

Model Building and Parameter Estimation for Electrodialysis Systems

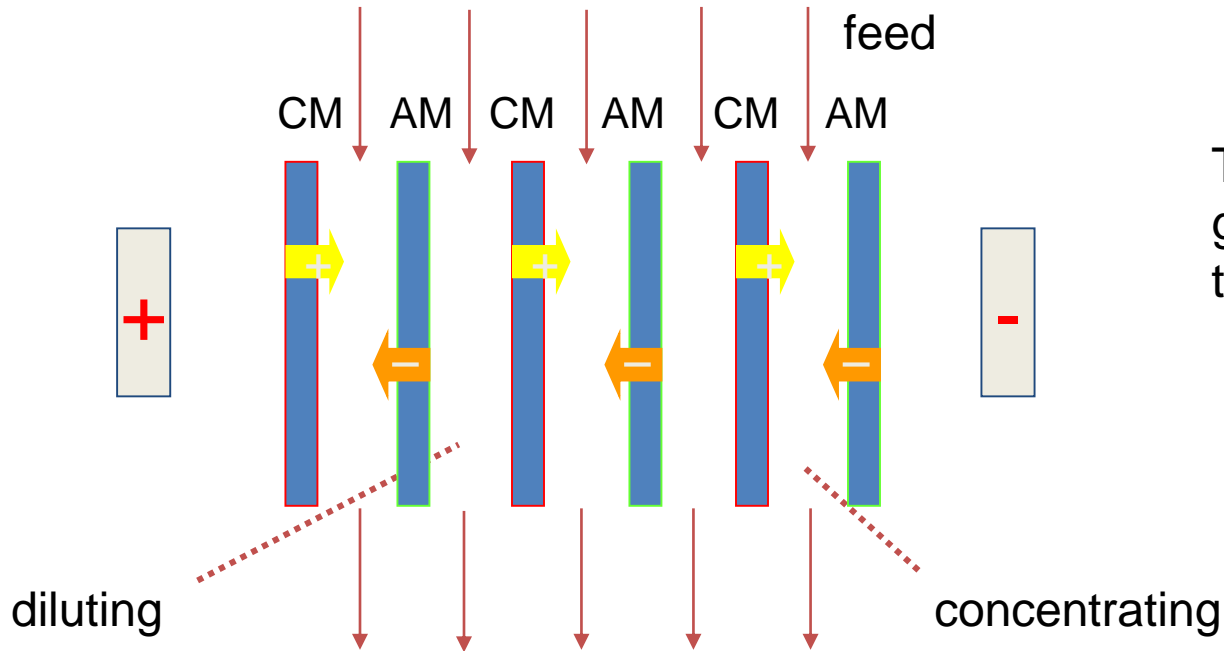
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Electrodialysis (ED)

Unit operation used to remove electrolytes from solutions and to concentrate electrolyte solutions. It uses two types of membranes consisting of a polymer skeleton and fixed charges arranged alternately in packs (of several hundred).



The electric field that is generated forces ions to cross membranes.

ED modeling

Water flux

$$J_W = \frac{t_W}{F} j + L_W \Delta \pi$$

Salt flux

$$J_B = \frac{t_B}{F} j + L_B \Delta c_B$$

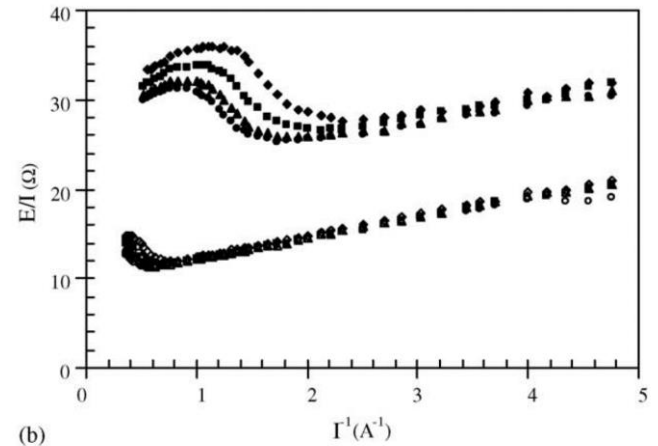
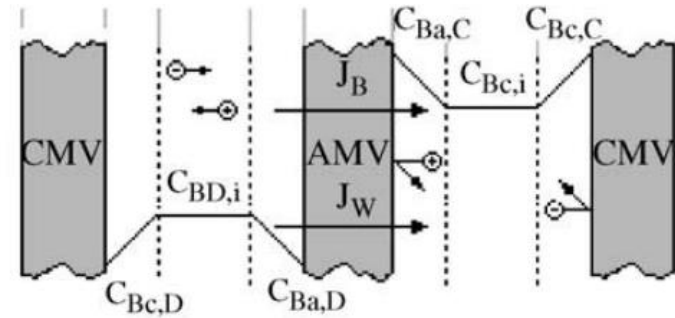
Electric potential

$$E + E_j + E_D = jr$$

Limiting
density

current

$$j_{\text{lim},c} = \frac{F c_B D_B}{\delta(t_c^+ - t^+)}$$



Determination of model parameters

Journal of Membrane Science 260 (2005) 90–111

www

Optimal strategy to model the electrodialytic recovery of a strong electrolyte

Marcello Fidaleo, Mauro Moresi*

- Electric conductivity measurements \longrightarrow t^+ , t^- , D° , k
- Desalting tests \longrightarrow t_B , t_W , L_B , L_W
- I-E experiments with only one type of membrane \longrightarrow E_{el} , R_a , R_c ,
 $I_{lim,a}$, $I_{lim,c}$, a_{me}

Determination of model parameters

Journal of Membrane Science 367 (2011) 220–232



Contents lists available at ScienceDirect

Journal of Membrane Science

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Electrodialytic desalting of model concentrated NaCl brines as such or enriched with a non-electrolyte osmotic component

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- Electric conductivity measurements \longrightarrow t^+ , t^- , D° , k
- Desalting tests \longrightarrow t_B , t_W , L_B , L_W
- I-E experiments with both types of membrane \longrightarrow E_{el} , $R_a + R_c$, I_{lim} , a_{me}

Determination of model parameters

CHEMICAL ENGINEERING RESEARCH AND DESIGN 105 (2016) 107–119



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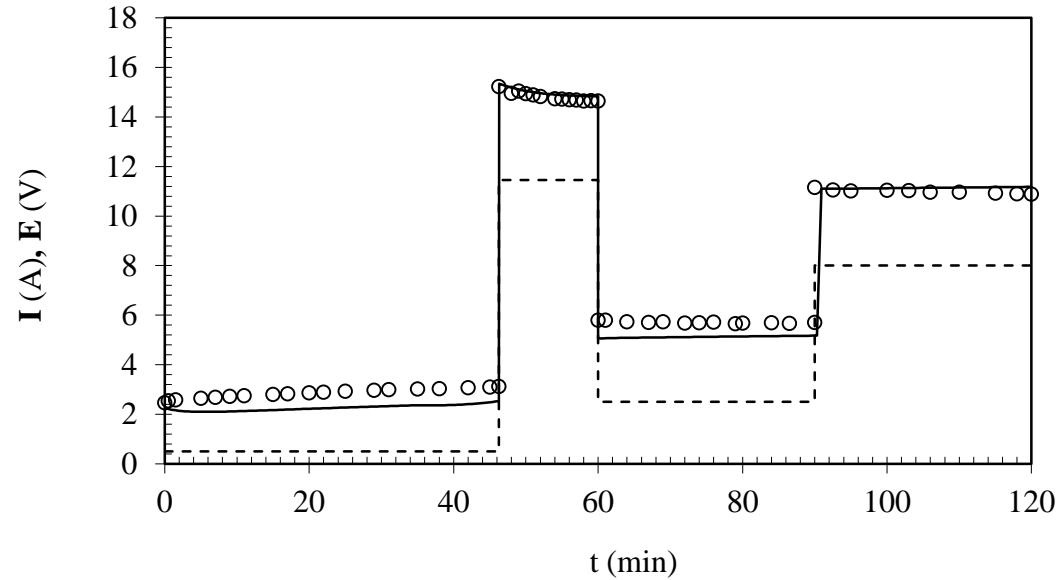
journal homepage: www.elsevier.com/locate/cherd

Optimal design of experiments for parameter identification in electro dialysis models

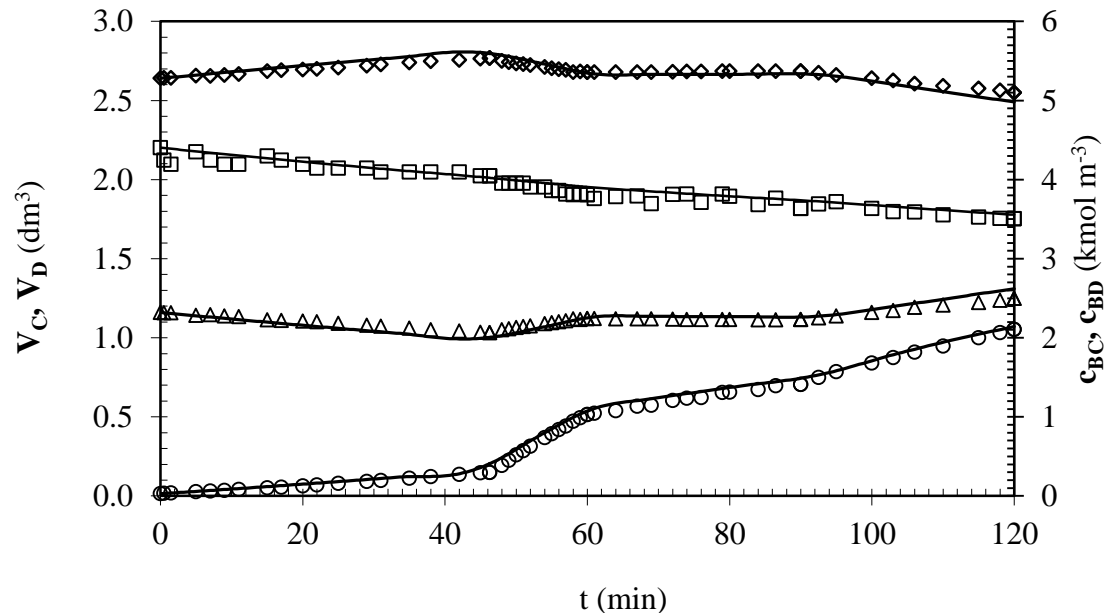
Federico Galvanin^a, Raffaele Marchesini^b, Massimiliano Barolo^b,
Fabrizio Bezzo^b, Marcello Fidaleo^{c,*}

- Electric conductivity measurements \longrightarrow t^+ , t^- , D° , k
- Desalting tests \longrightarrow t_B , t_W , L_B , L_W ,
 E_{el} , $R_a + R_c$, a_{me}

Design of experiments based on model



Given the model the optimal experiment for parameter estimation is designed.



The $I(t)$ trajectory that maximizes the information content of the experiment is determined.

Aim of this work

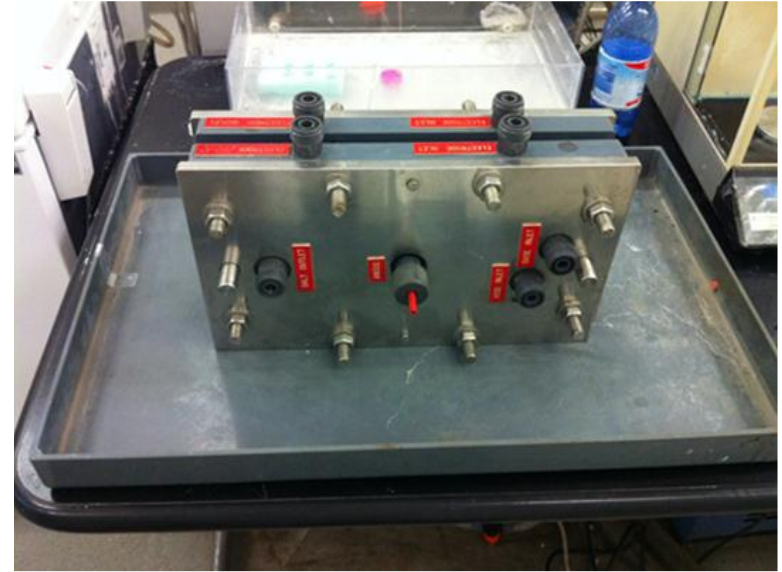
If we equip the plant with very precise online sensors for solution conductivity and volume and use a time dependent electric current function to feed the stack, can we estimate some model parameters with just one batch desalting experiment?

Can we accomplish this task by using COMSOL Multiphysics?

M&M: batch electro dialysis plant



ED plant control station



ED stack model EUR2 (Eurodia industrie SA)



Conductivity sensor



30 mm thread for general application

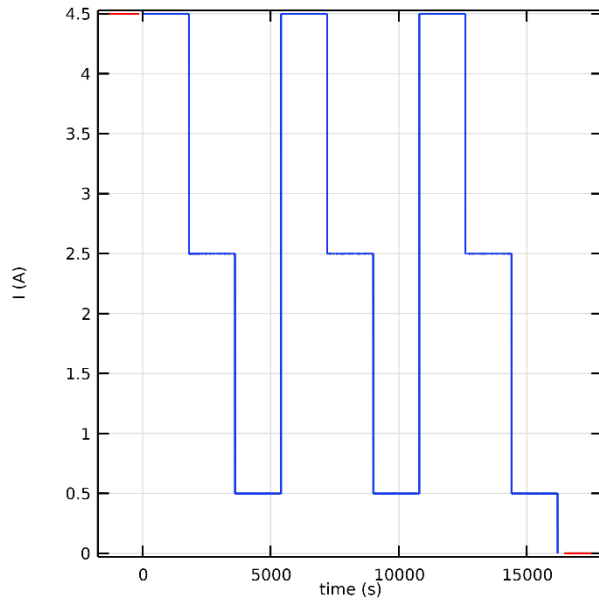
Level sensor



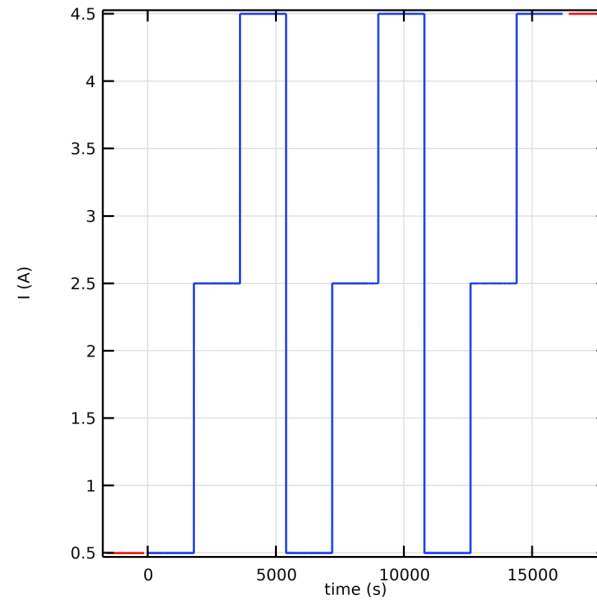
DC generator

Experimental plan

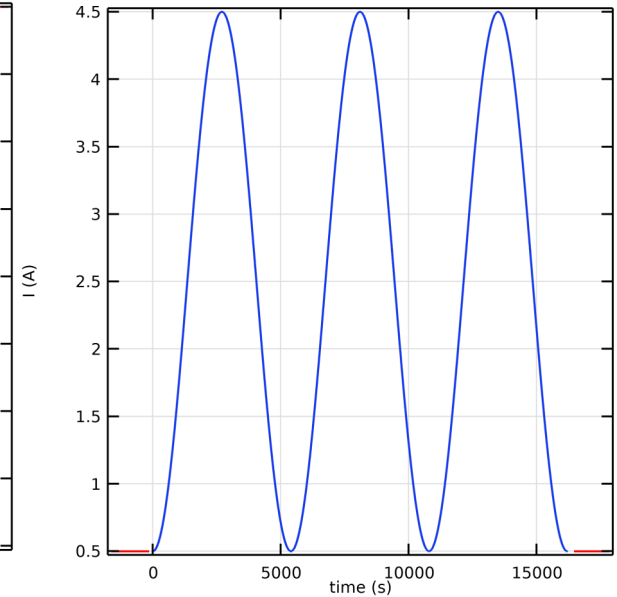
Three batch desalination experiments with different electric current inputs



decreasing step



increasing step



sinusoidal

Conductivity and level of solutions, electric current and potential acquired at 1 Hz sampling rate.

Model simulation and parameter estimation

Mathematical formulation

- 4 ODEs for concentrations (C) and volumes (V) of the solutions in the concentrating (C) and in the diluting (D) tanks
- 1 DAE for electric voltage (E)
- 4 parameters for water (L_W , t_W) and salt (L_B , t_B) transport properties

COMSOL implementation

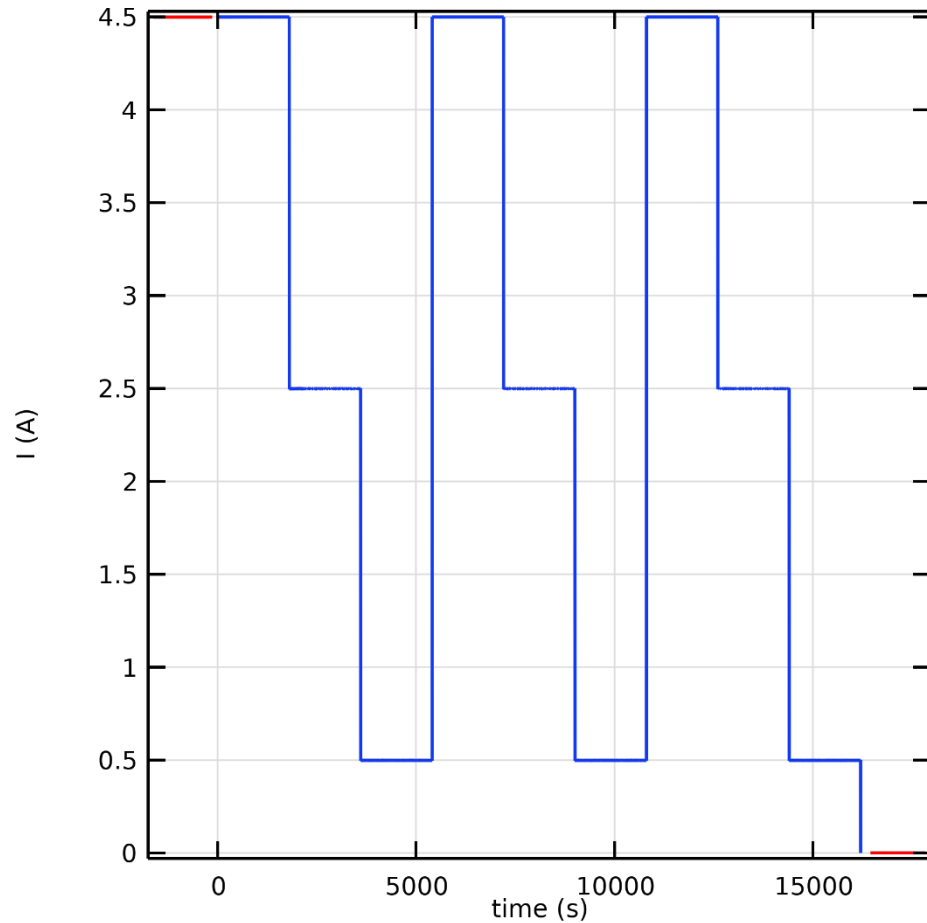
- 0D dimension, Mathematics, global ODEs and DAEs, parameter estimation

Name	f(u,ut,utt,t) (1)	Initial value (u_)	Initial value (u_t)	Description
VDd	$VDdt - (-WW * MW - WB * ...$	1	0	
VCd	$VCdt - (WW * MW + WB * ...$	1	0	
CBDd	$CBDdt + (CBDd * VDdt * ...$	1	0	
CBCd	$CBCdt + (+CBCd * VCdt * ...$	1	0	
Ed	$Ed - Eel / Eel + (ED * Ncell - ...$	1	0	
		0	0	

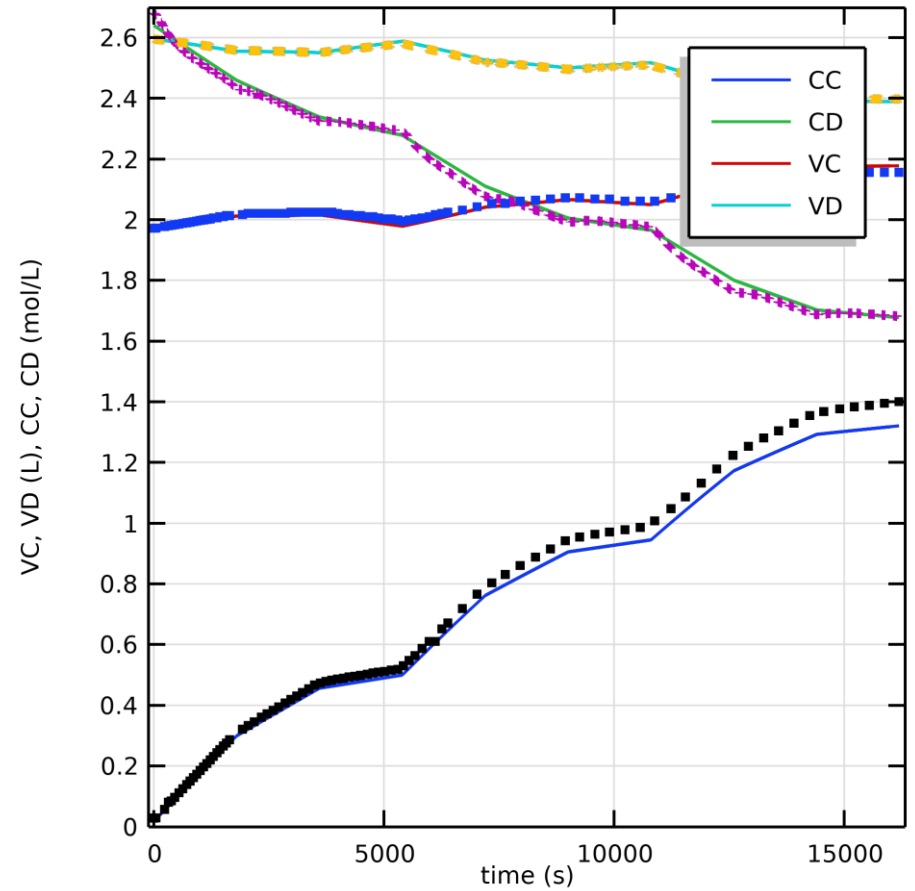
Results

Decreasing step pattern

Electric current

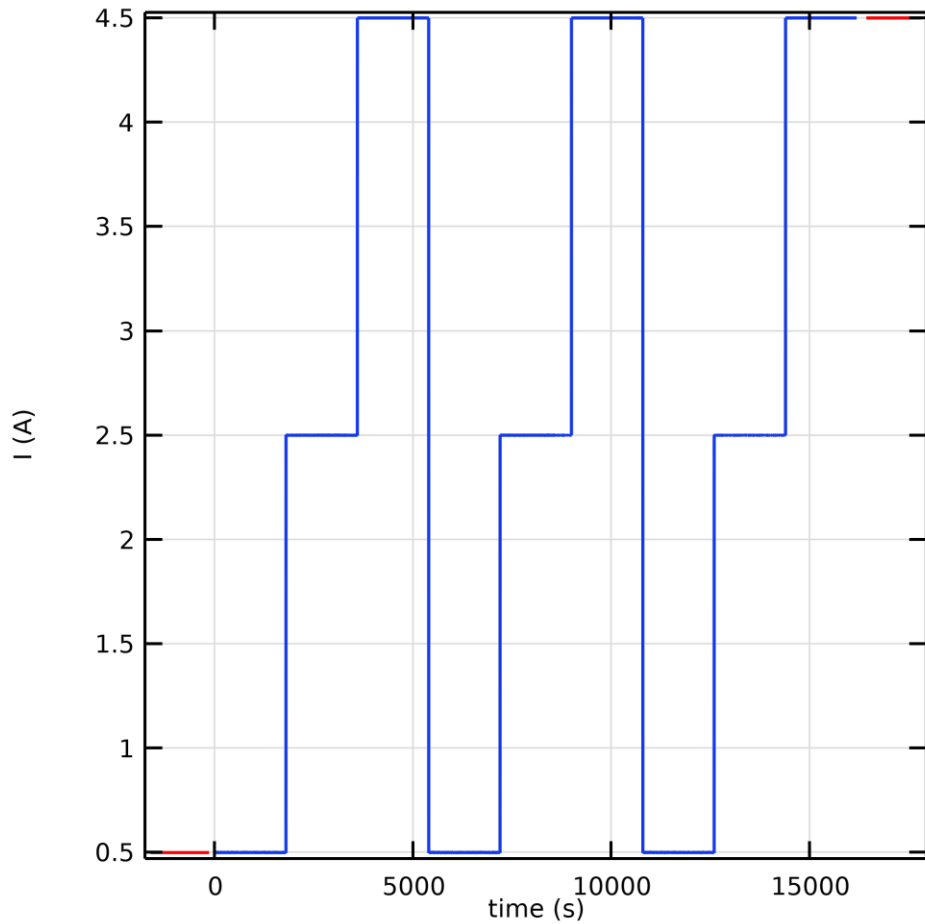


Volumes and concentrations

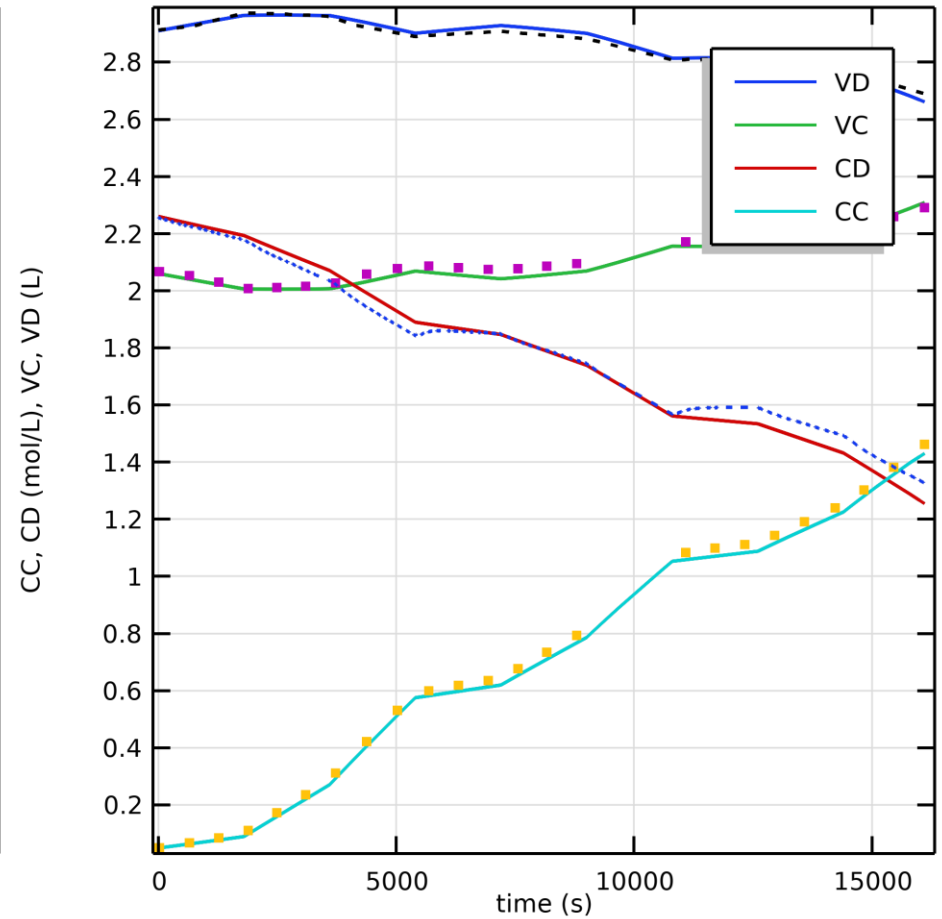


Increasing step pattern

Electric current

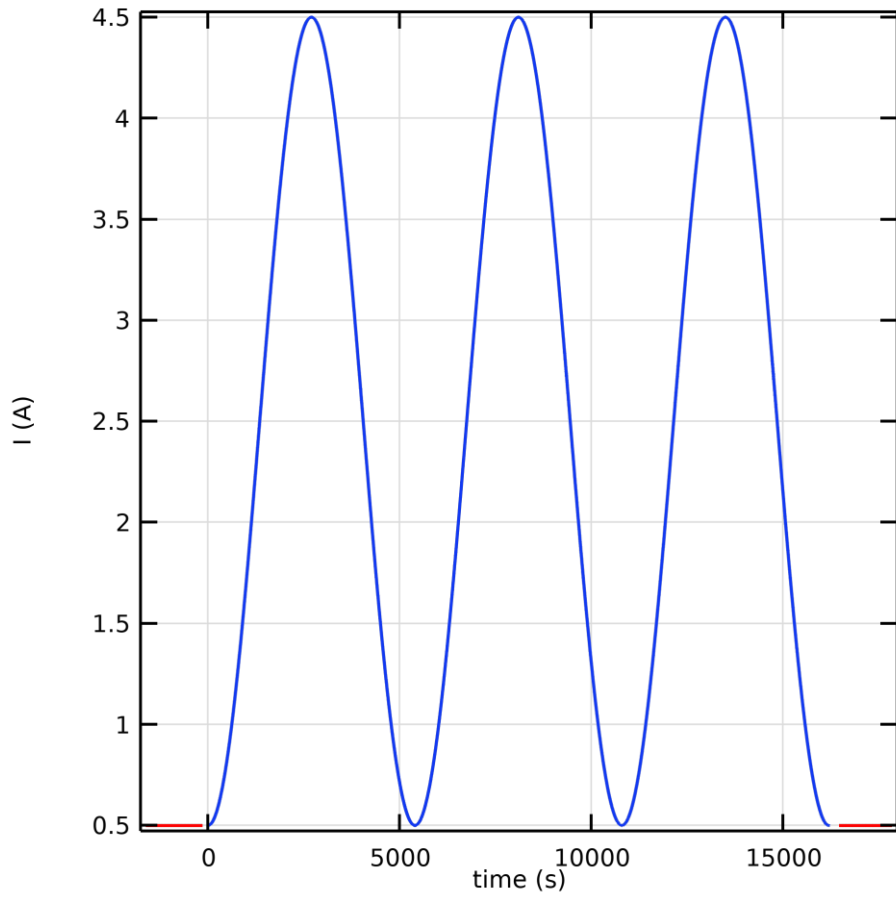


Volumes and concentrations

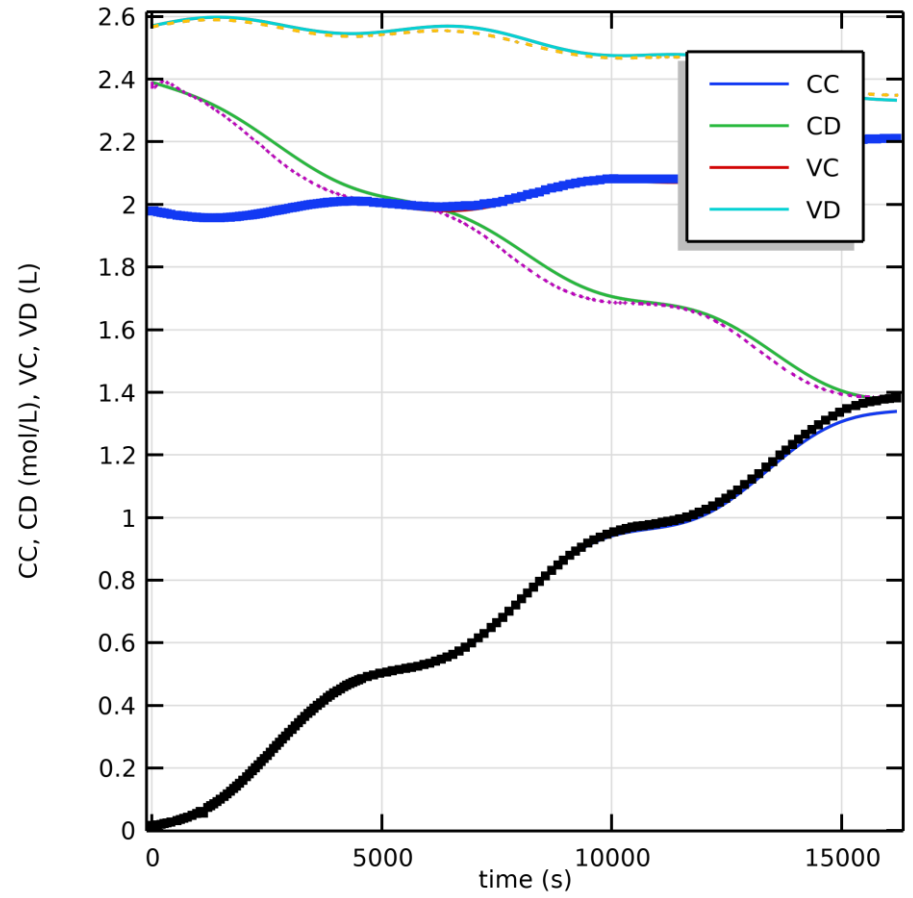


Sinusoidal pattern

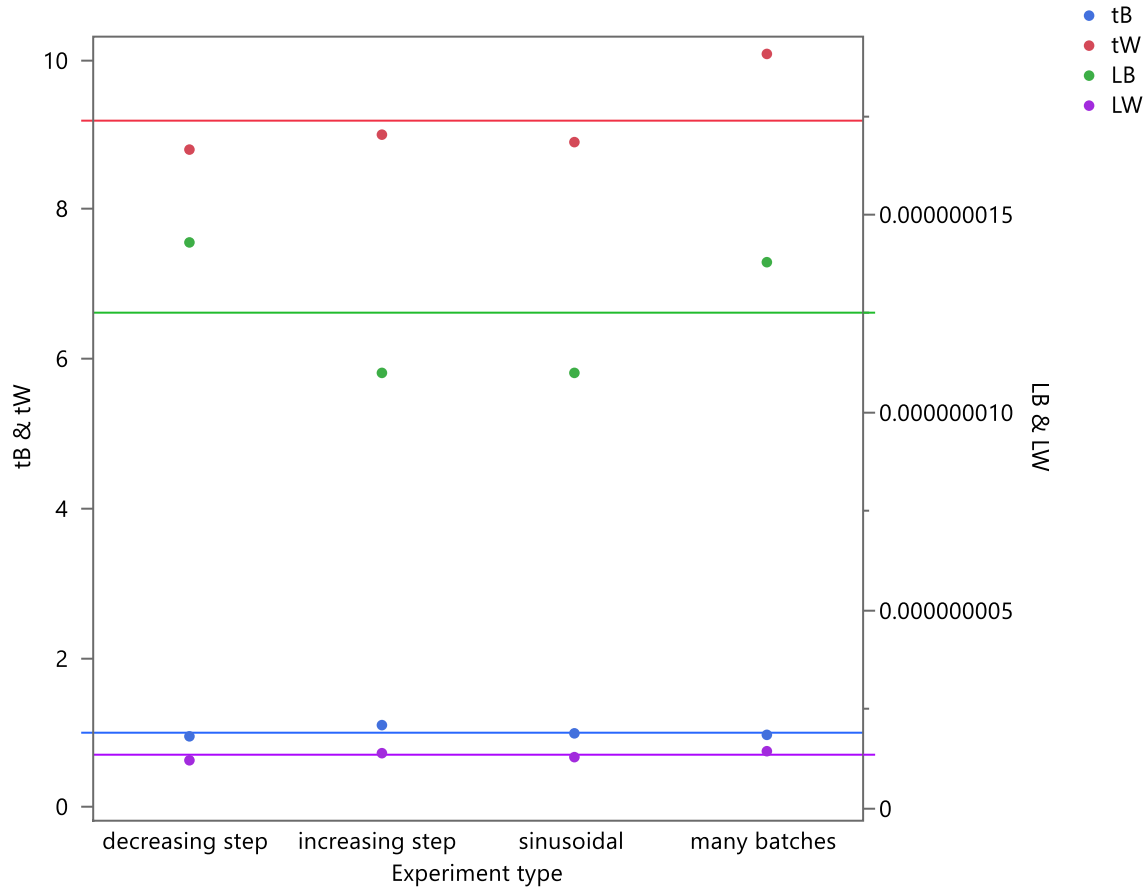
Electric current



Volumes and concentrations



Parameters estimate comparisons



It seems that parameter estimate is possible considering that the estimates are very close

Conclusions

- The use of online sensors allowed to acquire high-frequency and very precise measurements for concentrations and volumes.
- Model simulation and parameter estimates were easily carried out by using COMSOL Multiphysics.
- Further work is required to validate the results obtained by expanding the experimental data set.