SIMULACE VODÍKOVÝCH TECHNOLOGIÍ S VYUŽITÍM NÁHRADNÍCH MODELŮ ZALOŽENÝCH NA AI

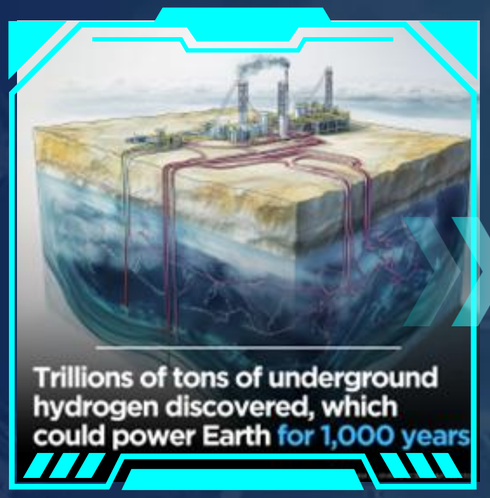
ZEUS

OZE

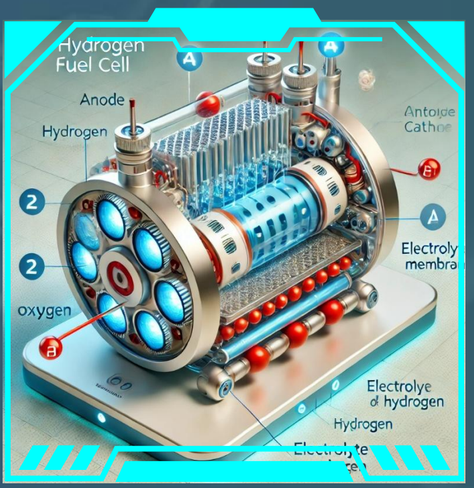
ELEKTROLYZÉRY

SKLADOVÁNÍ

NALEZIŠTĚ



PALIVOVÉ ČLÁNKY



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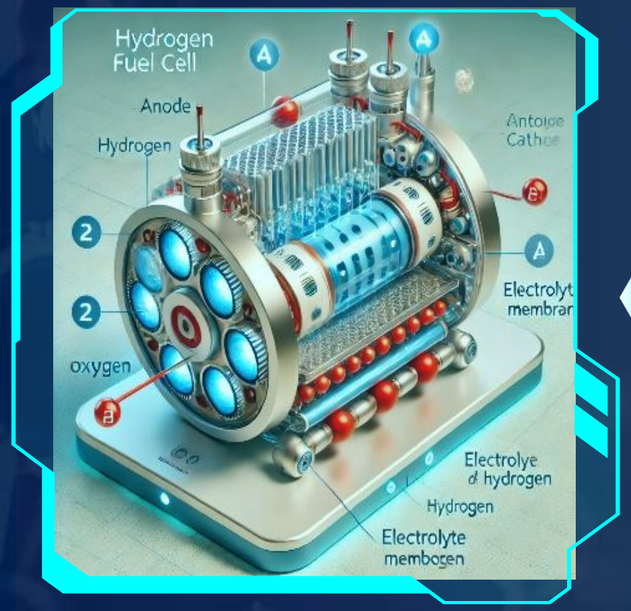
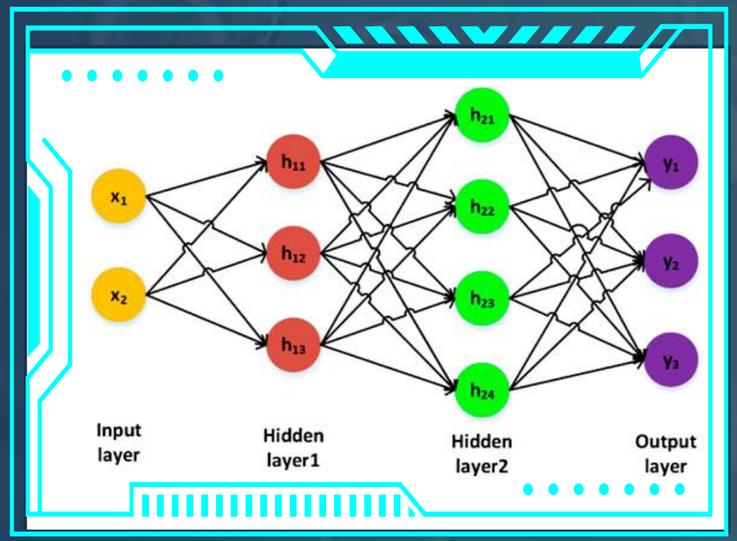
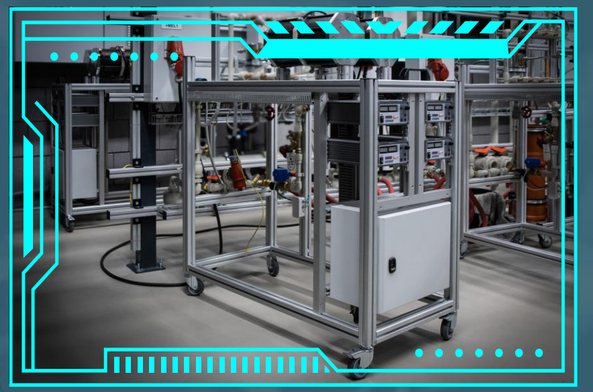
DIGITÁLNÍ DVOJČE



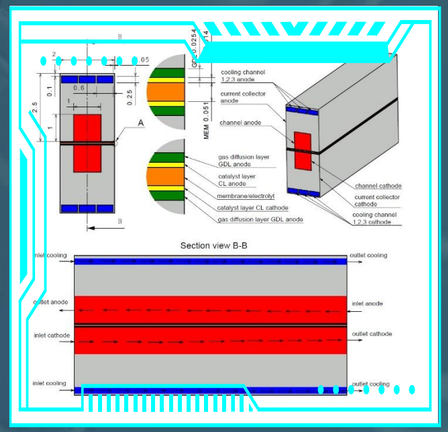
UMĚLÁ INTELIGENCE

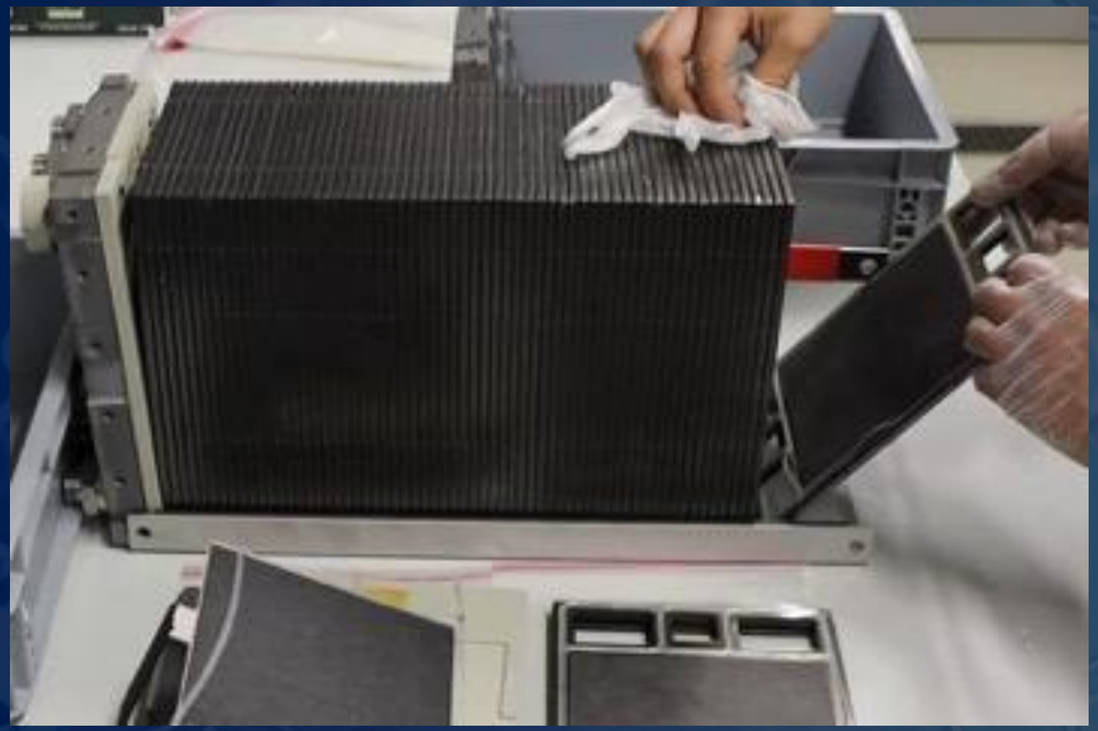


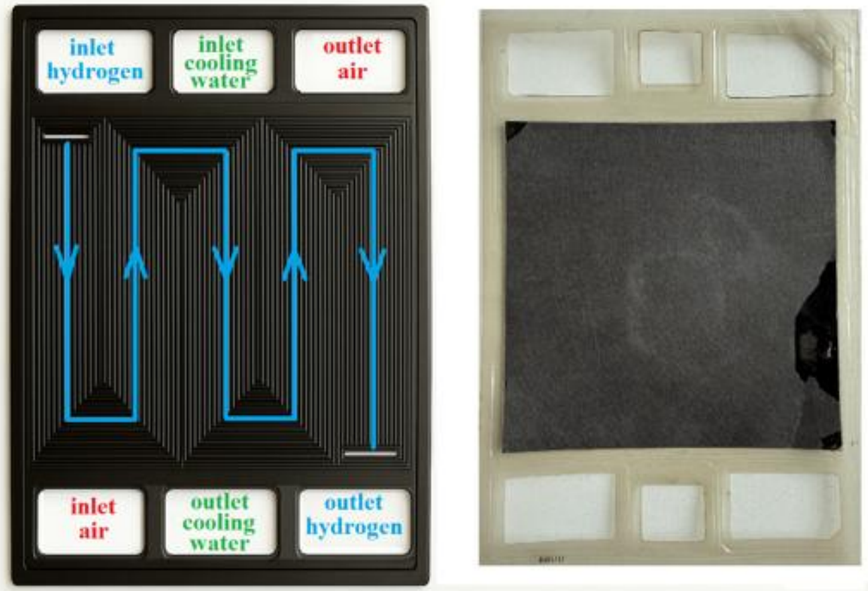
MĚŘENÍ



SIMULACE






inlet hydrogen
inlet cooling water
outlet air
inlet air
outlet cooling water
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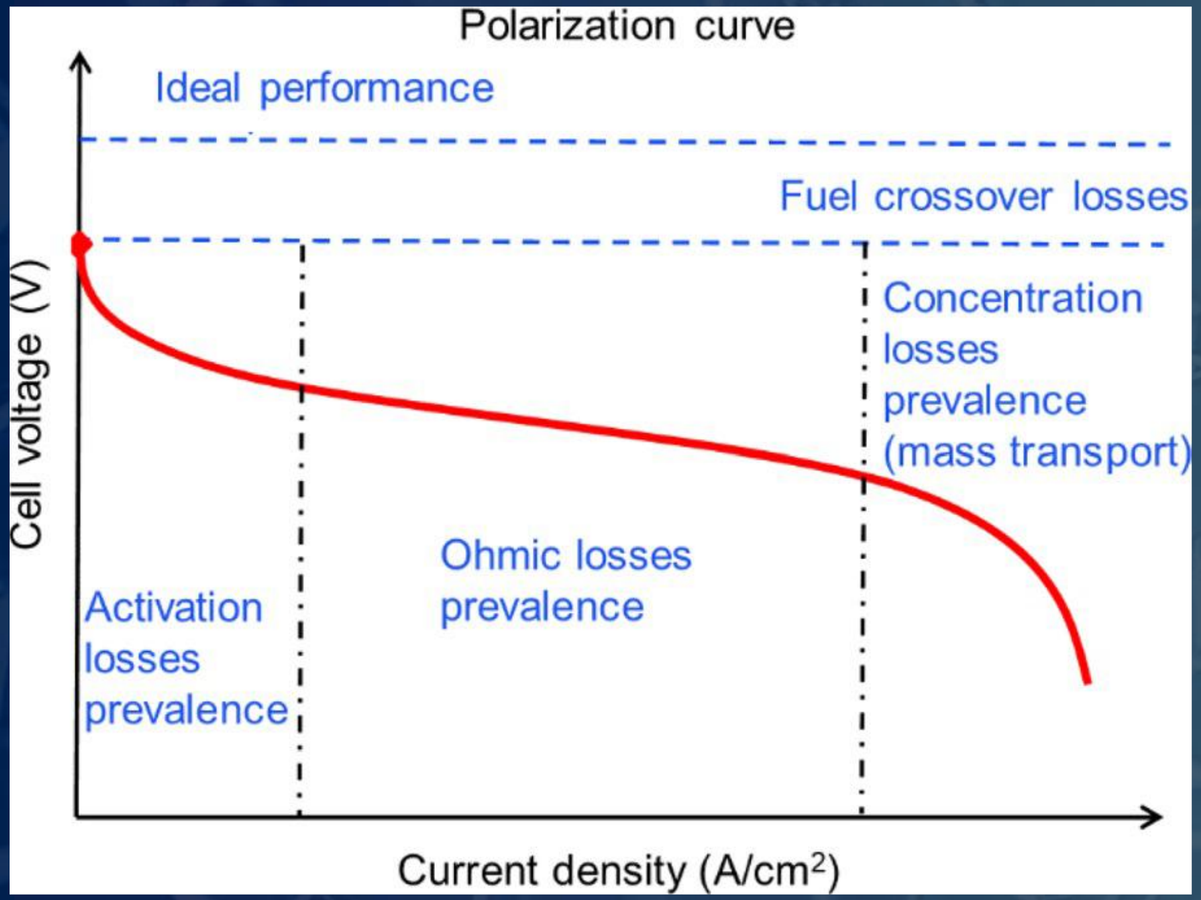
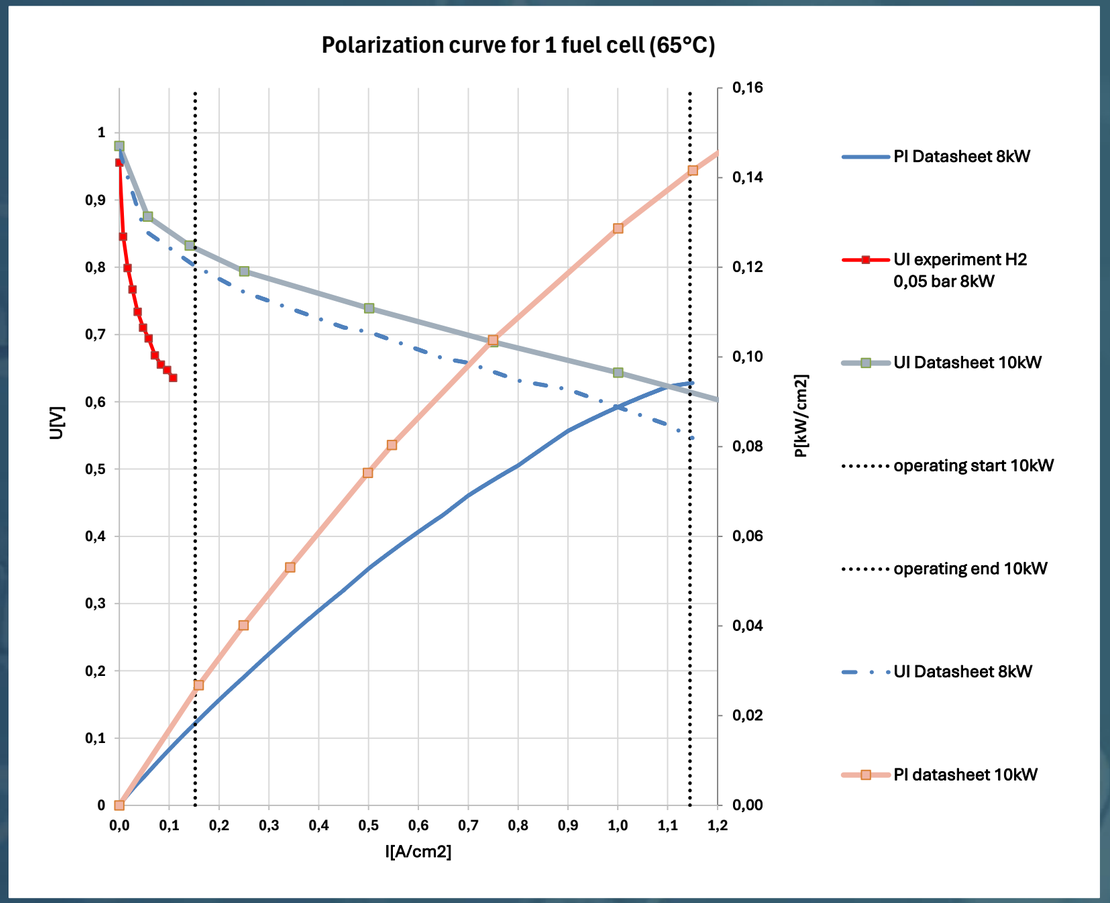
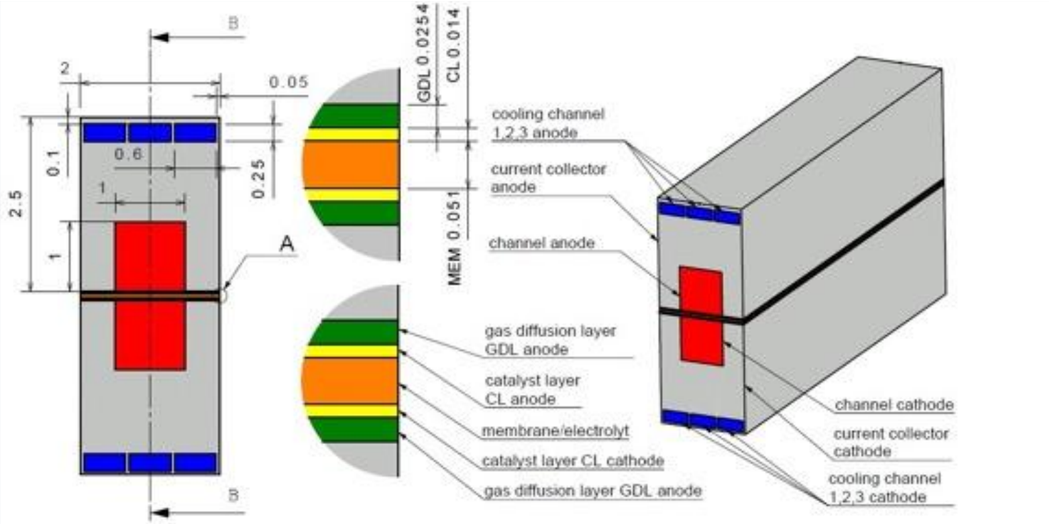
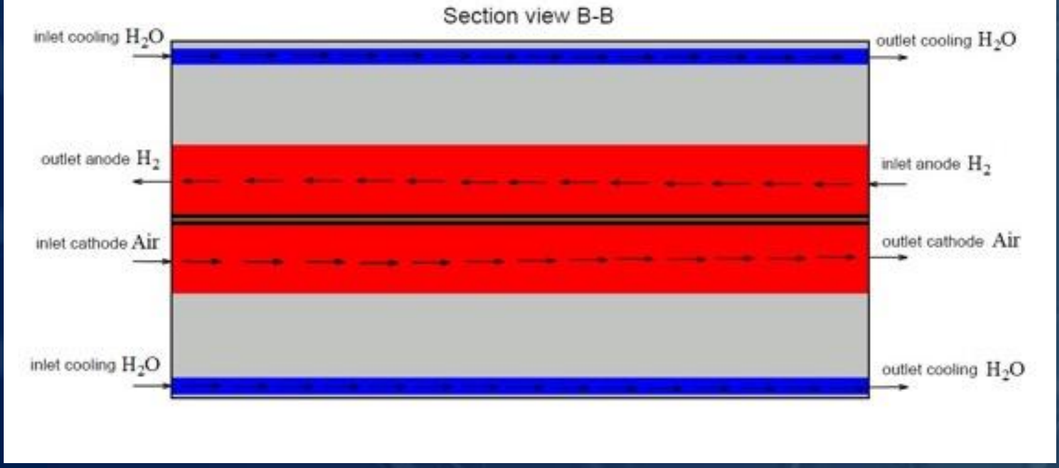
POLARIZAČNÍ KŘIVKA





CFD SIMULACE: MODEL





Anoda (Hydrogen Oxidation Reaction, HOR):

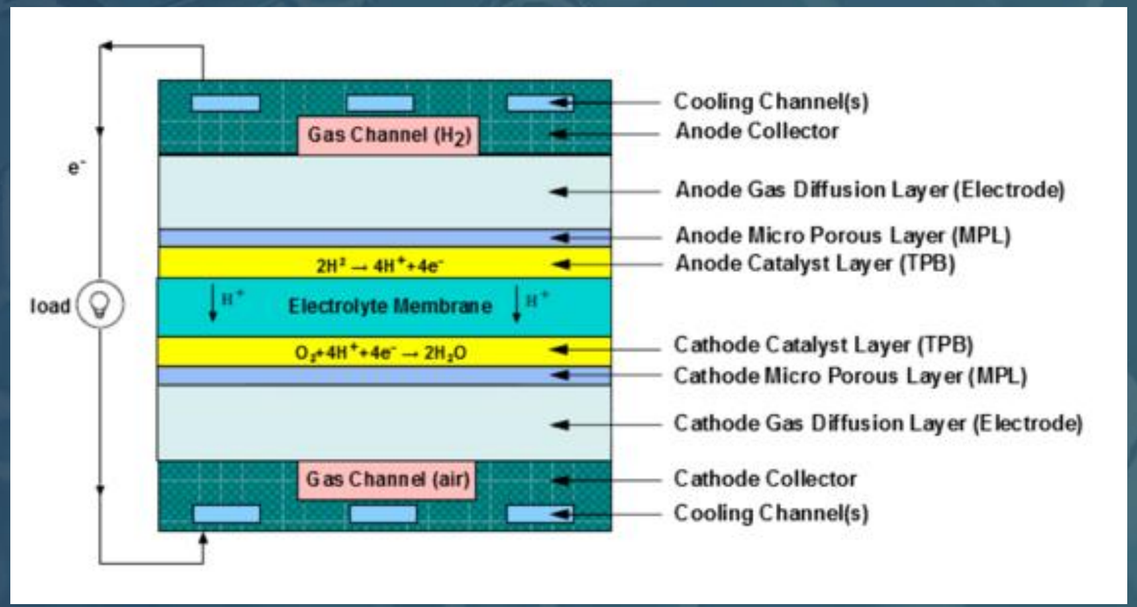
$$2H_2 \rightarrow 4H^+ + 4e^-$$

Katoda (Oxygen Reduction Reaction, ORR):

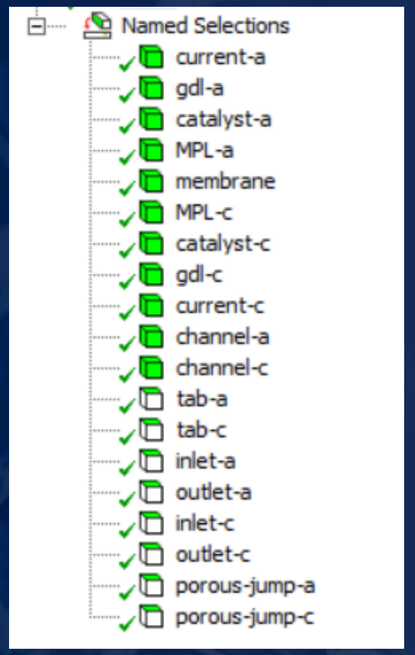
$$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$$

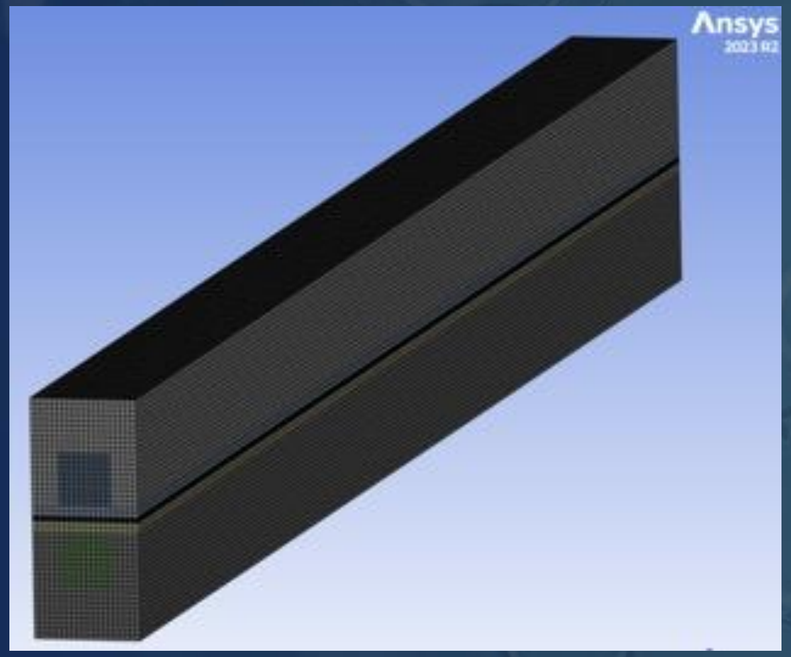
Celková reakce:

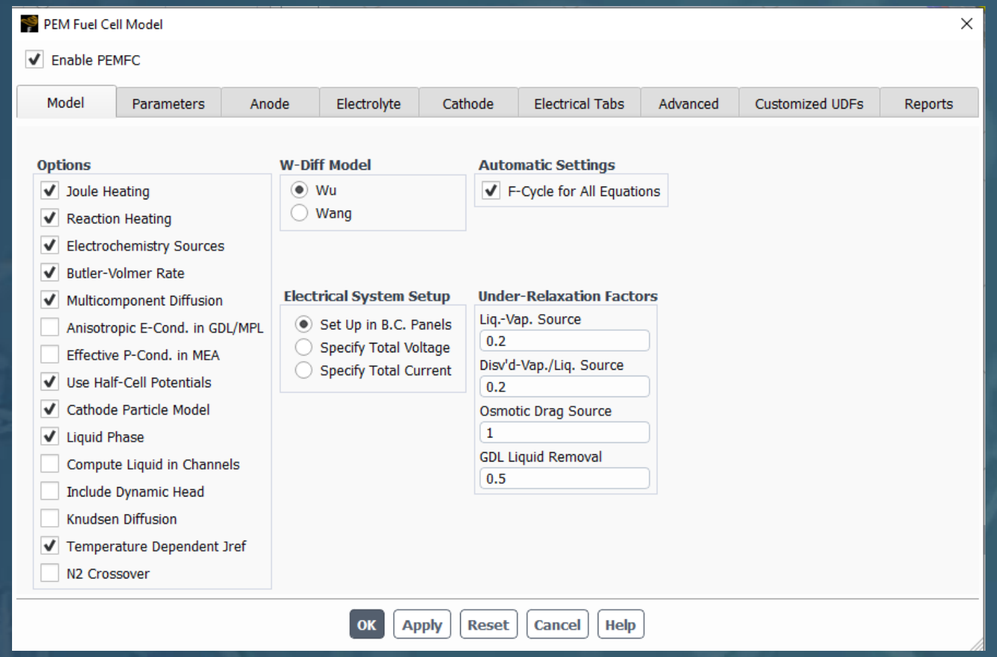
$$2H_2 + O_2 \rightarrow 2H_2O$$

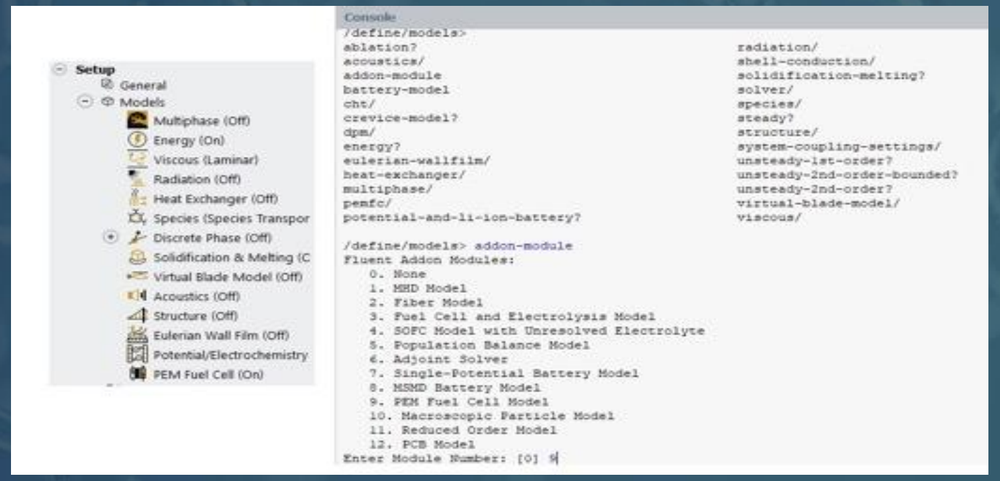


CFD SIMULACE: MODEL









CFD SIMULACE: ROVNICE

$$R_{an}=\left(\zeta_{an}\, j_{an}(T)\right)\left(\frac{[A]}{[A]_{ref}}\right)^{\gamma_{an}}\left(e^{\alpha_{an}^{an}F\eta_{an}/RT}-e^{-\alpha_{cat}^{an}F\eta_{an}/RT}\right)$$

$$E_{an}=0$$

$$j_{an}(T)=j_{an}^{ref}\,e^{-E_{an}/RT\left(1-T/T_{an}^{ref}\right)}$$

PEM Fuel Cell Model

Enable PEMFC

Model | Parameters | Anode | Electrolyte

Electrochemistry

Anode		Cathode	
J_ref (A/m2)	10000	J_ref (A/m2)	10
C_ref (kmol/m3)	1	C_ref (kmol/m3)	1
Con. Exponent	1	Con. Exponent	1
Exch. Coeff.(a)	1	Exch. Coeff. (a)	1
Exch. Coeff.(c)	1	Exch. Coeff. (c)	1
Std. State E0(V)	0	Std. State E0 (V)	1.22884
Entropy (j/kgmol-k)	0	Entropy (j/kgmol-k)	-163300

PEM Fuel Cell Model

Enable PEMFC

Model | Parameters | Anode | Electrolyte | Cathode | Electrical Tabs | Advanced | Customized UDFs | Reports

Electrochemistry

Anode		Cathode		Global	
J_ref (A/m2)	10000	J_ref (A/m2)	10	I_leak (A/m2)	0
C_ref (kmol/m3)	1	C_ref (kmol/m3)	1	Std. Temp. for U0(K)	298.15
Con. Exponent	1	Con. Exponent	1	Std. Press. for U0(Pa)	100000
Exch. Coeff.(a)	1	Exch. Coeff. (a)	1		
Exch. Coeff.(c)	1	Exch. Coeff. (c)	1		
Std. State E0(V)	0	Std. State E0 (V)	1.22884		
Entropy (j/kgmol-k)	0	Entropy (j/kgmol-k)	-163300		

Liquid Phase		Other Parameters	
Expon't Diff_gas	2.5	Gas-Disv'ed Phase	0.5
Expon't J_ref	2.5	Mod. Coef. OSM_drag	1
Expon't K_rel	3	Eq. W. Cont. at a=1	9.2
Expon't Liq_coverage	1	Eq. W. Cont. at s=1	16.8
Liq.-Disv'ed Phase	0.5	N2 Crossover Factor	0.001
Liquid Density	982		
Liq. Thermal Cond.	0.6		
Liq. Diff. in Chan.	1e-05		
V_liq/V_gas in Chan.	0.005		

OK | Apply | Reset | Cancel | Help

$$R_{cat}=\left(\zeta_{cat}\, j_{cat}(T)\right)\left(\frac{[C]}{[C]_{ref}}\right)^{\gamma_{cat}}\left(e^{\alpha_{an}^{cat}F\eta_{cat}/RT}+e^{-\alpha_{cat}^{cat}F\eta_{cat}/RT}\right)$$

Model | Parameters | Anode | Electrolyte

Electrochemistry

Anode		Cathode	
J_ref (A/m2)	10000	J_ref (A/m2)	10
C_ref (kmol/m3)	1	C_ref (kmol/m3)	1
Con. Exponent	1	Con. Exponent	1
Exch. Coeff.(a)	1	Exch. Coeff. (a)	1
Exch. Coeff.(c)	1	Exch. Coeff. (c)	1
Std. State E0(V)	0	Std. State E0 (V)	1.22884
Entropy (j/kgmol-k)	0	Entropy (j/kgmol-k)	-163300

Liquid Phase

Expon't Diff_gas	2.5	r_s
Expon't J_ref	2.5	γ_j
Expon't K_rel	3	b
Expon't Liq_coverage	1	θ
Liq.-Disv'ed Phase	0.5	γ_{ld}
Liquid Density	982	ρ_l
Liq. Thermal Cond.	0.6	k_l

$$D_i=\varepsilon^{1.5}(1-s^{r_s})D_i^0\left(\frac{p_0}{p}\right)^{\gamma_p}\left(\frac{T}{T_0}\right)^{\gamma_t}$$

$$R_j=(1-s)^{\gamma_j}R_j$$

$$K_r=s^{b}$$

$$S_{gd}=(1-s^{\theta})\gamma_{gd}M_{w,H_2O}\frac{\rho_l}{EW}(\lambda_{eq}-\lambda)$$

$$S_{ld}=s^{\theta}\gamma_{ld}M_{w,H_2O}\frac{\rho_l}{EW}(\lambda_{eq}-\lambda)$$

$$k_{eff}=s^{k_l}+(1-s)\left[\varepsilon k_{gas}+(1-\varepsilon)k_{solid}\right]$$

CFD SIMULACE: PARAMETRY

No.	Parameter Name	Symbol	Unit	Range (Dakota)	No.	Parameter Name	Symbol	Unit	Range (Dakota)
1	Reference current density (anode)	$J_{\mathrm{ref,an}}$	A/m^2	1000, 10000, 20000	39	CL (anode) permeability	K	m^2	$10^{-13}, 10^{-11}, 10^{-9}$
2	Reference current density (cathode)	$J_{\mathrm{ref,cat}}$	A/m^2	1, 10, 20	40	CL (anode) surface/volume ratio	ζ	1/m	10000, 200000, 1000000
3	Reference molar concentration H_2 (anode)	$C_{\mathrm{ref,an}}$	kmol/m^3	0.05, 1	41	CL (anode) hydrophobic contact angle	θ_c	°	90, 110, 135
4	Reference molar concentration O_2 (cathode)	$C_{\mathrm{ref,cat}}$	kmol/m^3	0.01, 1	42	CL (anode) activation energy for J_{ref}	E_i	J/kmol	5E+06, 8.314E+06, 1.2E+07
5	Concentration exponent (anode)	γ_{an}	–	0.3, 0.65, 1.0	43	CL (anode) reference temperature for J_{ref}	$T_{0,\mathrm{an}}$	K	338
6	Concentration exponent (cathode)	γ_{cat}	–	0.3, 0.65, 1.0	44	CL (anode) Leverett coeff. a	a	–	1.417
7	Transfer coefficient (anode)	α_{an}	–	0.3, 0.65, 1.0	45	CL (anode) Leverett coeff. b	b	–	2.12
8	Transfer coefficient (anode)	α_{an}	–	0.3, 0.65, 1.0	46	CL (anode) Leverett coeff. c	c	–	1.263
9	Transfer coefficient (cathode)	α_{cat}	–	0.3, 0.65, 1.0	47	CL (anode) condensation coeff.	γ_c	–	1E+06, 1E+08, 1E+10
10	Transfer coefficient (cathode)	α_{cat}	–	0.3, 0.65, 1.0	48	CL (anode) evaporation coeff.	γ_e	–	1E+06, 1E+08, 1E+10
11	Reversible potential (anode)	$U_{0,\mathrm{an}}$	V	0	49	Membrane equivalent weight	EW	kg/kmol	800, 1100, 1250
12	Reversible potential (cathode)	$U_{0,\mathrm{cat}}$	V	1.229	50	Membrane protonic conduction coeff.	β_{mem}	–	0.5, 1, 2
13	Entropy (anode)	ΔS_{an}	J/kmolK	-130000	51	Membrane protonic conduction exponent	ω_i	–	0.5, 1, 2
14	Entropy (cathode)	ΔS_{cat}	J/kmolK	-32660	52	Membrane water diffusivity coeff.	η_λ	–	0.1, 1, 2
15	Leakage current density	I_{leak}	A/m^2	0	53	Membrane permeability	K	m^2	$10^{-13}, 10^{-11}, 10^{-9}$
16	Standard temperature	T_0	K	298.15	54	GDL (cathode) porosity	ϵ	–	0.4, 0.75, 0.9
17	Standard pressure	p_0	Pa	101325	55	GDL (cathode) permeability	K	m^2	$10^{-13}, 10^{-11}, 10^{-9}$
18	Exponent Diffusion gas	r_s	–	1.5, 2.5, 3.5	56	GDL (cathode) hydrophobic contact angle	θ_c	°	90, 110, 135
19	Exponent J_{ref}	γ_j	–	1.5, 2.5, 3.5	57	GDL (cathode) water removal coef.	Θ	s/m	1E-05, 5E-05, 1E-04
20	Exponent relative permeability	b	–	2, 3, 4	58	GDL (cathode) Leverett coeff. a	a	–	1.417
21	Exponent liquid coverage	θ	–	0.2, 1, 1.8	59	GDL (cathode) Leverett coeff. b	b	–	2.12
22	Liq.-Dissolved Phase	γ_{ld}	–	0.25, 0.5, 1, 1.5	60	GDL (cathode) Leverett coeff. c	c	–	1.263
23	Liquid density	ρ_l	kg/m^3	982	61	GDL (cathode) condensation coeff.	γ_c	–	1E+06, 1E+08, 1E+10
24	Liquid thermal conductivity	k_l	W/mK	0.6	62	GDL (cathode) evaporation coeff.	γ_e	–	1E+06, 1E+08, 1E+10
25	Gas-dissolved Phase	γ_{gd}	–	0.25, 0.5, 0.75	63	CL (cathode) porosity	ϵ	–	0.4, 0.75, 0.9
26	Osmotic drag coefficient	η_{osm}	–	0.5, 1, 1.5	64	CL (cathode) permeability	K	m^2	$10^{-13}, 10^{-11}, 10^{-9}$
27	Eq. water content at a=1	λ_a	–	9.2	65	CL (cathode) surface/volume ratio	ζ	1/m	10000, 200000, 1000000
28	Eq. water content at s=1	λ_s	–	16.8	66	CL (cathode) hydrophobic contact angle	θ_c	°	90, 110, 135
29	GDL (anode) porosity	ϵ	–	0.4, 0.75, 0.9	67	CL (cathode) activation energy for J_{ref}	E_i	J/kmol	5E+06, 8.314E+06, 1.2E+07
30	GDL (anode) permeability	K	m^2	$10^{-13}, 10^{-11}, 10^{-9}$	68	CL (cathode) reference temperature for J_{ref}	$T_{0,\mathrm{cat}}$	K	343
31	GDL (anode) hydrophobic contact angle	θ_c	°	90, 110, 135	69	CL (cathode) product of O_2 solubility	$K_w D_w$	m^2/s	1E-9, 1E-8, 1E-7
32	GDL (anode) water removal coef.	Θ	s/m	1E-05, 5E-05, 1E-04	70	CL (cathode) catalyst particle radius	r_p	m	1E-9, 5E-8, 1E-8
33	GDL (anode) Leverett coeff. a	a	–	1.417	71	CL (cathode) ionomer resistance	R_{ion}	s/m	50, 100, 300
34	GDL (anode) Leverett coeff. b	b	–	2.12	72	CL (cathode) Leverett coeff. a	a	–	1.417
35	GDL (anode) Leverett coeff. c	c	–	1.263	73	CL (cathode) Leverett coeff. b	b	–	2.12
36	GDL (anode) condensation coeff.	γ_c	–	1E+06, 1E+08, 1E+10	74	CL (cathode) Leverett coeff. c	c	–	1.263
37	GDL (anode) evaporation coeff.	γ_e	–	1E+06, 1E+08, 1E+10	75	CL (cathode) condensation coeff.	γ_c	–	1E+06, 1E+08, 1E+10
38	CL (anode) porosity	ϵ	–	0.4, 0.75, 0.9	76	CL (cathode) evaporation coeff.	γ_e	–	1E+06, 1E+08, 1E+10
					77	Coolant density	ρ_c	kg/m^3	998.2

CFD SIMULACE: PARAMETRY

FIXNÍ

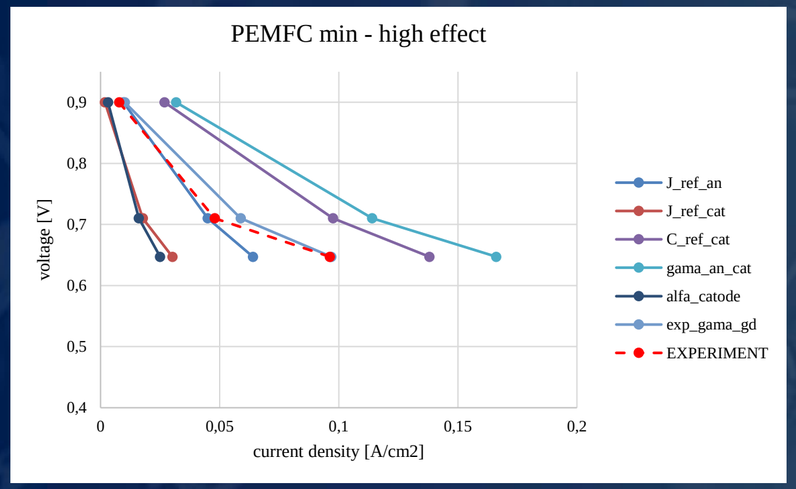
No.	Parameter Name	Symbol	Unit	Fixed Value / Range
1	Reversible potential (anode)	$U_{0,\mathrm{an}}$	V	0
2	Reversible potential (cathode)	$U_{0,\mathrm{cat}}$	V	1.229
3	Entropy (anode)	ΔS_{an}	J/kmolK	-130000
4	Entropy (cathode)	ΔS_{cat}	J/kmolK	-32660
5	Leakage current density	I_{leak}	A/m^2	0
6	Standard temperature	T_0	K	298.15
7	Standard pressure	p_0	Pa	101325
8	Liquid density	ρ_l	kg/m^3	982
9	Liquid thermal conductivity	k_l	W/mK	0.6
10	Eq. water content at a = 1	λ_a	–	9.2
11	Eq. water content at s = 1	λ_s	–	16.8
12	GDL (anode) Leverett coefficient a	a	–	1.417
13	GDL (anode) Leverett coefficient b	b	–	2.12
14	GDL (anode) Leverett coefficient c	c	–	1.263
15	CL (anode) reference temperature for J_{ref}	$T_{0,\mathrm{an}}$	K	338
16	CL (anode) Leverett coefficient a	a	–	1.417
17	CL (anode) Leverett coefficient b	b	–	2.12
18	CL (anode) Leverett coefficient c	c	–	1.263
19	Membrane permeability	K	m^2	10^{-13}, 10^{-11}, 10^{-9}
20	GDL (cathode) Leverett coefficient a	a	–	1.417
21	GDL (cathode) Leverett coefficient b	b	–	2.12
22	GDL (cathode) Leverett coefficient c	c	–	1.263
23	CL (cathode) reference temperature for J_{ref}	$T_{0,\mathrm{cat}}$	K	343
24	CL (cathode) Leverett coefficient a	a	–	1.417
25	CL (cathode) Leverett coefficient b	b	–	2.12
26	CL (cathode) Leverett coefficient c	c	–	1.263
27	Coolant density	ρ_c	kg/m^3	998.2

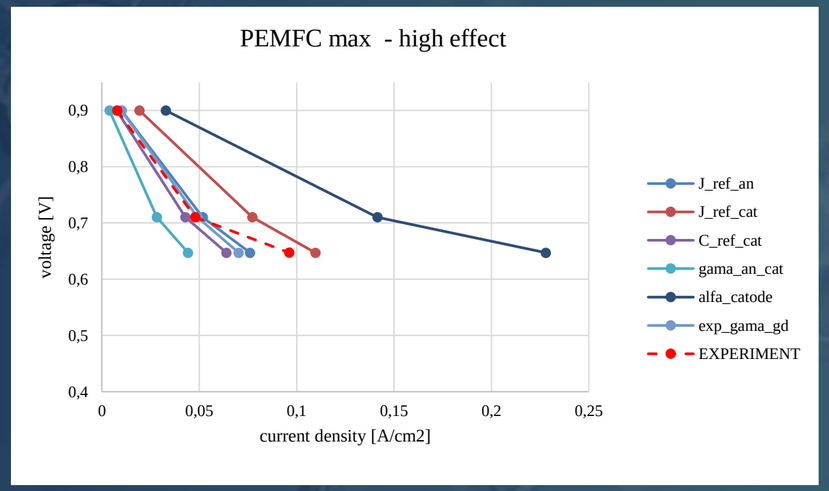
PROMĚNNÉ

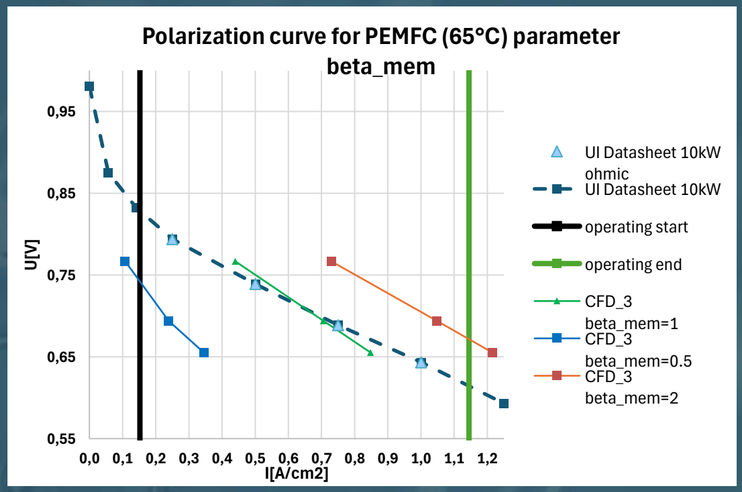
No.	Parameter Name	Symbol	Unit	Range (Dakota)
1	Reference current density (anode)	$J_{\mathrm{ref,an}}$	A/m^2	1000, 10000, 20000
2	Reference current density (cathode)	$J_{\mathrm{ref,cat}}$	A/m^2	1, 10, 20
3	Reference molar concentration H_2 (anode)	$C_{\mathrm{ref,an}}$	kmol/m^3	0.05, 1
4	Reference molar concentration O_2 (cathode)	$C_{\mathrm{ref,cat}}$	kmol/m^3	0.01, 1
5	Concentration exponent (anode)	γ_{an}	–	0.3, 0.65, 1.0
6	Concentration exponent (cathode)	γ_{cat}	–	0.3, 0.65, 1.0
7	Transport coefficient (anode)	α_{anode}	–	0.3, 0.65, 1.0
8	Transport coefficient (cathode)	$\alpha_{\mathrm{cathode}}$	–	0.3, 0.65, 1.0
9	Exponent: diffusion gas	r_s	–	1.5, 2.5, 3.5
10	Exponent: J_{ref}	γ_j	–	1.5, 2.5, 3.5
11	Exponent: relative permeability	b	–	2, 3, 4
12	Exponent: liquid coverage	θ	–	0.2, 1, 1.8
13	Exponent: liquid–dissolved phase	γ_{ld}	–	0.25, 0.5, 1, 1.5
14	Exponent: gas–dissolved phase	γ_{gd}	–	0.25, 0.5, 0.75
15	Osmotic drag coefficient	η_{osm}	–	0.5, 1, 1.5
16	GDL/CL porosity	ε	–	0.4, 0.75, 0.9
17	GDL/CL absolute permeability	K	m^2	1E-16, 1E-12, 1E-08
18	GDL/CL hydrophobic contact angle	θ_c	°	90, 110, 135
19	Water removal coefficient (GDL/CL)	Θ	s/m	1E-05, 5E-05, 1E-04
20	Condensation rate coefficient (GDL/CL)	γ_c	–	1E+06, 1E+08, 1E+10
21	Evaporation rate coefficient (GDL/CL)	γ_e	–	1E+06, 1E+08, 1E+10
22	Catalyst layer surface-to-volume ratio (anode)	ζ	1/m	10000, 200000, 1000000
23	Activation energy for J_{ref}	E_i	J/kmol	5E+06, 8.314E+06, 1.2E+07
24	Membrane equivalent weight	EW	kg/kmol	800, 1100, 1250
25	Membrane protonic conduction coefficient	β_{mem}	–	0.5, 1, 2
26	Membrane protonic conduction exponent	ω_i	–	0.5, 1, 2
27	Membrane water diffusivity coefficient	η_λ	–	0.1, 1, 2
28	Cathode CL product of O_2 solubility and diffusivity	$K_w D_w$	m^2/s	1E-9, 1E-8, 1E-7
29	Cathode CL catalyst particle radius	r_p	m	1E-9, 5E-8, 1E-8
30	Cathode CL ionomer resistance	R_{ion}	s/m	50, 100, 300

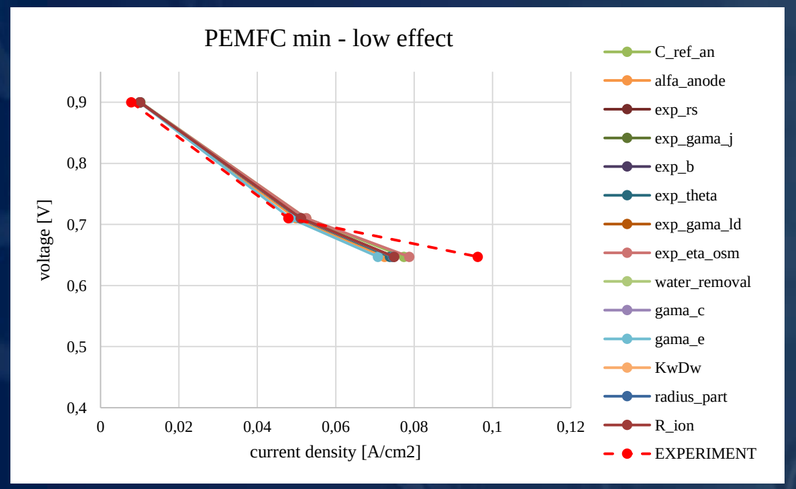
ZEUS

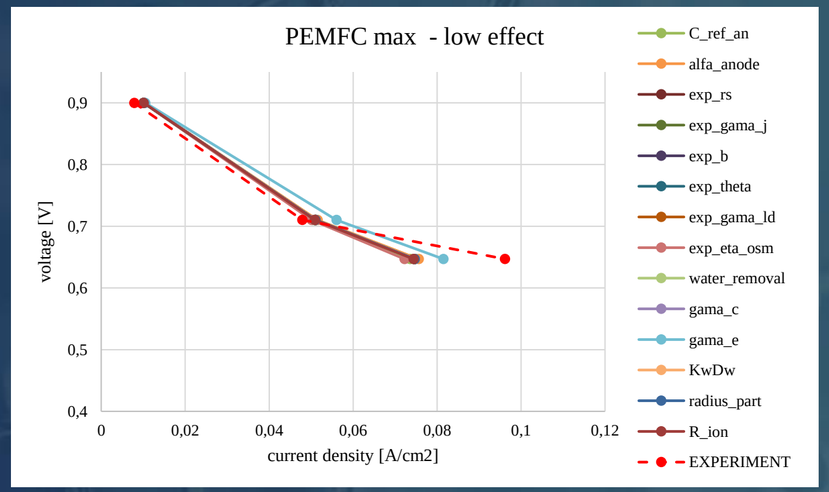
CFD SIMULACE: CITLIVOSTNÍ ANALÝZA

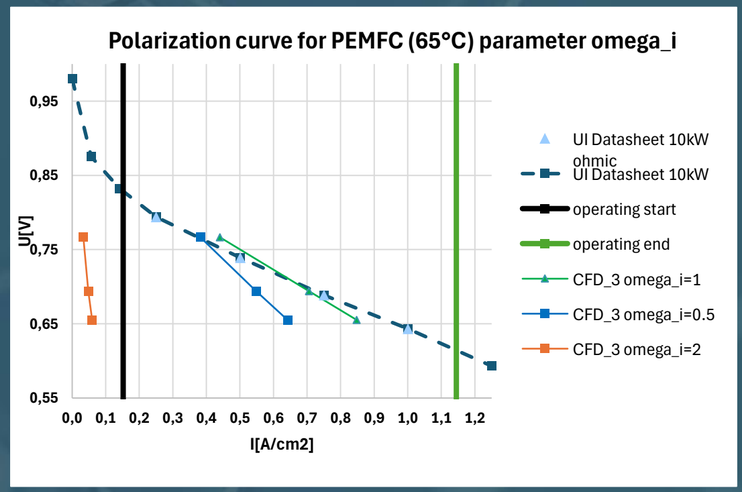






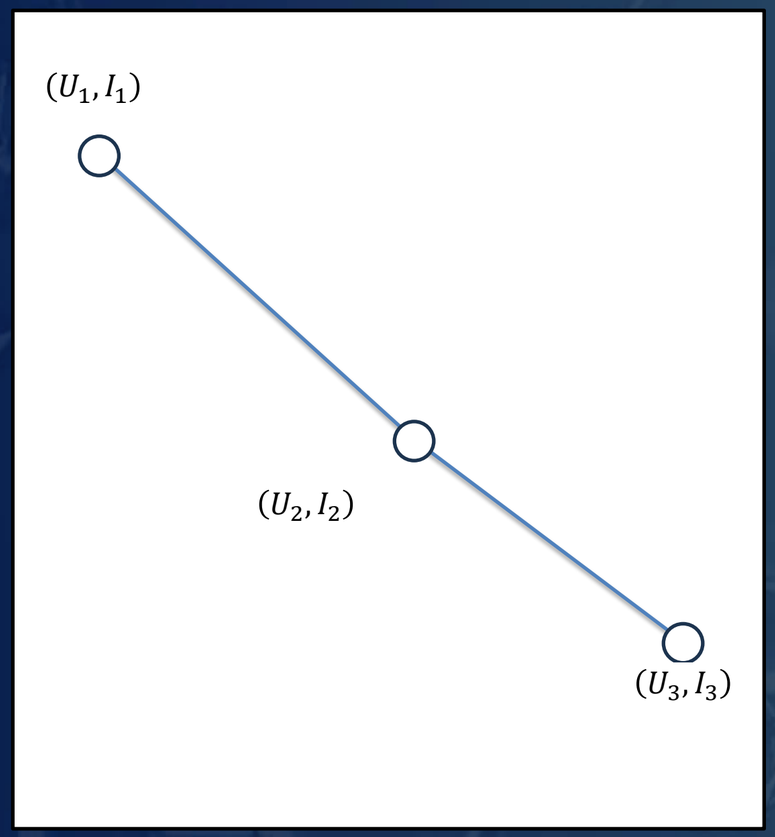






AI: DEFINICE ÚLOHY

Nalézt sadu parametrů P odpovídající volt-ampérové charakteristice $\{(\mathrm{U_j}, \mathrm{I_j})\}$ pro $\mathrm{j} \in \{1, 2, 3\}$



Vytvořit **náhradní model (surrogate model)** pro odhad P s pomocí gradientní optimalizace.

$$f_\Theta : P \times U \to I,$$

$$f_\Theta : I \to P.$$

AI: NÁVRH ŘEŠENÍ

Krok 1:

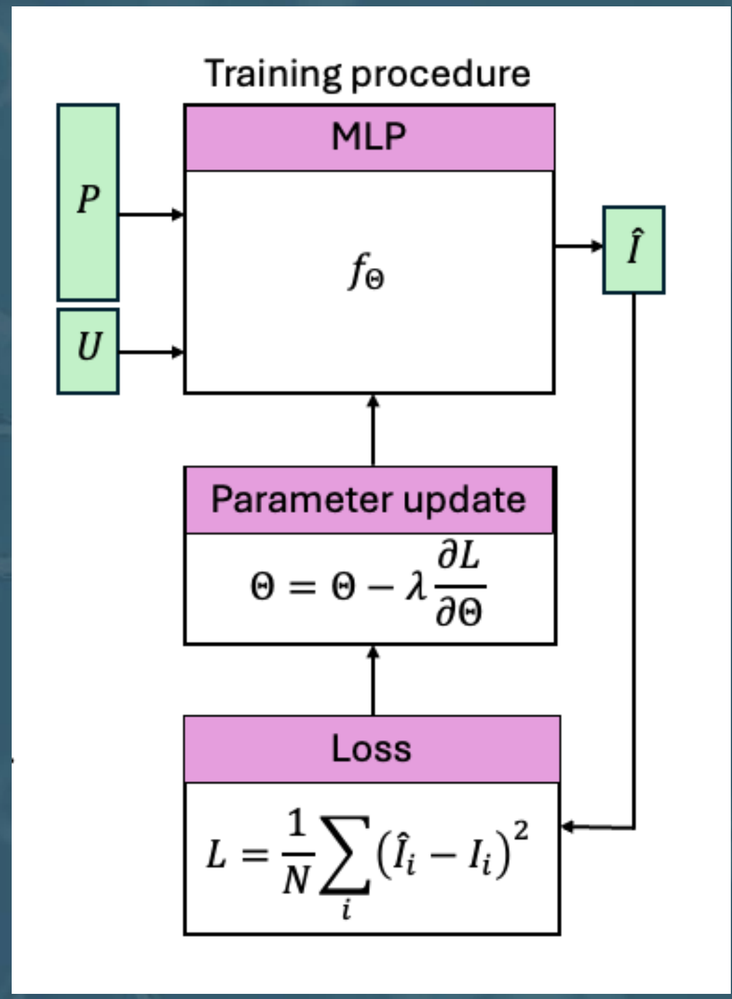
- Očištění a transformace dat
- Normalizace hodnot P, U, I tak, aby byly v konkrétním rozsahu $\langle a, b \rangle$.
- Odstranění odlehlých hodnot
- Rozdělení dat na trénovací a testovací

Krok 2:

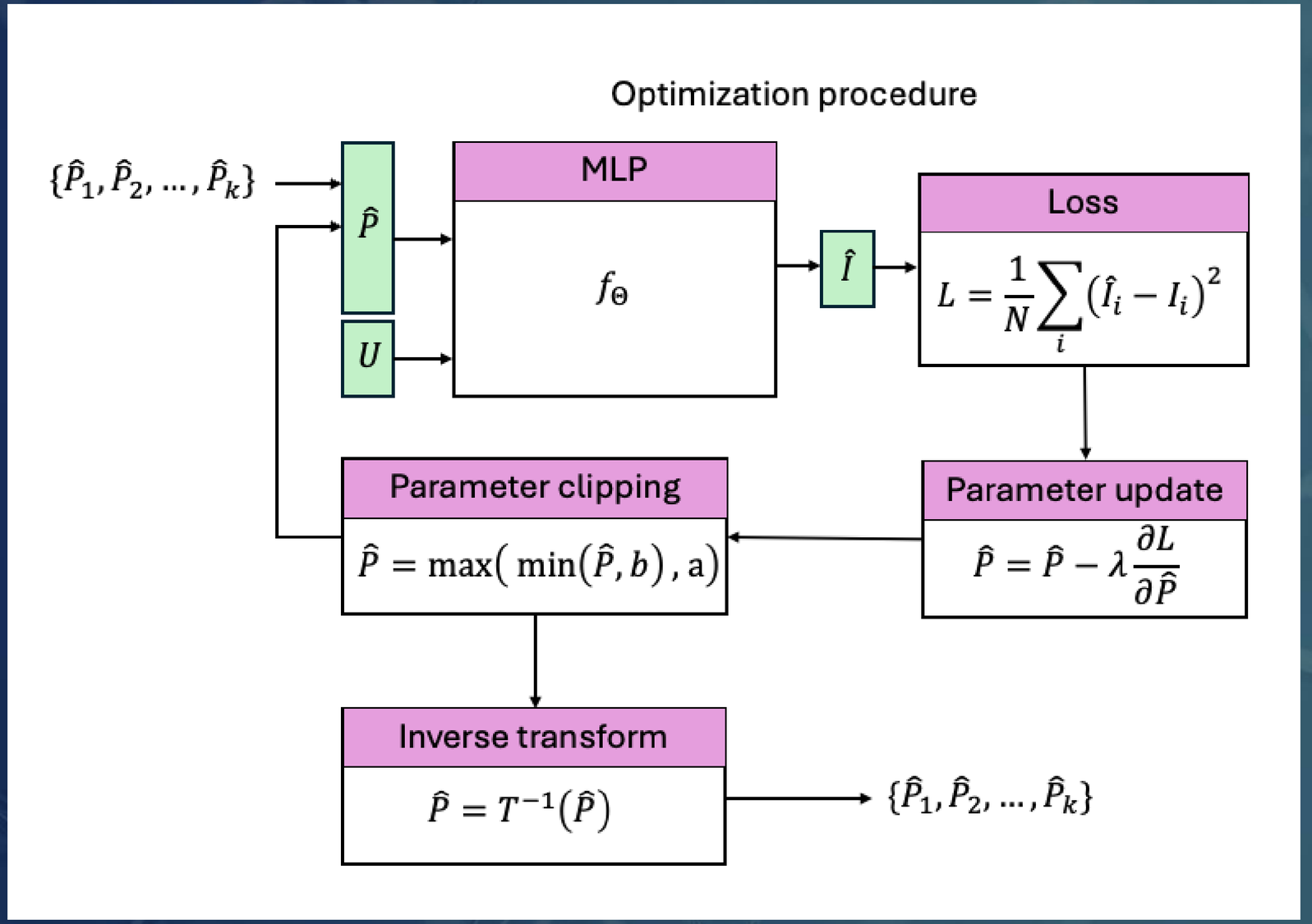
- Definice vhodné architektury modelu: Vícevrstvý perceptron.
- Experimenty s:
  - počtem skrytých vrstev
  - aktivačními funkcemi
  - normalizacemi vrstev
  - hodnotami dropoutu

Krok 3: Trénink náhradního modelu:

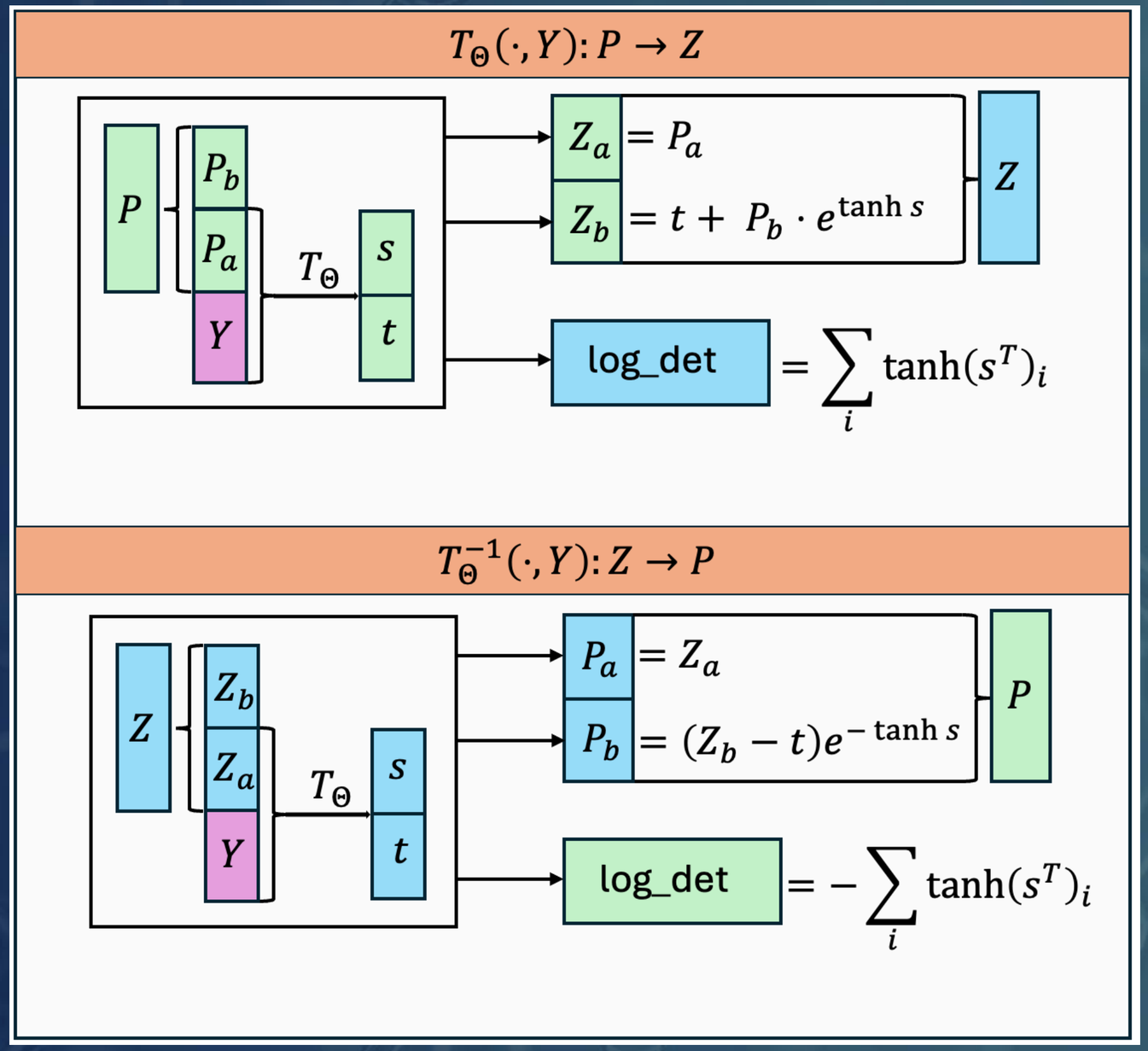
- Výběr vhodné optimalizační metody (AdamW).
- Výběr vhodného plánovače rychlosti učení (cyklická rychlost učení).
- Monitoring ztrátové funkce



AI: ODHAD PARAMETRŮ



AI: DALŠÍ KROK



ZEUS

Zvýšení odolnosti energetických sítí v kontextu dekarbonizace, decentralizace a udržitelného socioekonomického rozvoje

CZ.02.01.01/00/23_021/0008759

Operační program Jan Amos Komenský

Spolufinancováno Evropskou unií

MINISTERSTVO ŠKOLSTVÍ, MLÁDEŽE A TĚLOVÝCHOVY