Research for Sustainable Technologies

DECHEMA
FORSCHUNGSINSTITUT
Stiftung bürgerlichen Rechts

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DMFC Model with COMSOL

Comsol conference, Munich, 12.10.2016

Materials
Chemical Engineering
Biotechnology

COMSOL CONFERENCE
2016 MUNICH

State-of-the art and challenges of Direct Methanol Fuel Cell

- **Commercial available DMFC for off-grid applications :** The Company, owner of the globally established EFOY COMFORT and EFOY Pro fuel cell generator brands, has sold over **35,000** of its systems into a large number of industrial, defense and consumer applications: http://www.sfc.com/en/markets/overview

EFOY Pro 12000 Duo (SFC AG, Brunnthal)
24 V / 20,8 A
48 V /10.4 A
Max. nominal power **500 W**
640 x 441 x 310 mm = **87,5 l**
Weight: **33 kg**

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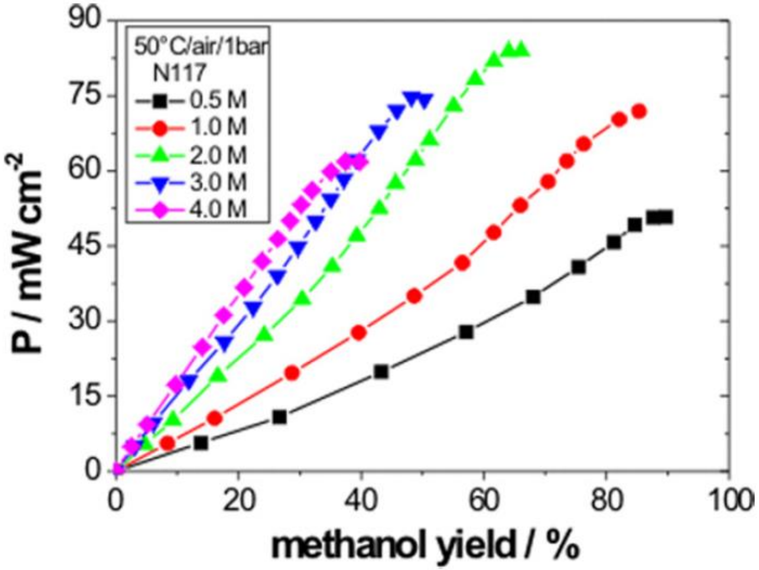
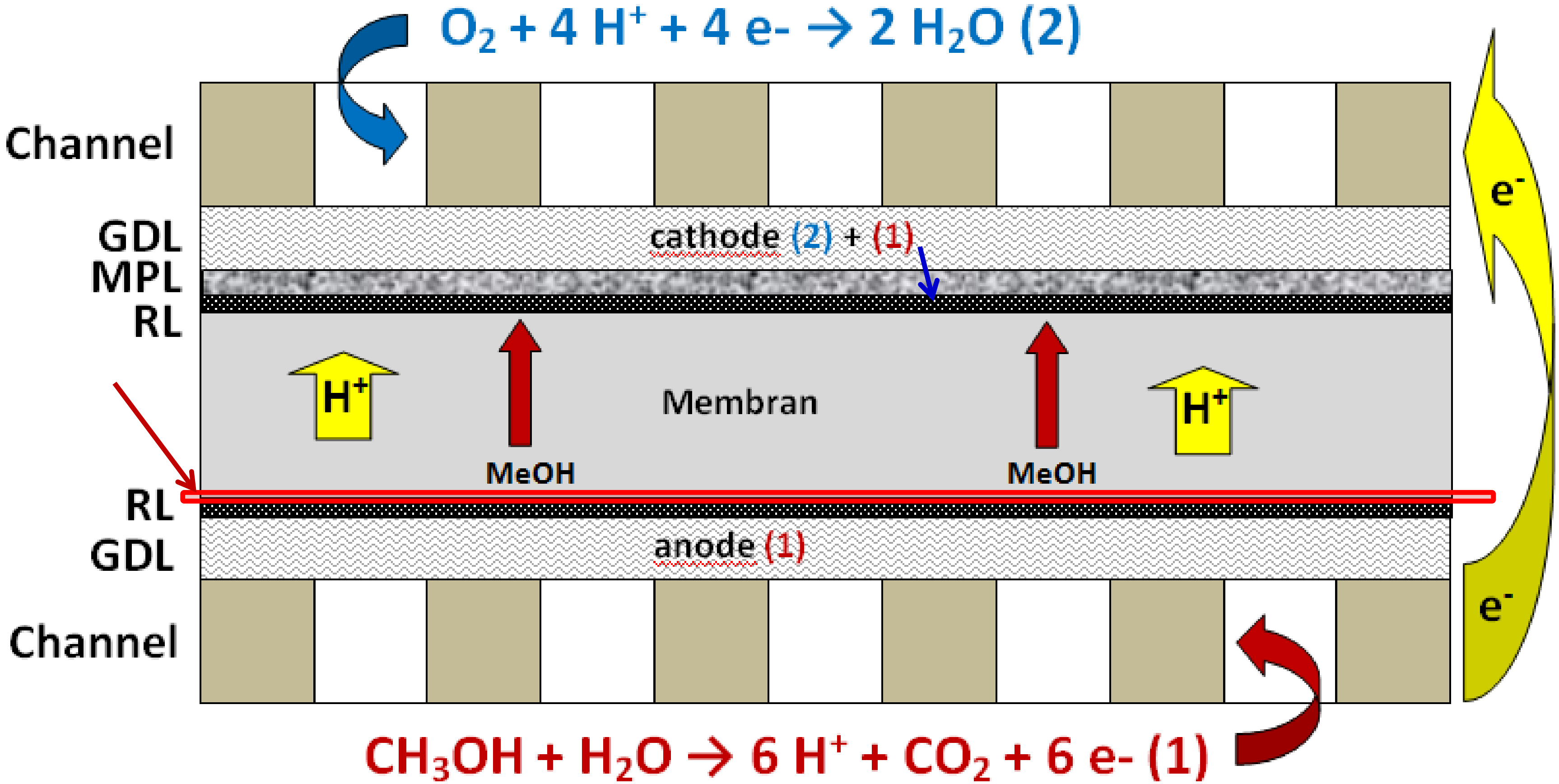


- **Main challenges to overcome:**

- Increase of both power density and methanol yield!
- Limitation of methanol cross-over through PEM membrane
- reduce Catalyst loading

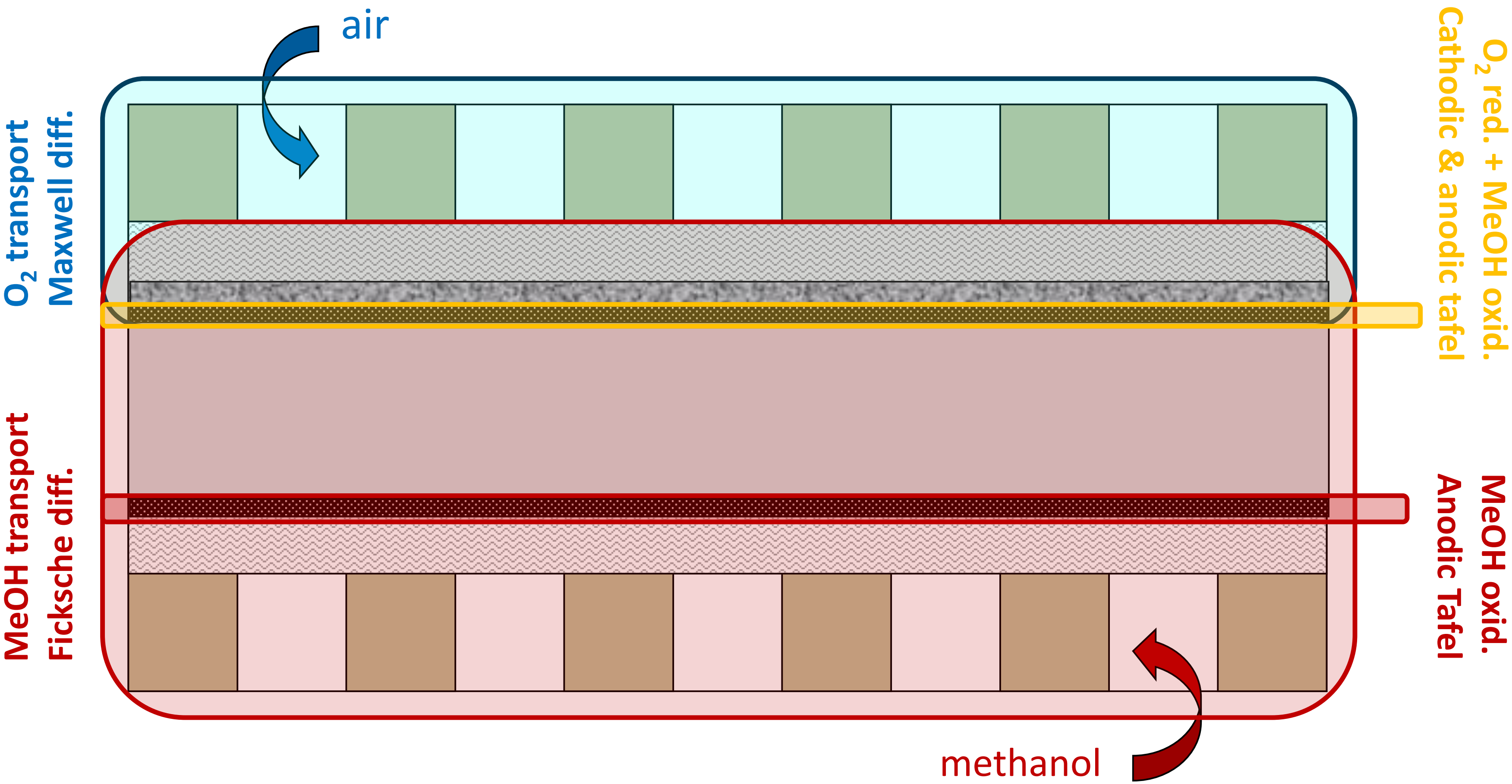
* N. Bogolowski, J.F. Drillet, Chemical Engineering Journal 270 (2015) 91

Principle of Direct Methanol Fuel Cell



➢ **Optimal case: C_{MeOH} at RL_a/membrane interface = 0**

Domains and physics



➢ **Assumptions: - no transport of molecular O_2 through Nafion membrane**
- no methanol transport from RL cathode to channel cathode

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Physics

Electronic/Ionic charge balance	Ohm's law	$I = \sigma\, \Delta \cdot V$
Charge transfer kinetics for η <<	Butler-Volmer	$i_a = i_0 * (\frac{c_{meoh}}{c_{meoh,ref}})\ exp\ (\frac{\alpha_{a,a}}{R * T} F * \eta_a)$ with $i_0 = F\, k_0\, c_{ox}^{\alpha}\, c_{red}^{(1-\alpha)}$
Charge transfer kinetics for η >>	Tafel	$i_{loc} = i_0\, 10^{\eta/Aa}$, $i_{loc} = -i_0\, 10^{\eta/Ac}$
Concentration dependency of i_0		$i_0 = i_{0\_MORa} * (rfcs.c\_wMeOH_a / c_{MeOH.ref})$
Charge transport in electrolyte	Nernst-Planck	$N_i = -D_i \nabla c_i - z_i u_i F c_i \nabla \Phi + c_i u$
Coupled mass transport in free channel and porous electrode	Navier-Stokes	$\rho \frac{\partial u}{\partial t} + \nabla \cdot [-\eta(\nabla u + \nabla u^T) + pI] = -\rho(u \cdot \nabla)u$
	Brinkman	$\frac{\rho}{\varepsilon_p}\frac{\partial u}{\partial t} + \nabla \cdot \left[-\eta \frac{\eta}{\varepsilon_p}(\nabla u + \nabla u^T) + pI\right] = -\frac{\eta}{k} u$
Mass balances in gas phase in gas channels and porous electrodes	Fick	$-\nabla \cdot (-D \cdot \nabla c + c \cdot u) = 0$
	Maxwell-Stefan	$-\nabla \cdot [-\rho\omega_i \sum_{j=1}^{N} D_{ij} \left\{\frac{M}{M_j}\left(\nabla\omega_j + \omega_j \frac{\nabla M}{M}\right) + \left(x_j - \omega_j \frac{\nabla p}{p}\right)\right\} + \omega_i \rho u] = 0$

A_a = anodic Tafel slope (V decade^{-1})
c = concentration ($mol\ m^{-3}$)
D = diffusion coefficient ($m^2\ s^{-1}$)
F = Faraday constant ($C\ mol^{-1}$)
i_a = anodic current density ($A\ m^{-2}$)
i_0 = exchange current density ($A\ m^{-2}$)
I = current (A)
N_i = charge transport in electrolyte ($mol\ m^{-2}\ s^{-1}$)
p = pressure (Pa)
u = velocity ($m\ s^{-1}$)
V = potential (V)
z = number of electron ($-$)
α = symetrie factor ($-$)
η = dynamic viscosity ($Pa \cdot s$)
η_a = anodic overpotential (V)
ε_p = porosity ($-$)
κ = permeability (m^2)
Φ = potential in electrolyte (V)
ρ = density ($kg\ m^{-3}$)
σ = conductivity ($S\ m^{-1}$)
II = Tensor

Geometry

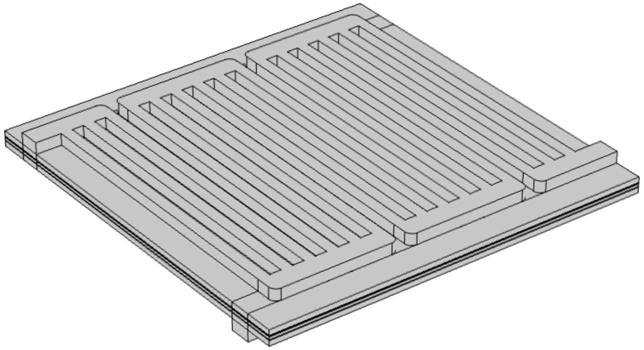
- **WP8 + extrude** opposite direction: H_ch + H_GDLc + H_MPLc + H_RLc+ H_M + H_Rla + H_GDLa

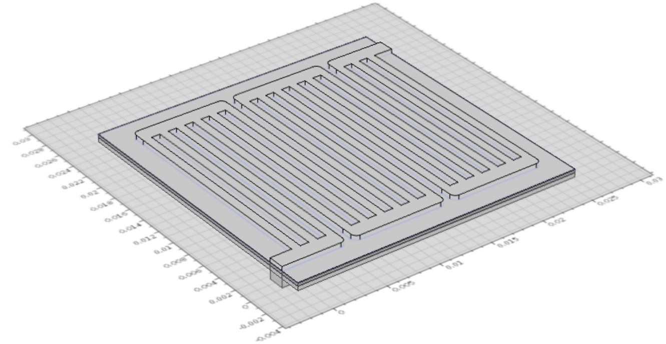
- **WP8**: channel cathode

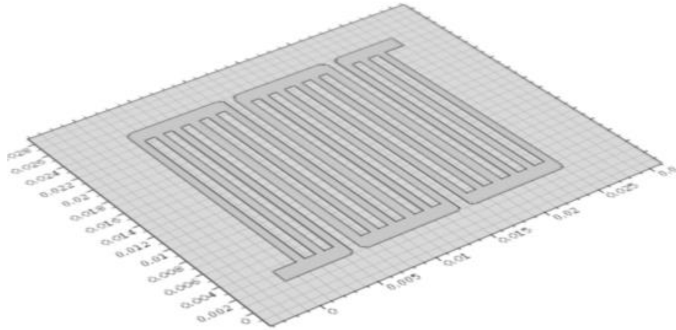
- **WP7 + extrude**: GDL cathode
- **WP6 + extrude**: MPL cathode
- **WP5 + extrude**: RL cathode
- **WP4 + extrude**: Membrane
- **WP3 + extrude**: RL anode
- **WP2 + extrude**: GDL anode

- **WP1 + extrude**: H_ch + H_GDLa + H_Rla + H_M + H_RLc + H_GDLc + H_MPLc

- **WP1**: channel anode

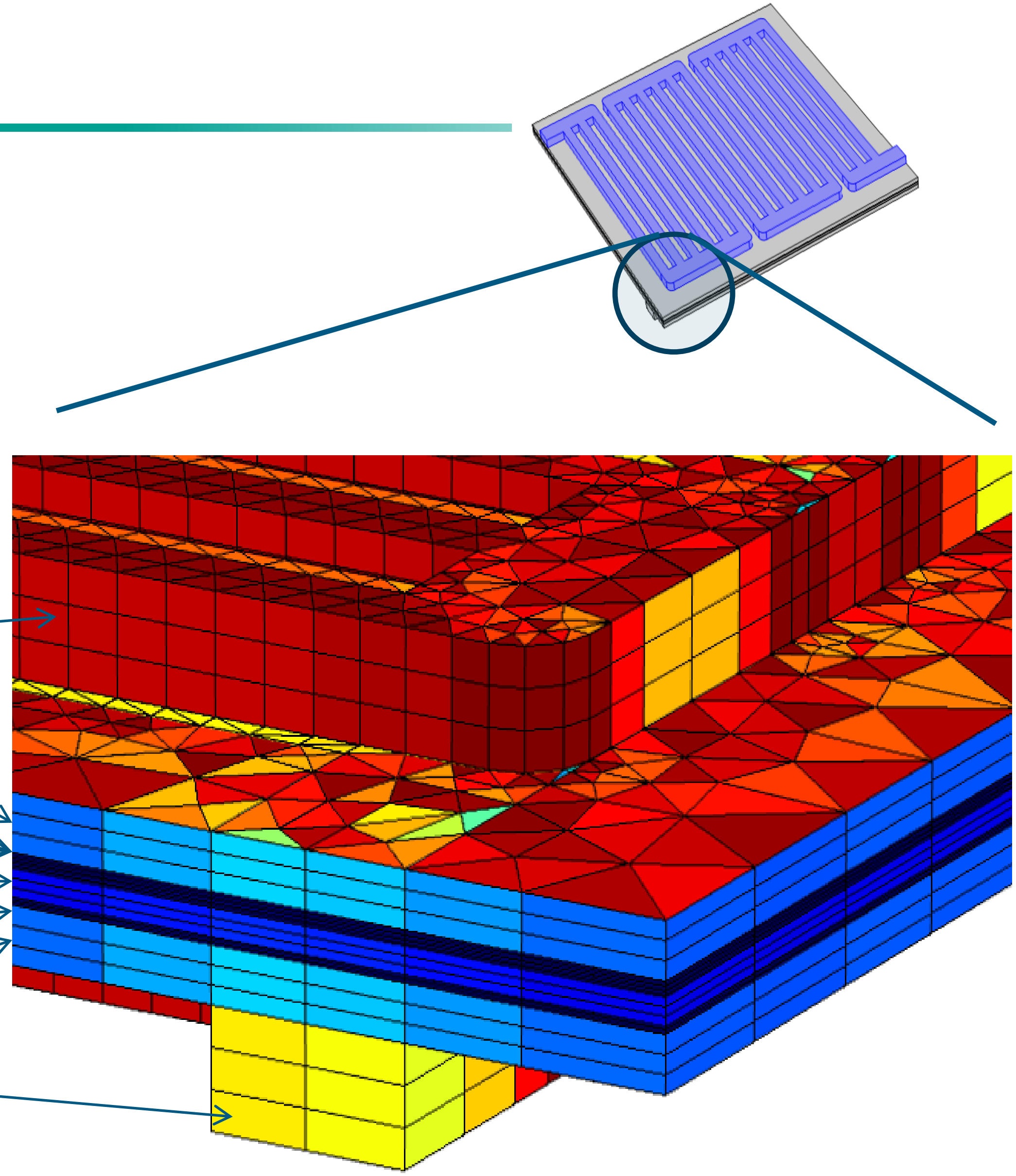






Mesh

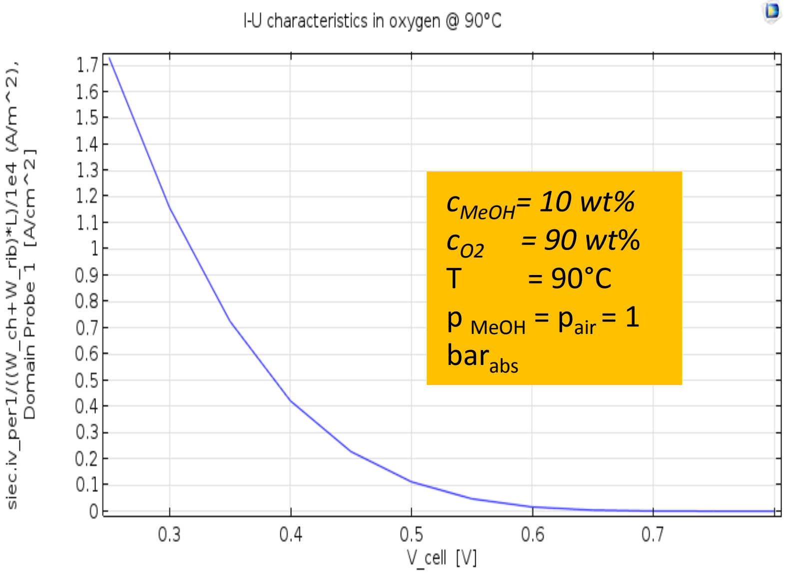
- **Size:** fine
- **Free Triangular**
- **Swept:** generates **hexahedrons**
    - **Ditribution: 3** elements
- **Complete mesh** consists of
    - **253020** domain elements
    - **172658** boundary elements
    - **32654** edge elements.



- Air Channel cathode
- Gas Diffusion Layer GDLc
- Micro Porous layer MPLc
- Reaction Layer RLc
- Membrane
- Reaction Layer RLa
- Gas diffusion Layer GDLa
- MeOH Channel inlet

U_I characteristic in function of practical reaction equilibriums E_0

	V_{cell} V	w_{O2_in} wt%	$E_{0.MORa}$ V	$E_{0.MORc}$ V	$E_{0.ORRc}$ V	I_{max} A cm^{-2}
04.07.2016	0.8	0.9	0.45	0.6	1	0.39
12.07.2016	0.8	0.9	0.35	0.6	1.1	1.85
10.08.2016	0.8	0.9	0.35	0.6	1.23	div
16.08.2016	**0.8**	**0.9**	**0.35**	**0.6**	**1.2**	**1.75**
22.08.2016	0.8	0.9	0.25	0.6	1.2	3.3
05.09.2016	0.8	0.9	0.3	0.55	1.2	div.
07.09.2016	0.8	0.9	0.25	0.55	1.2	div.
12.09.2016	0.8	0.9	0.35	0.6	1.15	1.85
19.09.2016	0.8	0.9	0.35	0.55	1.1	1.2
23.09.2016	0.8	0.2	0.35	0.55	1.1	0.015
29.09.2016	0.8	0.2	0.35	0.55	1.15	div.
04.10.2016	0.8	0.2	0.35	0.6	1.15	0.040



➢ **Fuel cell performance is strongly dependent on experimentally parameters such as E_0, exchange current density i_0, Tafel slope b**

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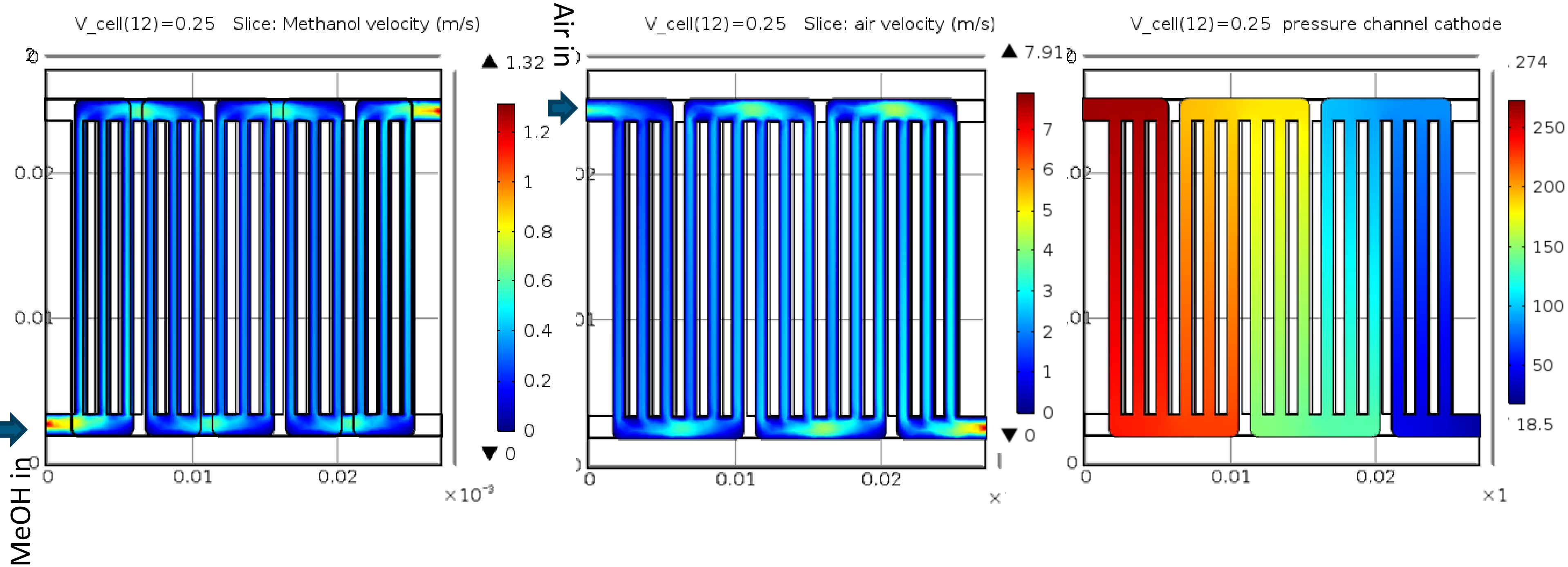
MeOH/air velocity and pressure profiles in channels @ 0,25 V



- ➢ **Fluids velocity/Flow fields geometry should be adapted/optimized for better fuel repartition**
- ➢ **This is a laboratory cell; more complex geometry in prototypes are usually used**

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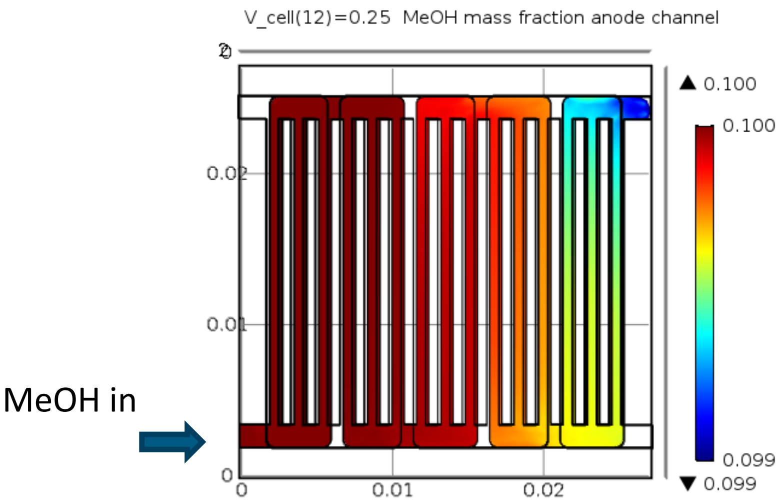
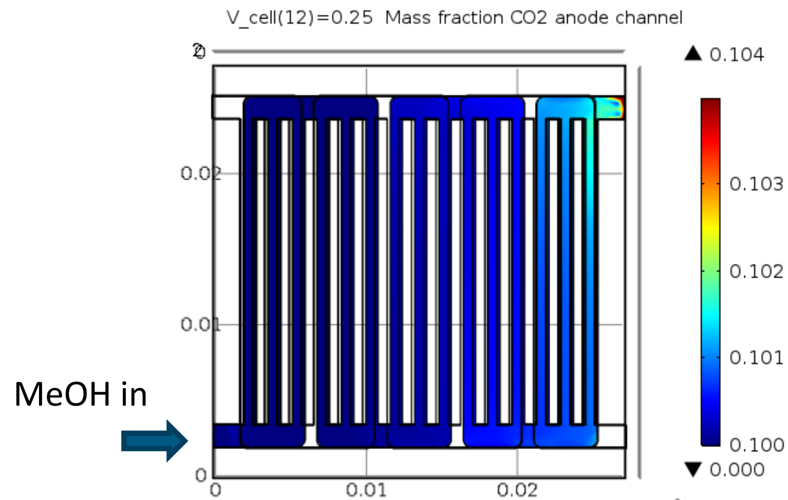
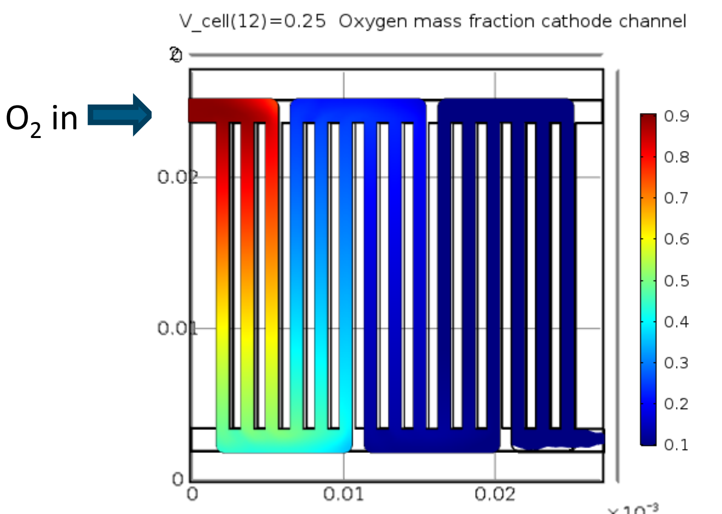
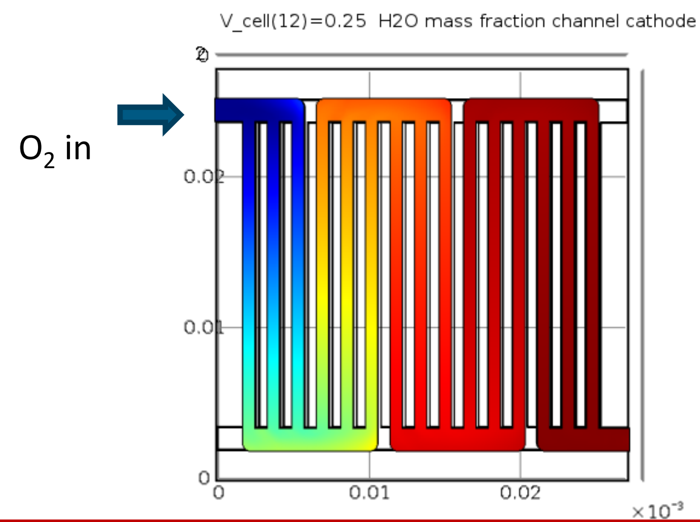
Mass fraction distribution of reactants & products @ 0,25 V









➢ **No relevant MeOH mass transport limitation; H_2O enrichment in cathode flow field channels**

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Conclusions & acknowlegements

➢ Next step: model extension **with** air & electro-osmotic drag implementation, as well as model validation.

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Thanks for your kind attention!