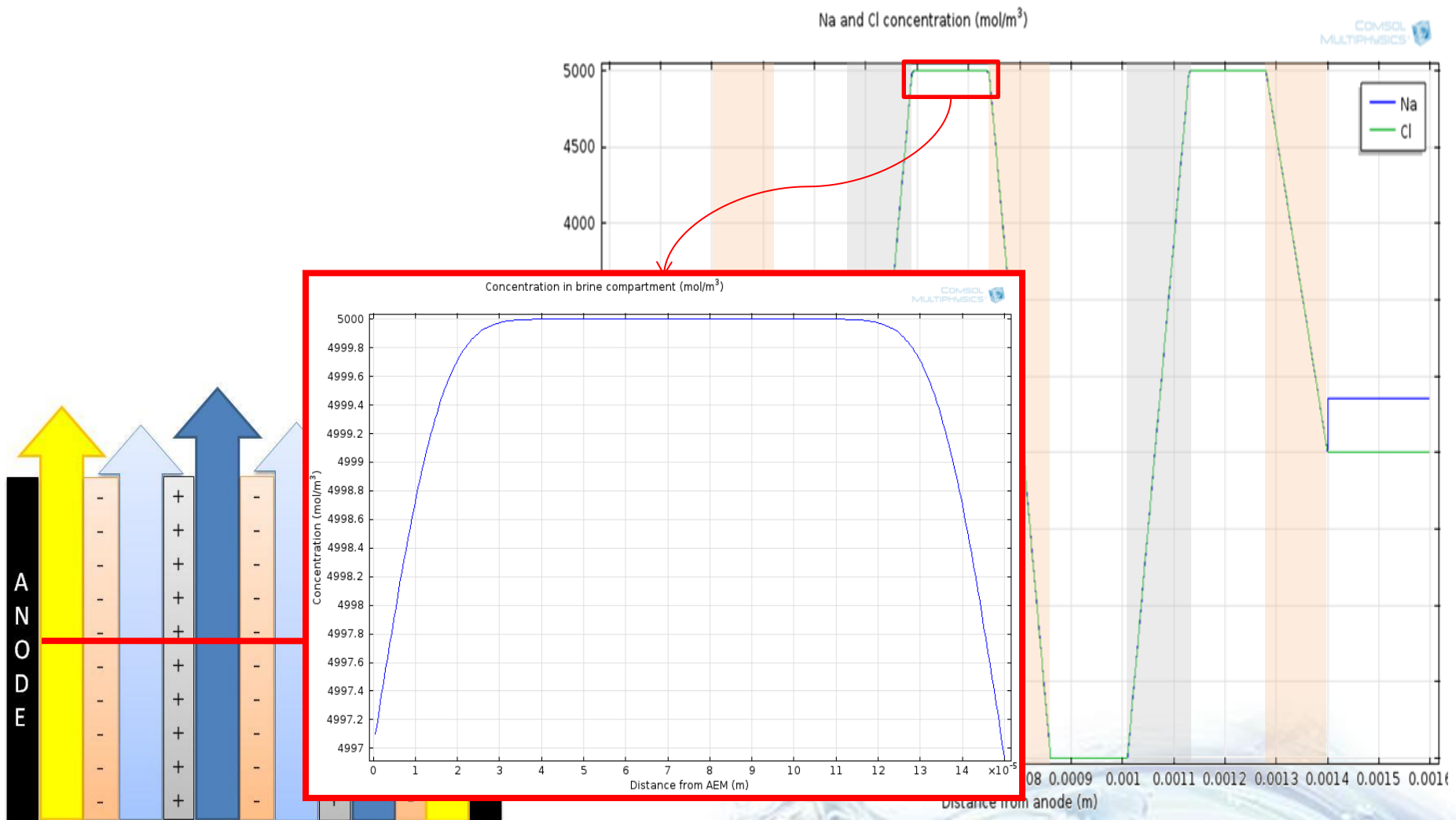


Model validation

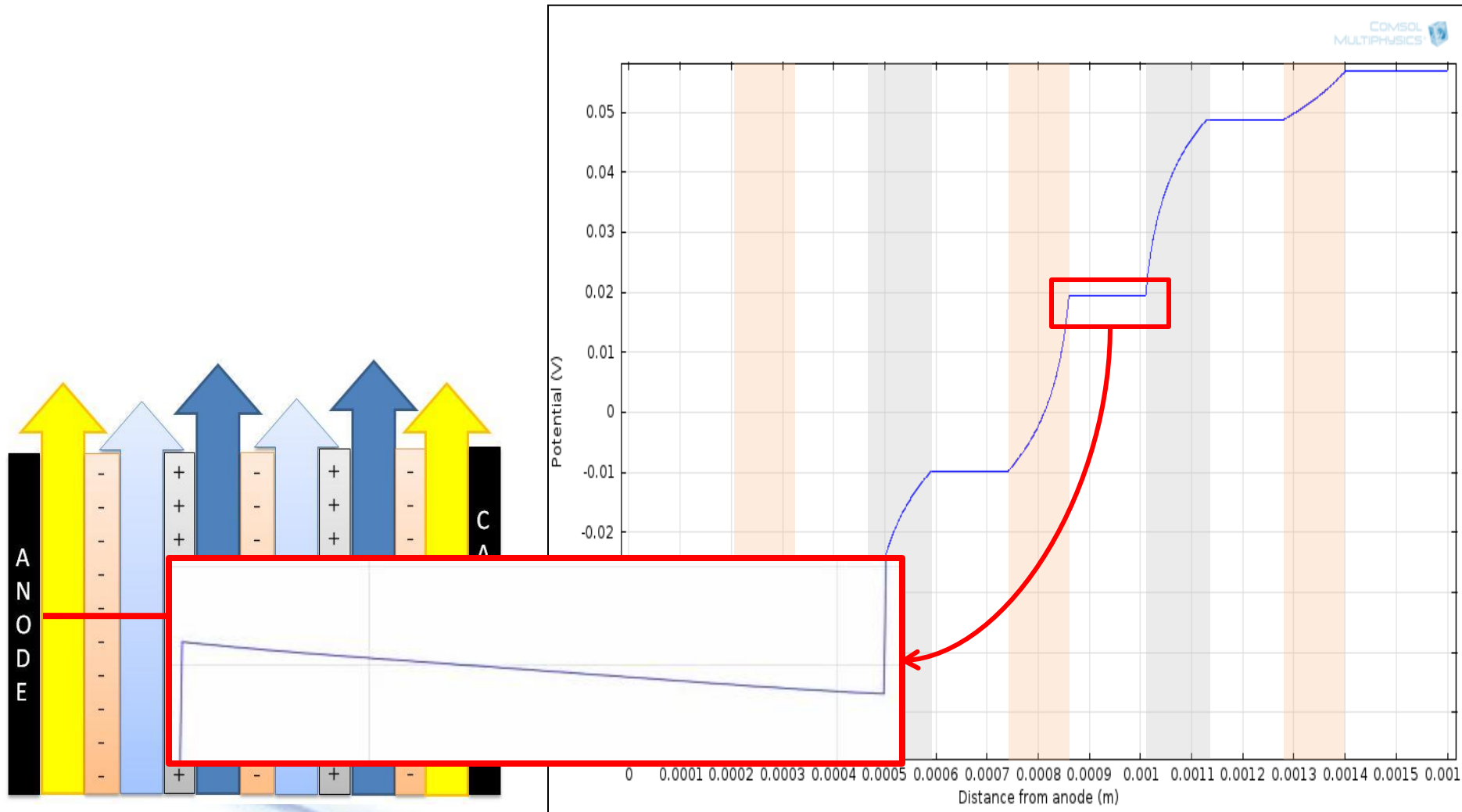


Experimental data collected with a 50 cell pairs stack, Fujifilm membranes, Deukum 270 μm spacers. Brine: 5 M NaCl. $T=20^\circ C$. Fluid velocity: 1 cm/s.

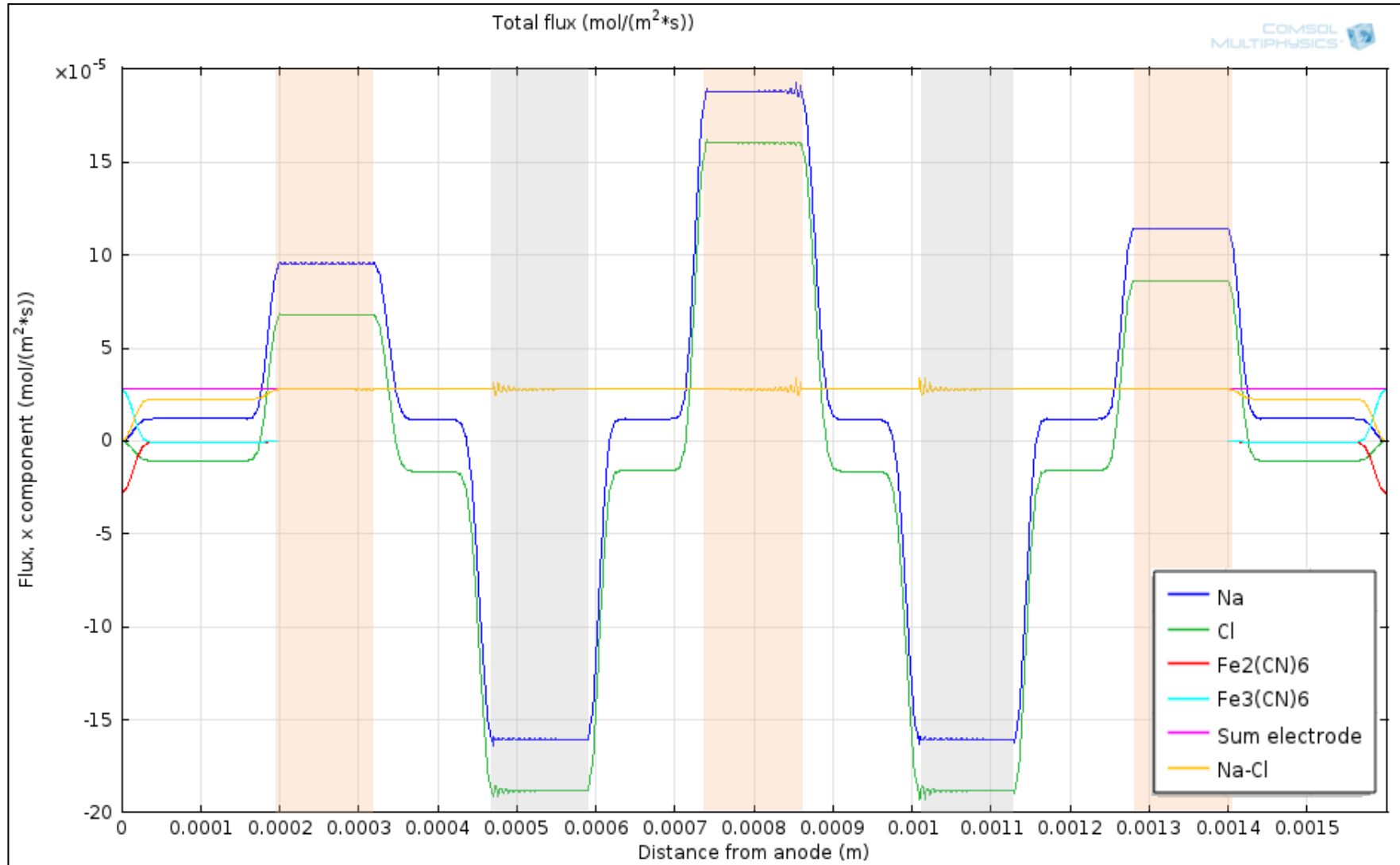
Concentration profiles along channels



Electric potential through the stack



Salt fluxes through membranes



Conclusions

- ✓ **Model validated** on experimental data under different conditions
- ✓ Simplified approach to simulate both **fluid dynamics/electrochemical phenomena**

Next steps

- **Activity coefficients** evaluation
- **Mechanical analysis** on membranes
- Description of **Donnan Potentials** across membranes

Acknowledgments



www.reapower.eu

Project title: *Reverse Electrodialysis Alternative Power Production*

Call identifier: FP7-ENERGY-2010-FET

(Future Emerging Technologies for Energy Applications)

The Future

of sustainable energy production



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***Thank you
for your attention***

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