Institute of Electronic Sensor Systems

Impact of material properties on the PEMFC performance: comprehensive computational study

Karpenko-Jereb L.

O u t l i n e

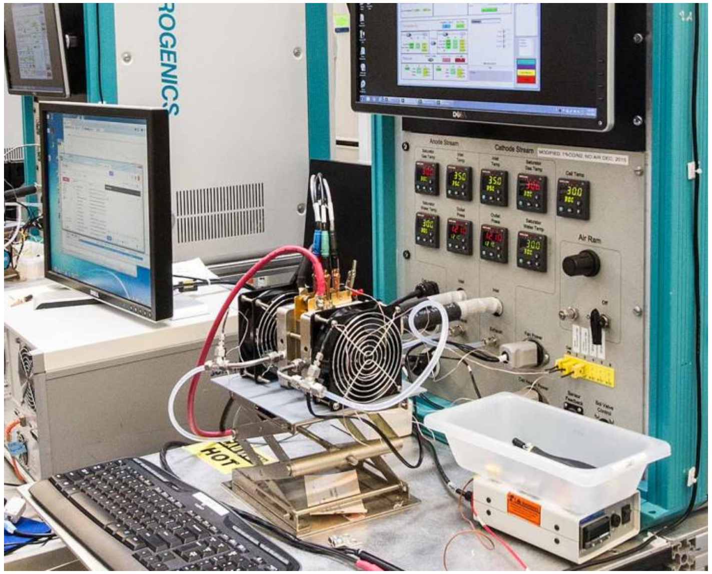
1. Introduction
2. Effect of material properties
3. Modelling chemical degradation

Conclusion & Acknowledgment

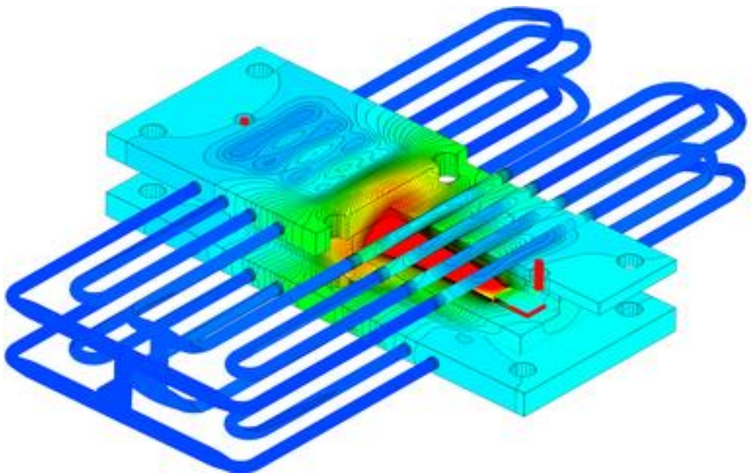
1. Introduction

What possibilities do we have to study and to develop PEMFCs?

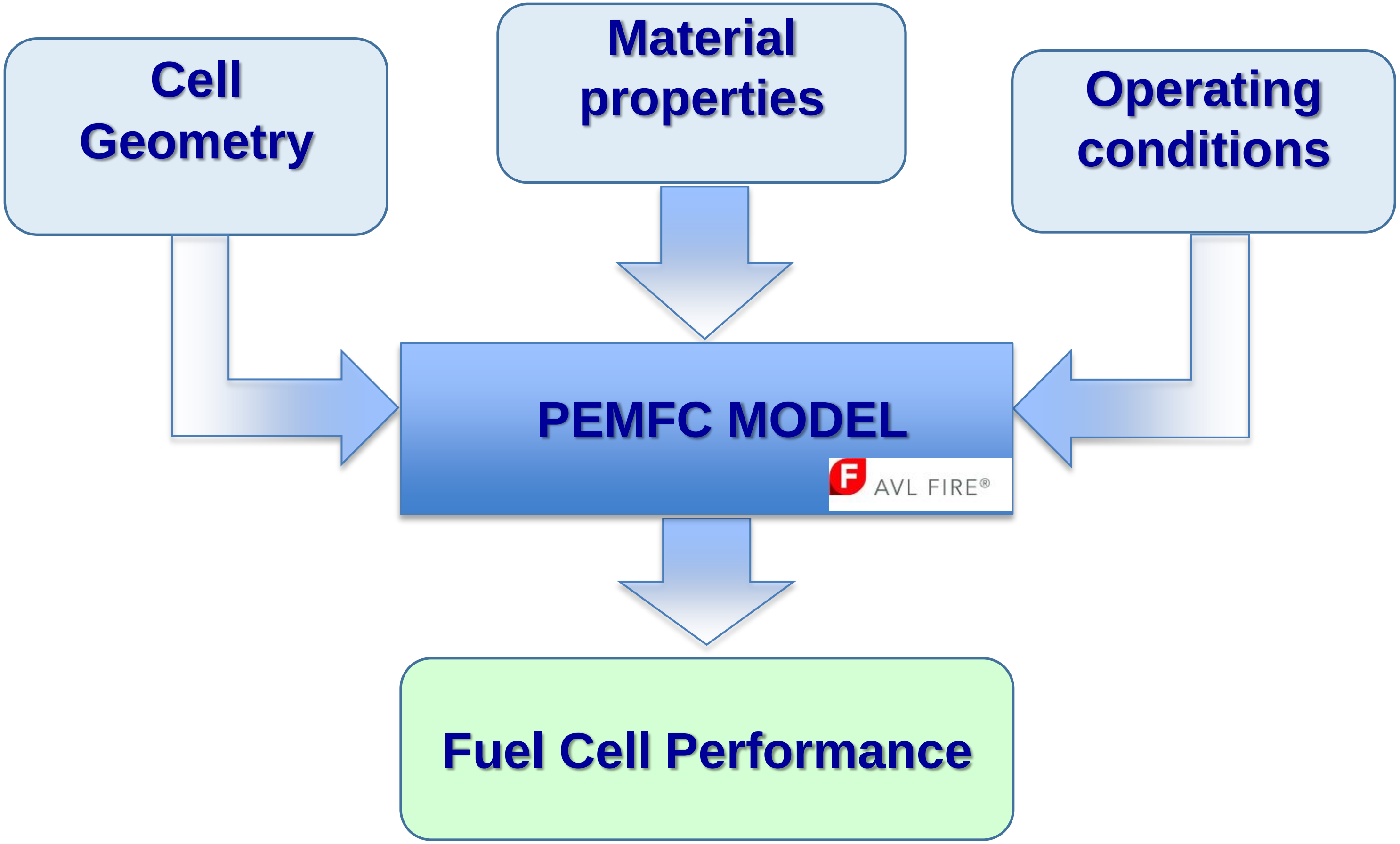
Experiments



Simulation



1. Introduction



[1] Karpenko-Jereb L. et al. // Int J Hydrogen Energy 39 (**2014**) 7077.
[2] Karpenko-Jereb L. et al. // Int J Hydrogen Energy 41 (**2016**) 13644.

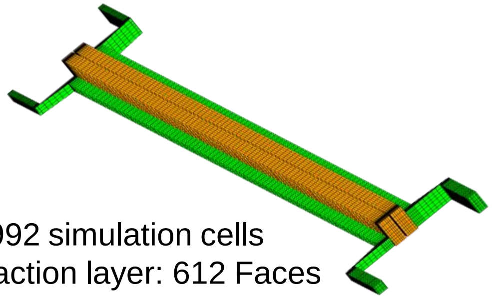
2. Effect of material properties

Cell Geometry

Material properties

Operating conditions

Single channel cell



13992 simulation cells
Reaction layer: 612 Faces

Catalyst Layers

Gas Diffusion Layer

Membrane

$RH_a = RH_c = 90\%$

$T = 70°\ C$

$\lambda a/\lambda c = 1.5/2.2$

$p_a = 101325$ Pa

Fuel Cell Performance

- Cell potential
- Power Density
- Membrane Over-potential
- Mean Water Concentration in PEM
- Total Water Flux in PEM
- Relative Humidity in CCL at interface to PEM

as a function of the current density

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Theoretical study of the influence of material parameters on the performance of a polymer electrolyte fuel cell

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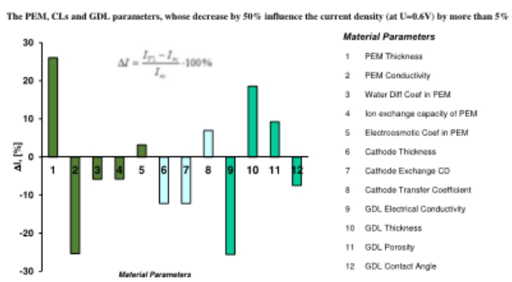
HIGHLIGHTS

- Material properties impacts on FC behaviour was studied by the CFD simulation.
- 25 parameters of PEM, GDL and CLs were investigated on single channel fuel cell.
- Conductivity and thickness of PEM, GDL have the most influence on FC efficiency.
- Parameters of the anode catalyst layer insignificantly affect the FC performance.

GRAPHICAL ABSTRACT



15 pages

Appendix C. Supplementary data

Supplementary data related to this article can be found at http://dx.doi.org/10.1016/j.jpowsour.2015.07.011.

26 pages

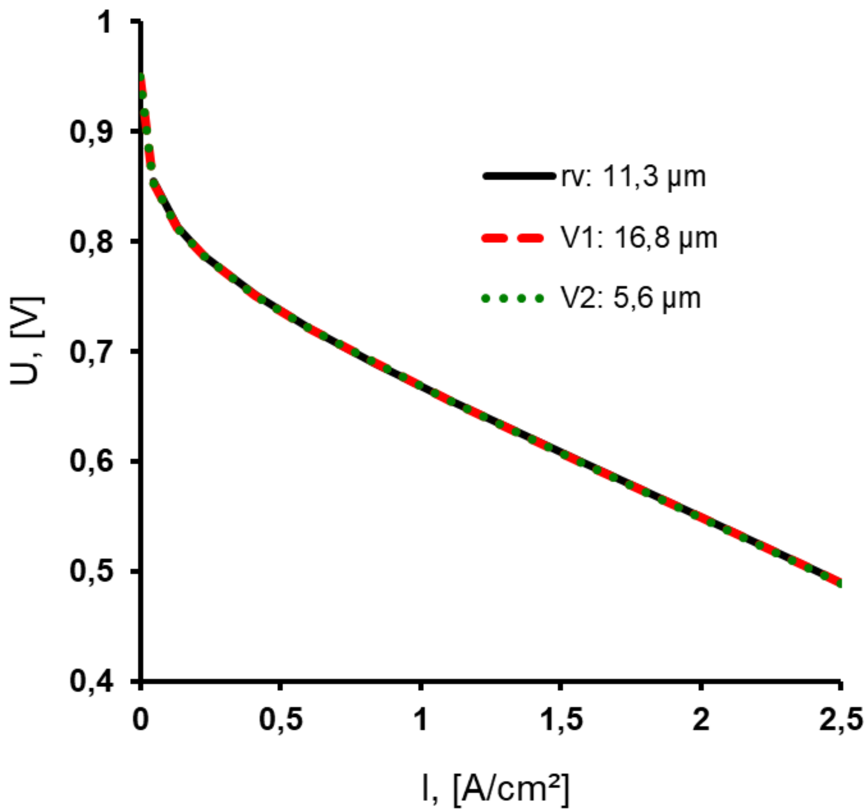
Karpenko-Jereb L. et al. // J Power Sources 297 (2015) 329.

Effect of material properties: tested parameters and values

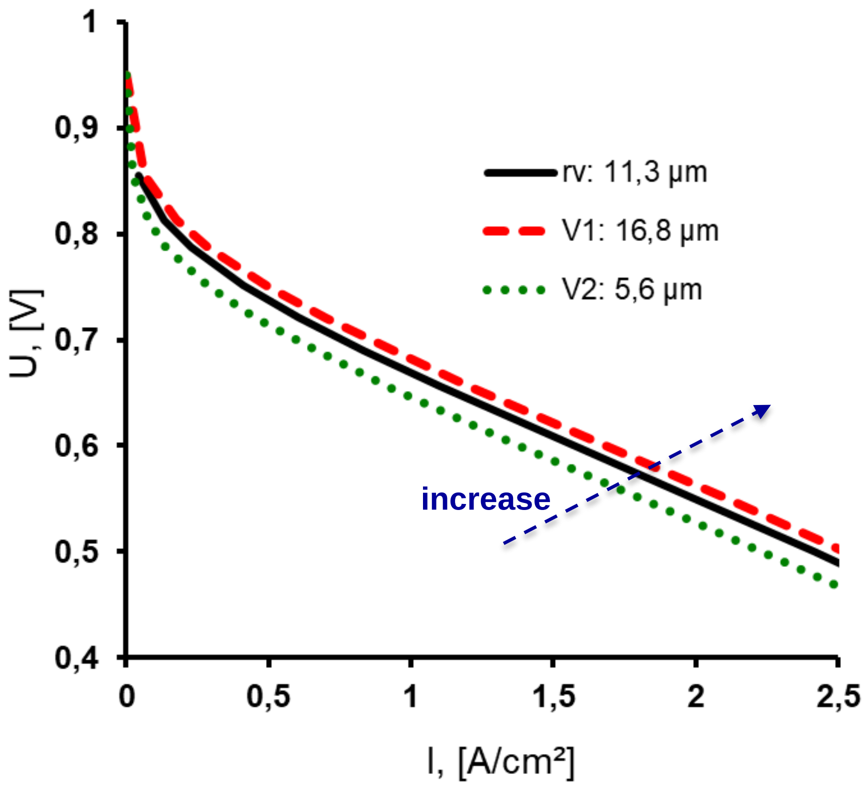
Domain		Parameter	Unit	Reference (rv)	Variation 1 (rv*1,5)	Variation 2 (rv*0,5)
PEM	**1**	**Ionic conductivity**	A/mV	5,34	2,68	1,34
	2	**Acid group concentration**	Kmol/m^3	1,90	2,85	0,95
	3	**Thickness**	m	3,50E-05	5,25E-05	1,75E-05
	4	**Water diffusion coefficient**	m^2/s	2,68E-11	4,02E-11	1,34E-11
	5	**Electro-osmotic coefficient**	-	1,08E-01	1,62E-01	5,41E-02
	6	**Diffusion coefficient of H_2**	m^2/s	2,09E-10	3,14E-10	1,05E-10
	7	**Diffusion coefficient of O_2**	m^2/s	9,73E-11	1,46E-10	4,87E-11
	8	**Diffusion coefficient of N_2**	m^2/s	9,73E-11	1,46E-10	4,87E-11
	9	**Henry coefficient H_2**	Pa	1,21E+08	1,82E+08	6,05E+07
	10	**Henry coefficient O_2**	Pa	5,14E+08	7,71E+08	2,57E+08
	11	**Henry coefficient N_2**	Pa	5,14E+08	7,71E+08	2,57E+08
CL	**12**	**Exchange current density at cathode**	A/m^3	3,2E+05	4,8E+05	1,6E+05
	13	**Exchange current density at anode**	A/m^3	1,00E+11	1,50E+11	5,00E+10
	14	**Transfer coefficient at cathode**	-	0,10	0,15	0,05
	15	**Transfer coefficient at anode**	-	0,50	0,75	0,25
	16	**Thickness of cathode**	m	1,13E-05	1,69E-05	5,63E-06
	17	**Thickness of anode**	m	1,13E-05	1,69E-05	5,63E-06
GDL	**18**	**Thickness**	m	3,00E-04	4,50E-04	1,50E-04
	19	**Inplane permeability**	m^2	2,33E-12	3,50E-12	1,17E-12
	20	**Throughplane permeability**	m^2	1,07E-14	1,61E-14	5,35E-15
	21	**Porosity**	-	0,78	0,98	0,59
	22	**Tortuosity**	-	1,50	1,88	1,13
	23	**Contact angle**	deg	122	152	92
	24	**Throughplane thermal conductivity**	W/mK	4,55	6,83	2,28
	25	**Throughplane electrical conductivity**	A/mV	8,49E+02	1,27E+03	4,24E+02

Effect of **thickness**

Anode CL thickness

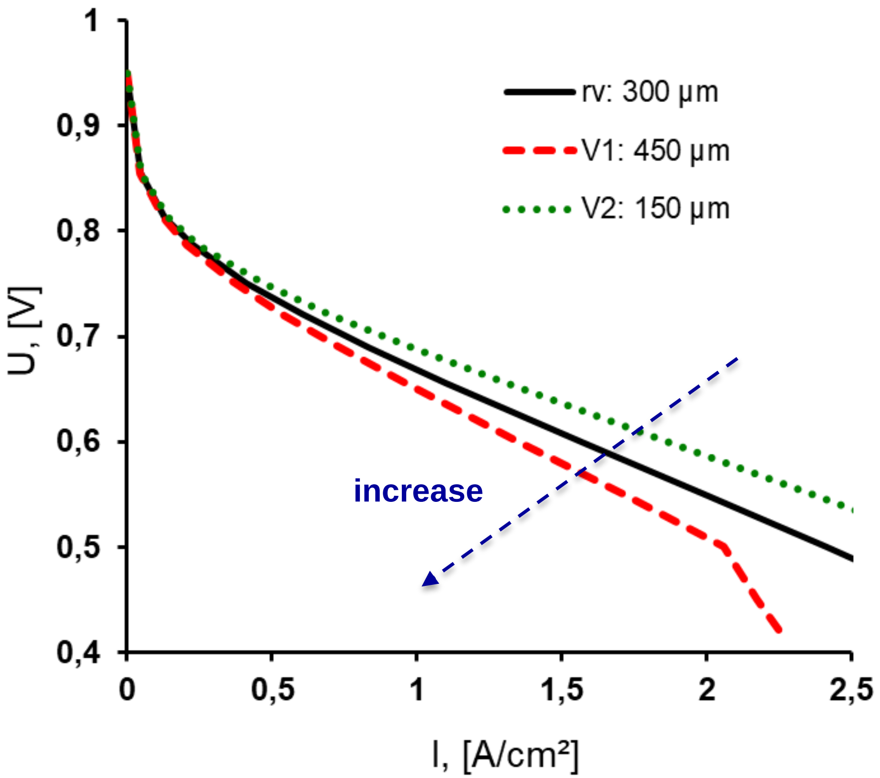


Cathode CL thickness

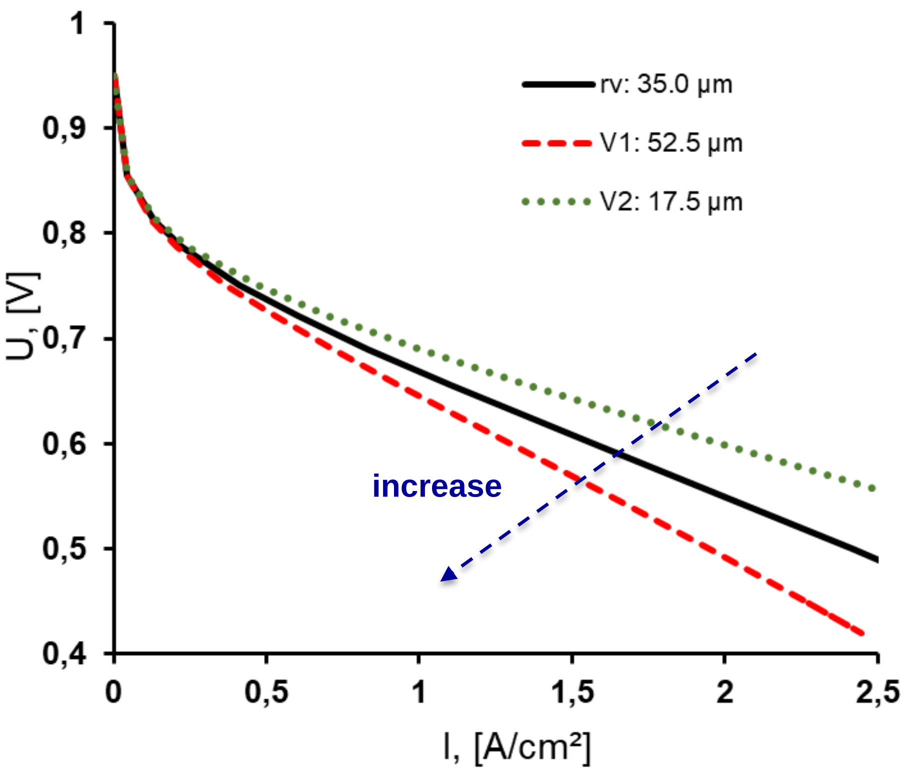


Effect of **thickness**

GDL thickness

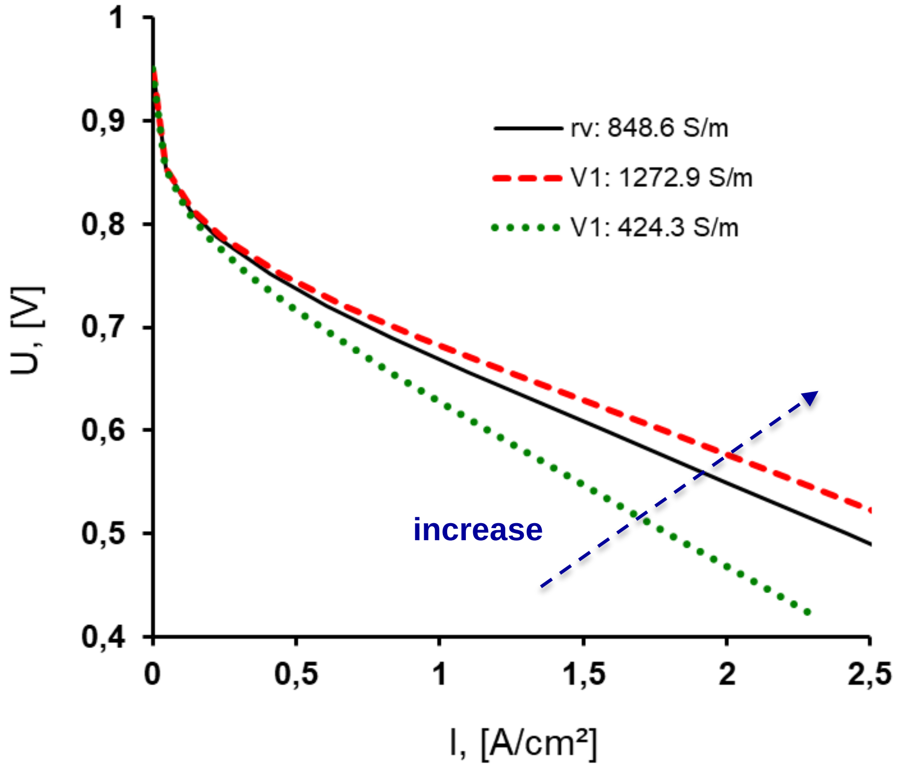


Membrane thickness

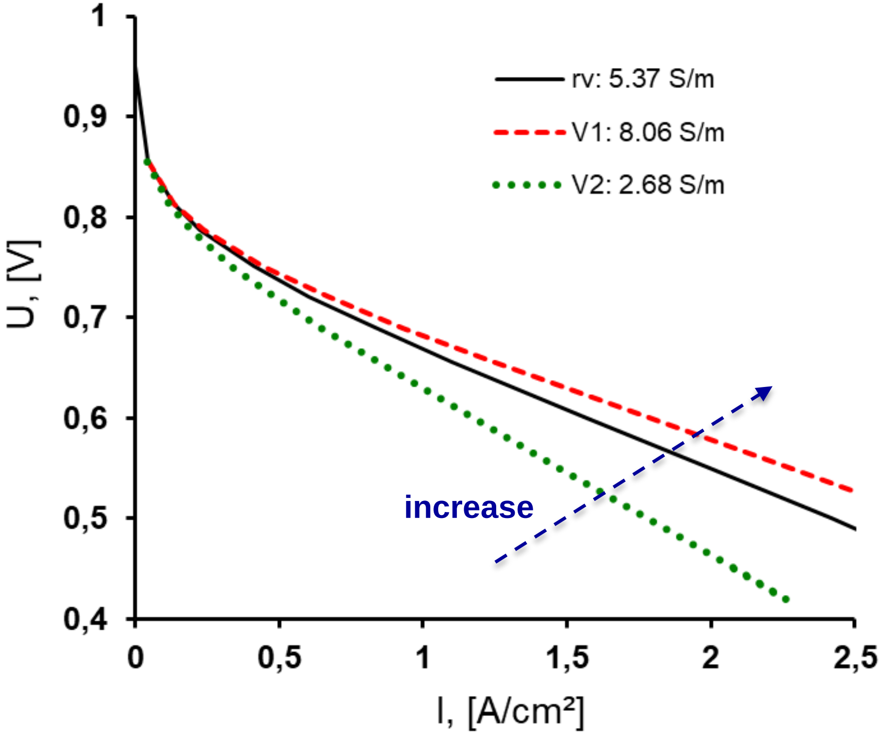


Effect of **conductivity**

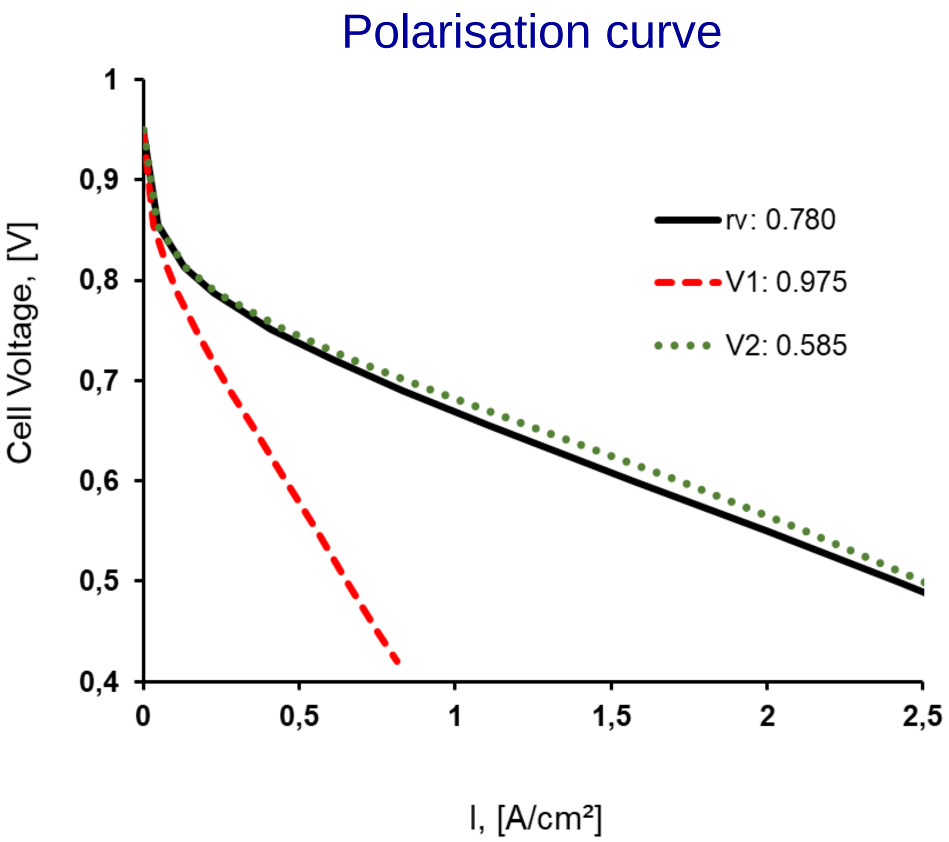
GDL conductivity

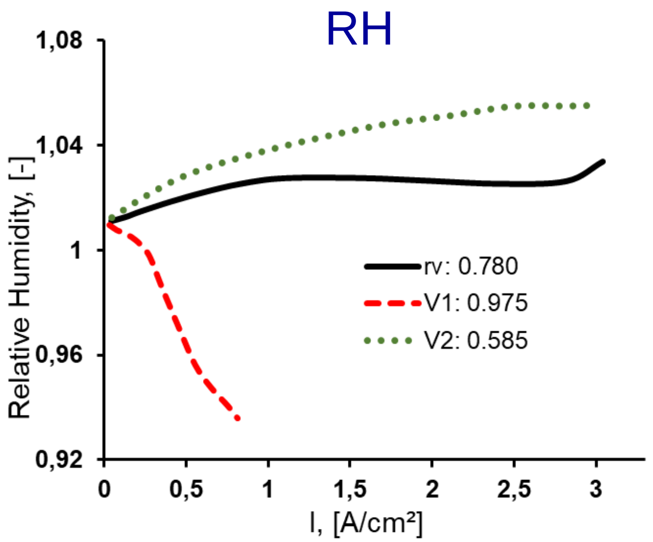


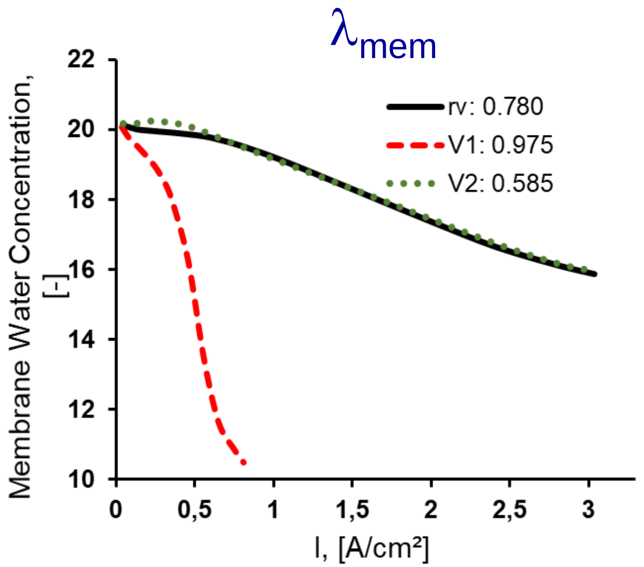
Membrane conductivity



Effect of **GDL porosity**

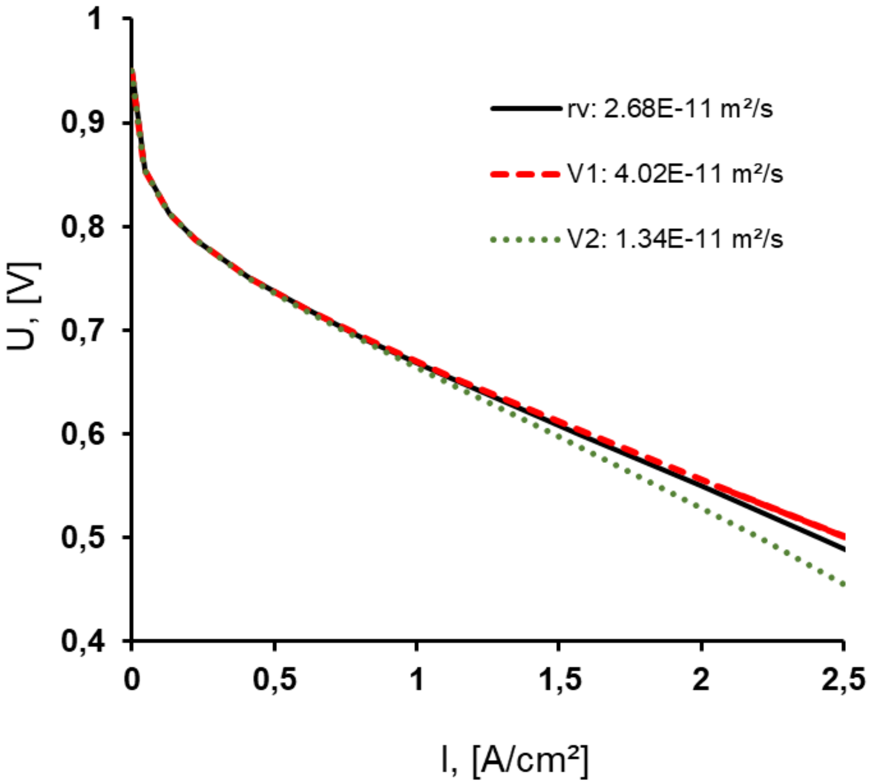




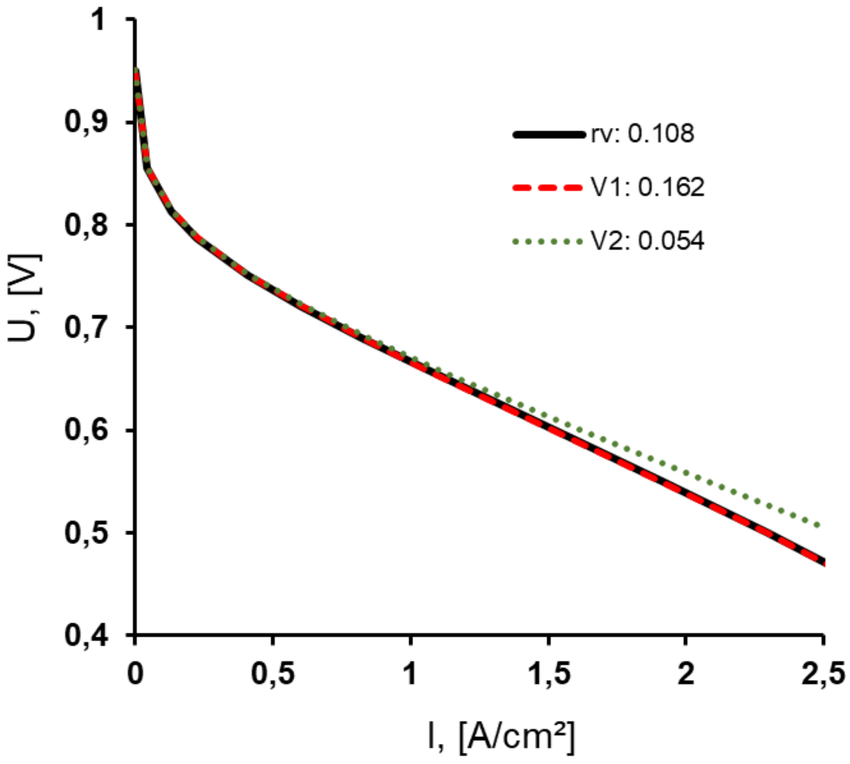


Effect of **water transport** coefficients **in PEM**

Diffusion coefficient

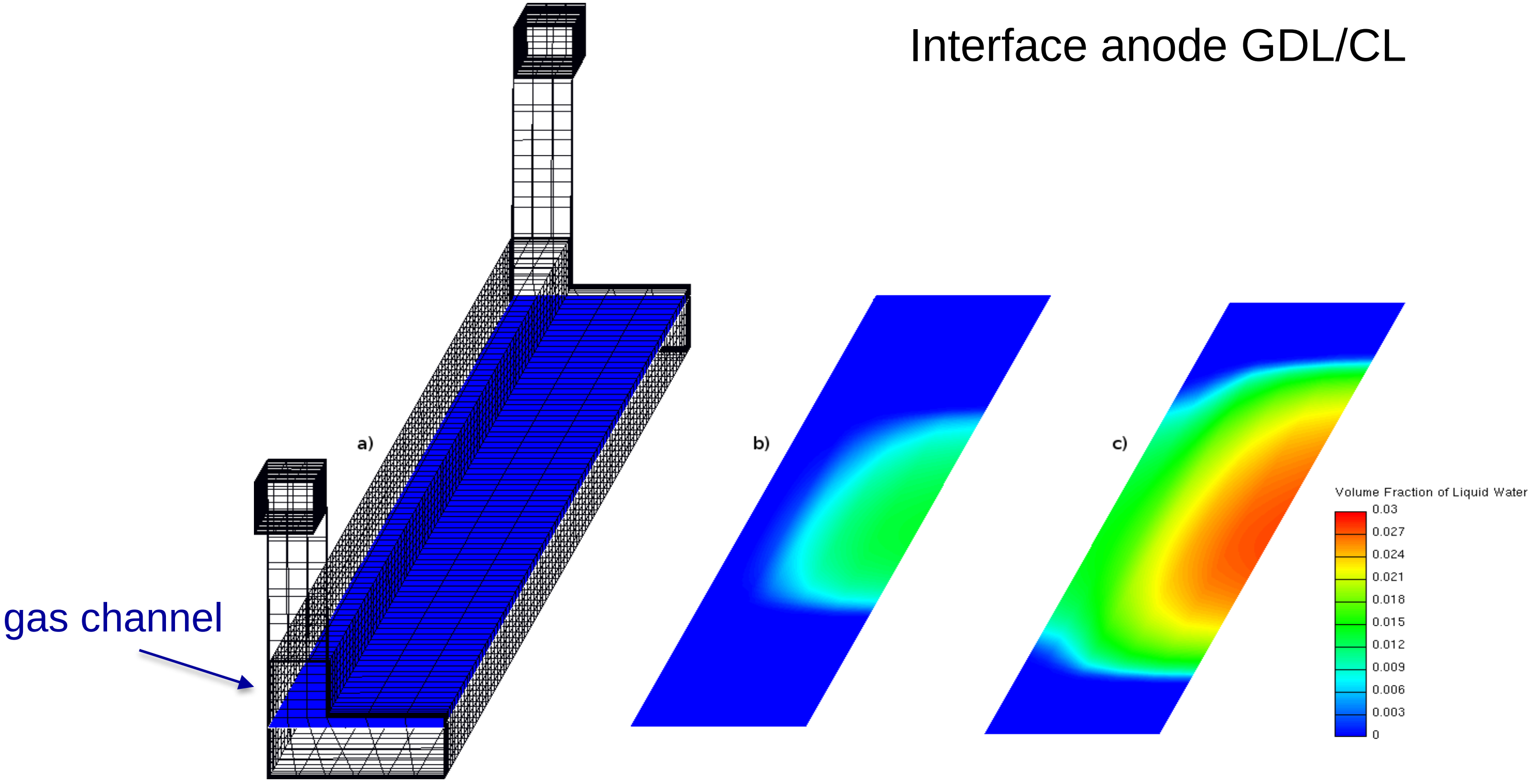


Electro-osmotic coefficient



Effect of **water diffusion** coefficient in PEM

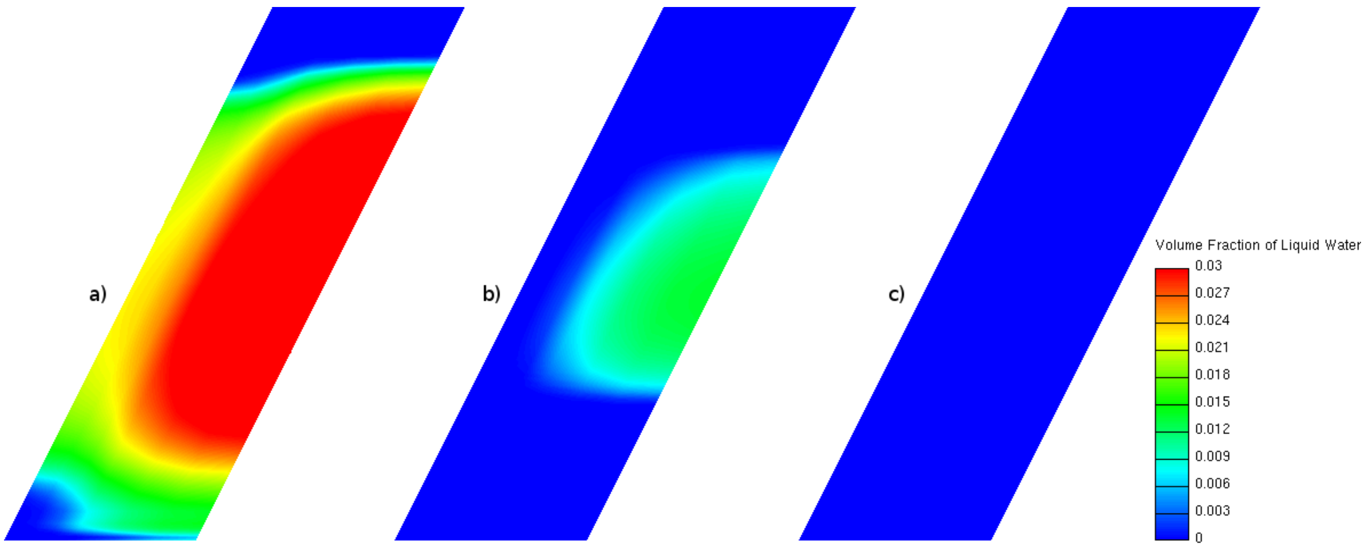
Interface anode GDL/CL



$d_w, 10^{-11} \left[{}^{m^2}/_{s}\right]$: **1.34** **2.68** **4.02**

Effect of **electro-osmotic** coefficient in PEM

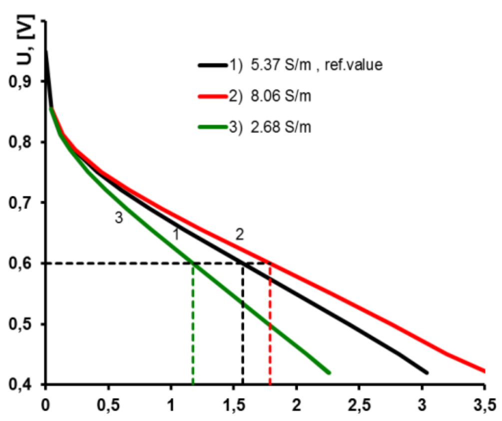
Interface anode GDL/CL



$c_{drag}, 10^{-1}$: **0.54** **1.08** **1.62**

2. Effect of material properties

Analysis



$$\Delta I = \frac{I_{V1} - I_{rv}}{I_{rv}} \cdot 100\%$$

$$\Delta I = \frac{I_{V2} - I_{rv}}{I_{rv}} \cdot 100\%$$

Summary

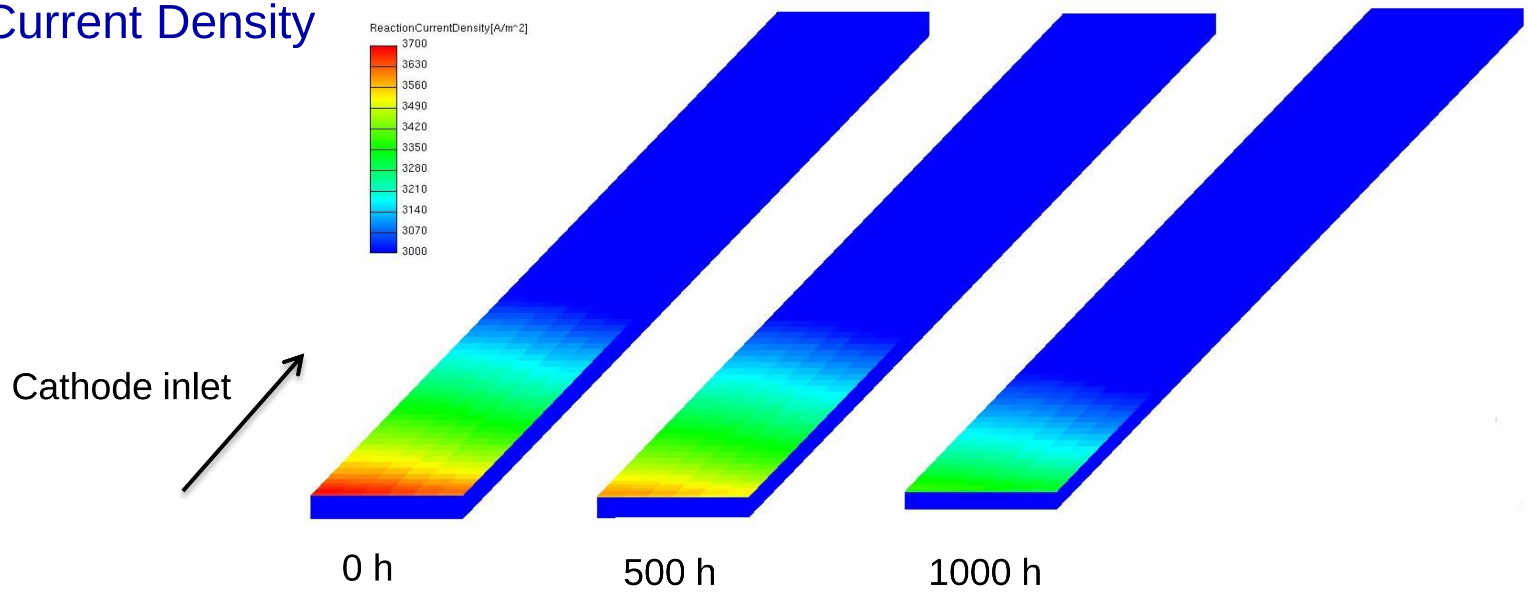
Tested Parameters	rv* 0.5	rv* 1.5
PEM	V2	V1
Thickness	+26%	-17%
Conductivity	-25%	+13%
Water Diffusion Coefficient	-6%	+2%
Acid Group Concentration	-6%	+2%
CL		
Cathode Thickness	-12%	+7%
Cathode Exchange at CD	-12%	+7%
Cathode Transfer Coefficient	+7%	-7%
GDL		
Electrical Conductivity	-25%	+13%
Thickness	+18%	-14%
Porosity	+9%	-70%
Contact Angle	-7%	+1%

Karpenko-Jereb L. et al. Theoretical study of the influence of material parameters on the performance of a polymer electrolyte fuel cell // Journal of Power Sources 297 (21452) (**2015**) 329-343, doi: 10.1016/j.jpowsour.2015.07.011

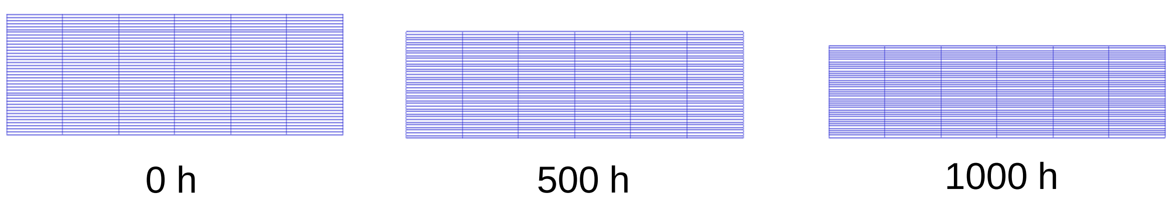
3. Modelling chemical degradation

Semi-empirical model of PEMFC chemical degradation

Current Density

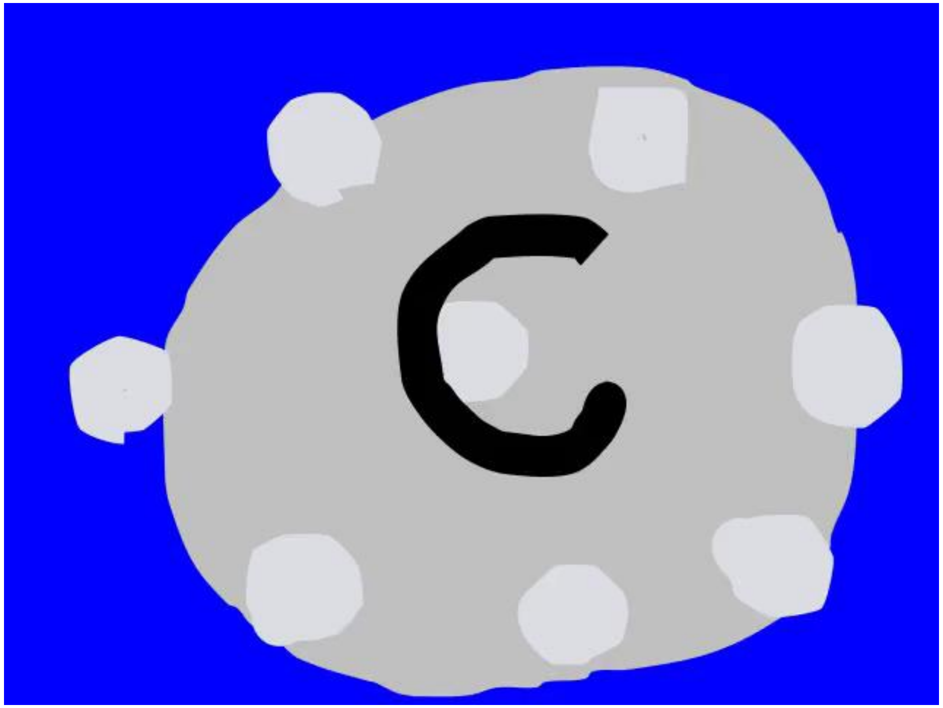


Membrane thickness



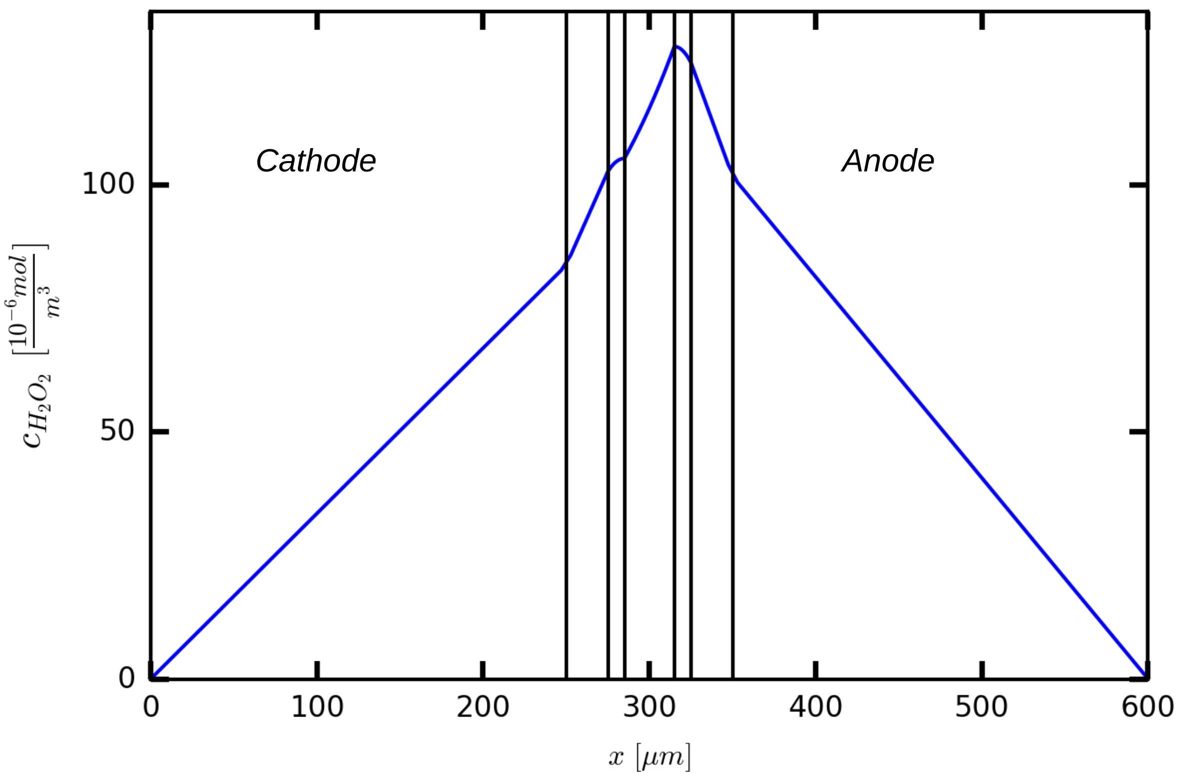
Karpenko-Jereb L. et al. **Membrane degradation model** for 3D CFD analysis of fuel cell performance as a function of time // Int J Hydrogen Energy 41 (**2016**) 13644-13656

Chemical degradation of the catalyst layer



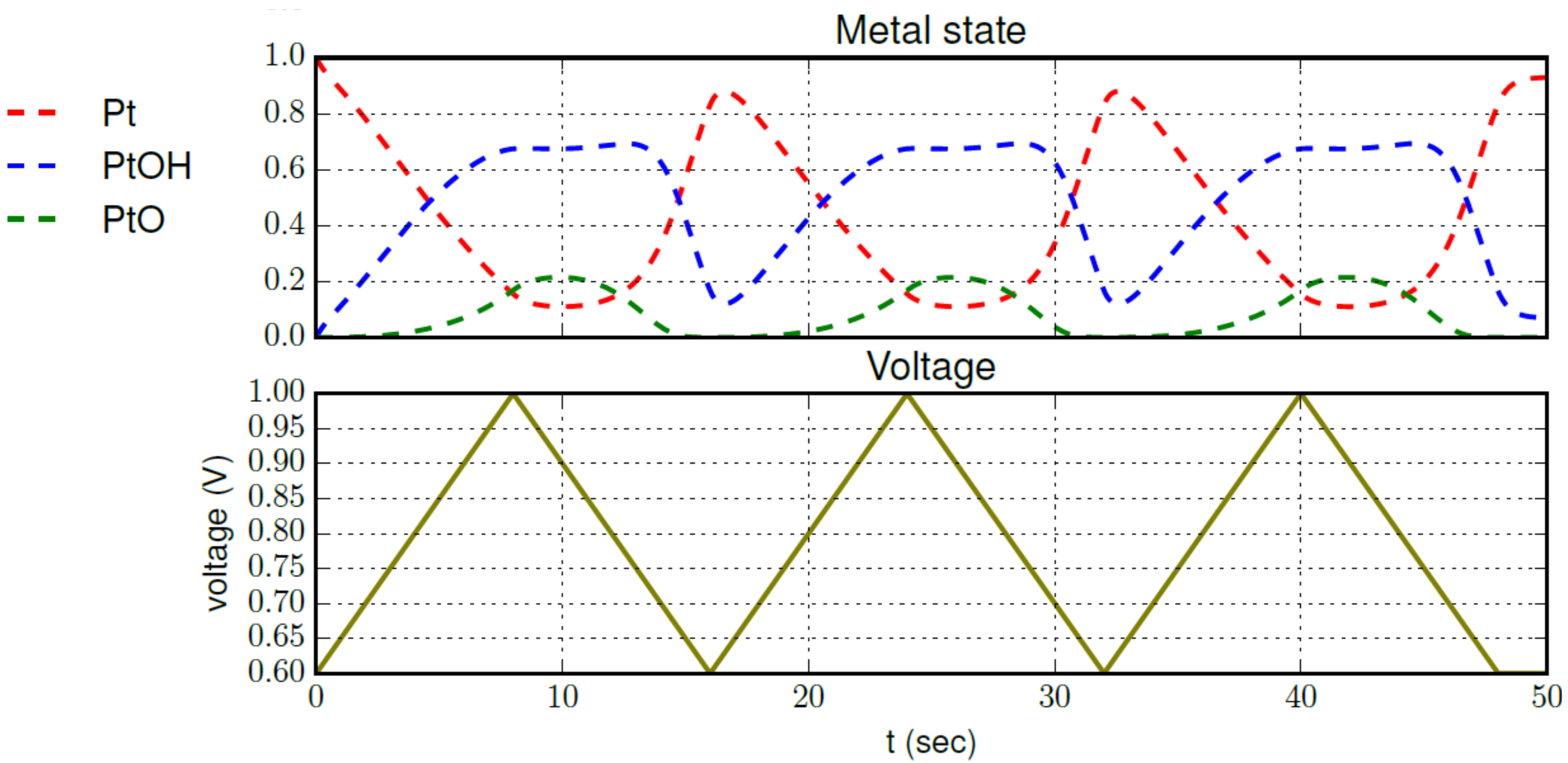
Pal Verebes. Animation of chemical degradation of the ionomer in the CL.**2017.**

Evolution of H_2O_2 distribution in LT-PEMFC during the ionomer degradation in CLs



Karpenko-Jereb, L., Verebes, P. et al. Modelling chemical degradation of ionomer in a polymer electrolyte fuel cell / International Congress on Membranes and Membrane Processes ICOM2017. San Francisco 29 July – 4 Aug 2017. USA.

Evolution of Pt surface composition during an AST of catalyst degradation



Conclusion

- The simulation tools enable to look inside the cells and serve as virtual sensors
- They save time and allow detecting phenomena which very often cannot be measured experimentally
- Modern development of the fuel cell is impossible without simulation tools. On the other hand, without experimental validation their further improvement is impossible

Acknowledment

Colleagues

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Dr. Fink Clemens
Dr. Tatschl Reinhard

Research Projects

- **2010-2012** PEM-MODEL Bridge 1, **FFG**
- **2012-2014** **ÖAD** Project with Poland
- **2012-2015** A3 FALCON, **FFG**
- **2015-2018** FC-DIAMOND, **FFG**

The Austrian Research Promotion Agency, FFG

The Austrian Agency for Int. Mobility and Cooperation, ÖAD

Questions

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