# CFD-Based Digital Twin of a PEM Fuel Cell with AI-Driven Surrogate Modelling

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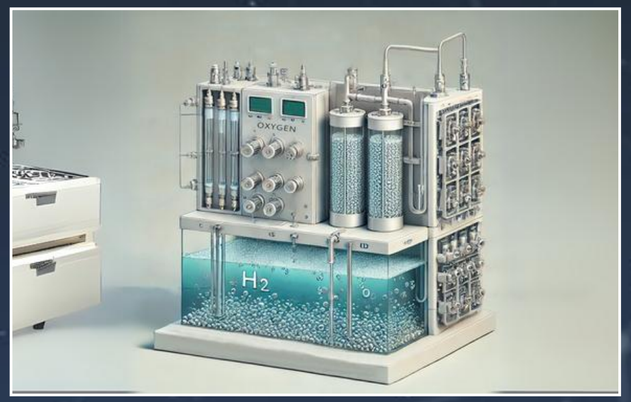
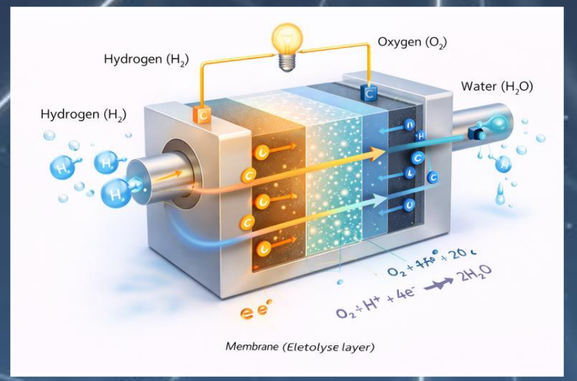
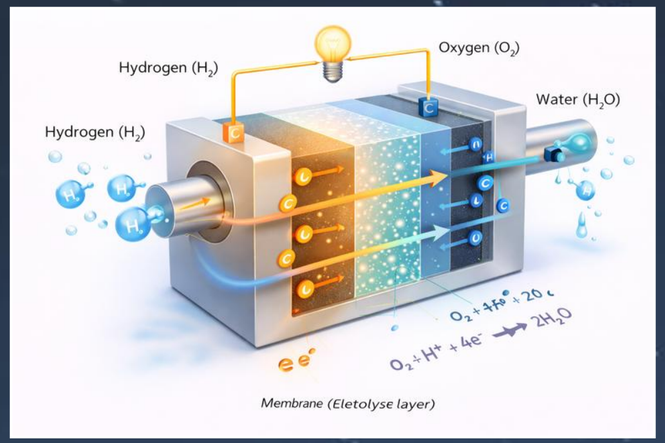
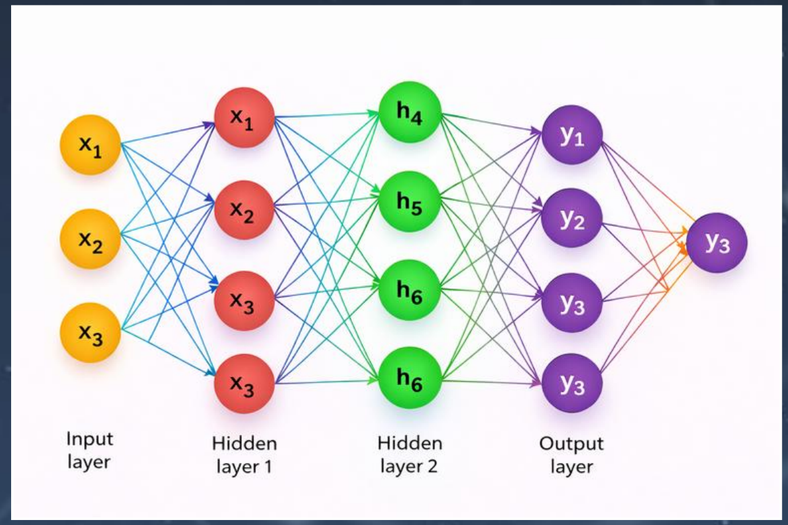
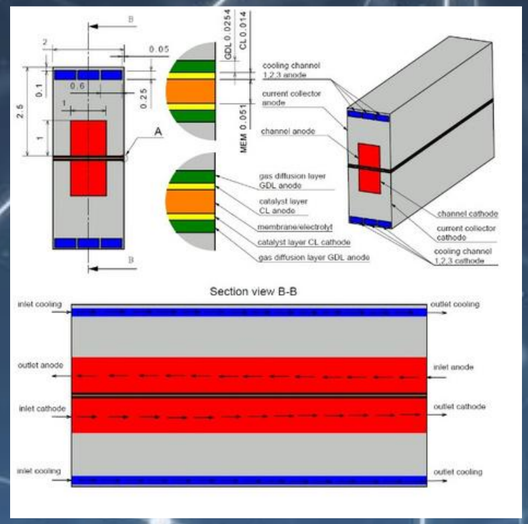




# Development of Digital Twin of PEM Fuel cell



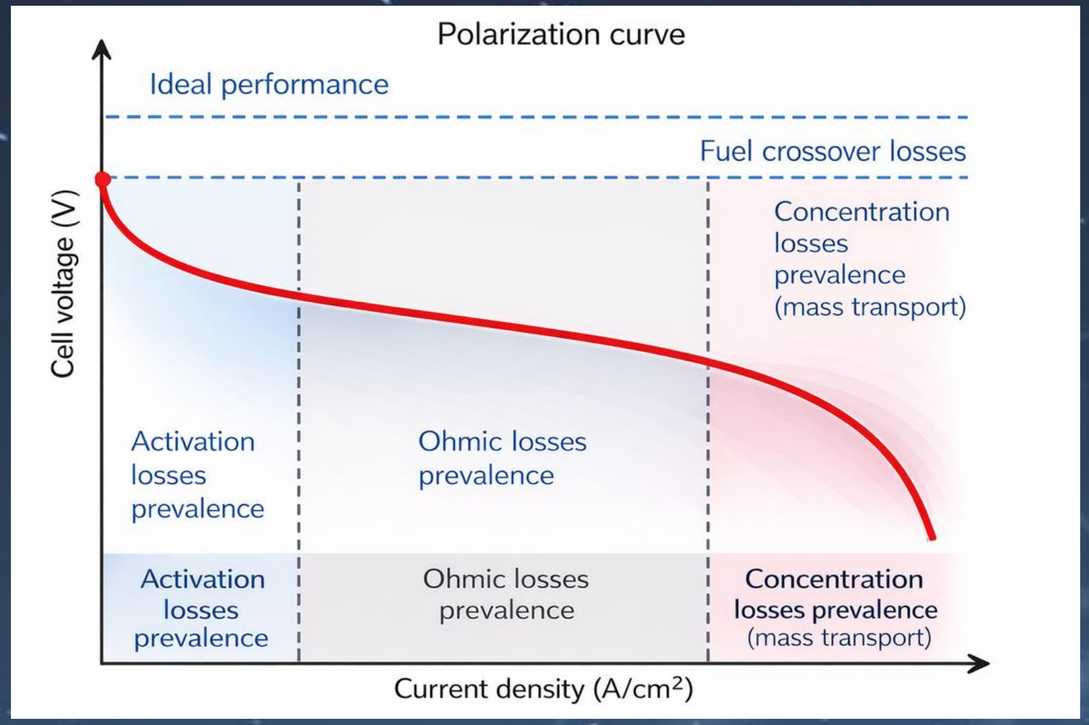



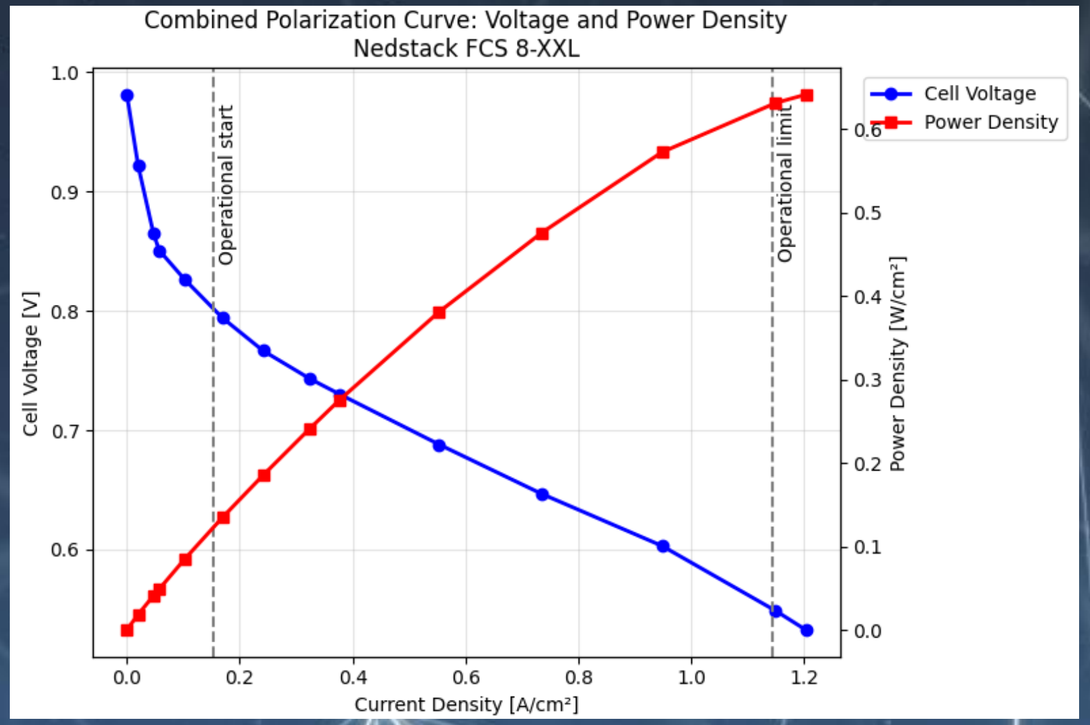


# Development of Digital Twin of PEM Fuel cell

# Polarisation curve





# CFD simulation



## Anode

(Hydrogen Oxidation Reaction)

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

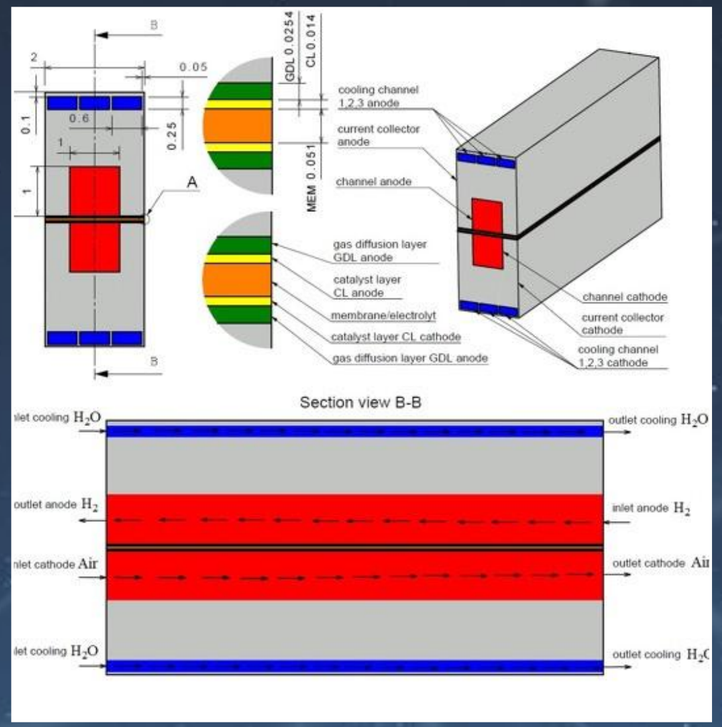
## Cathode

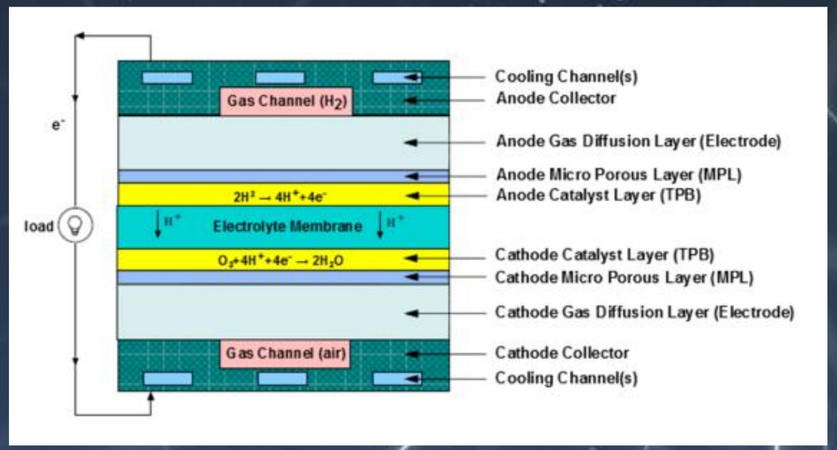
(Oxygen Reduction Reaction)

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

## Whole system

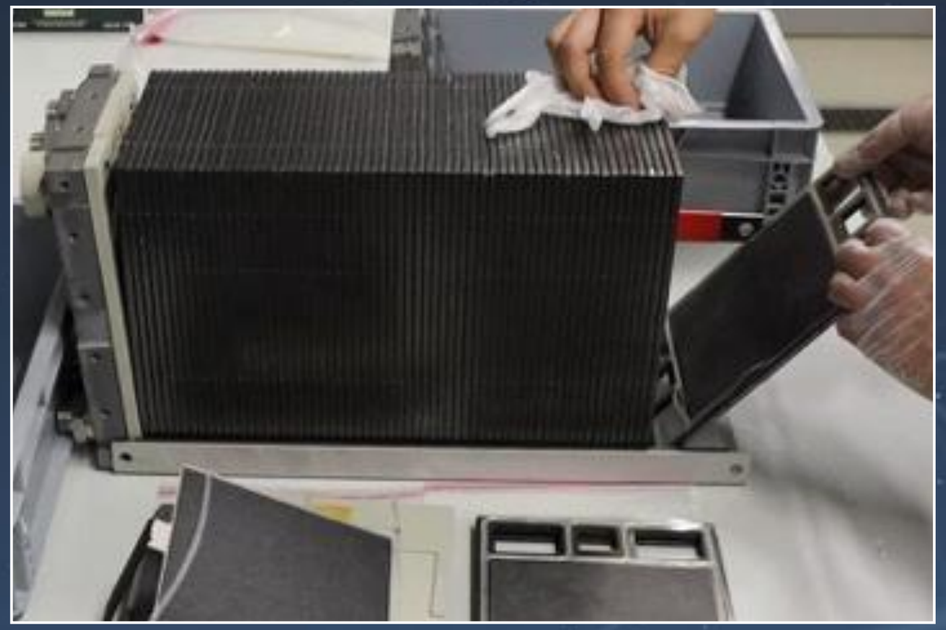
$$2H_2 + O_2 \rightarrow 2H_2O$$

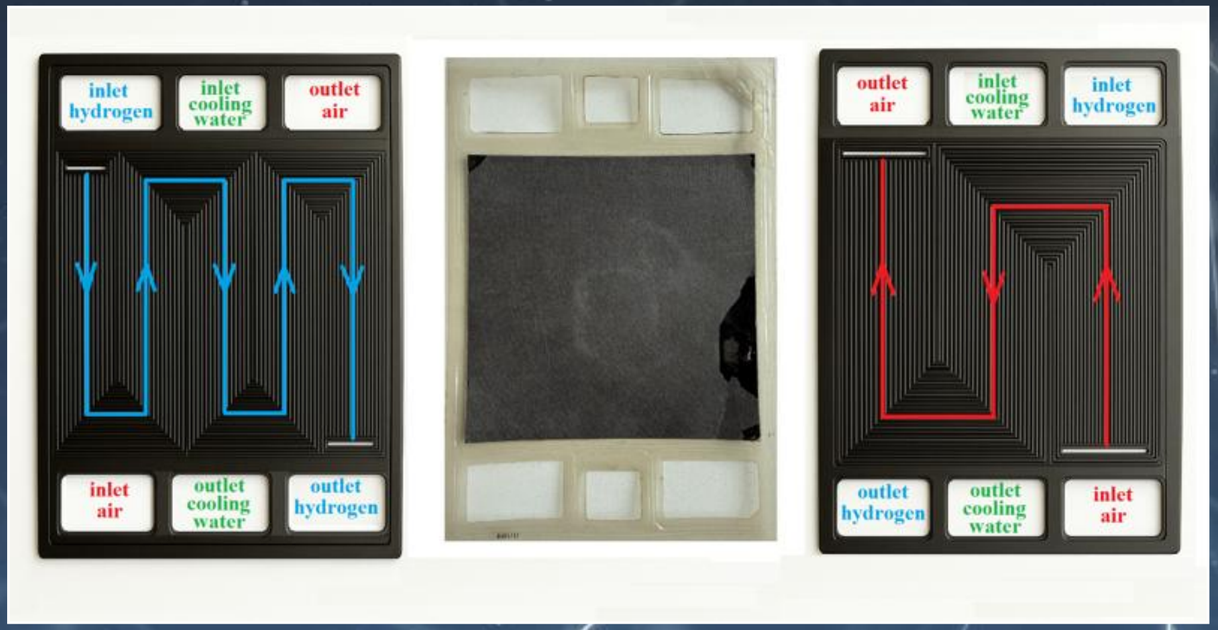


# PEM (Polymer Electrolyte Membrane) fuel cell

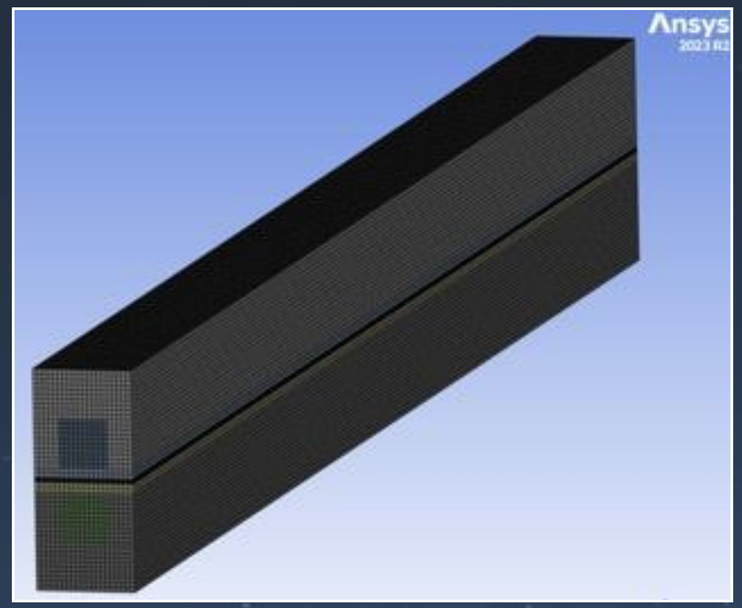


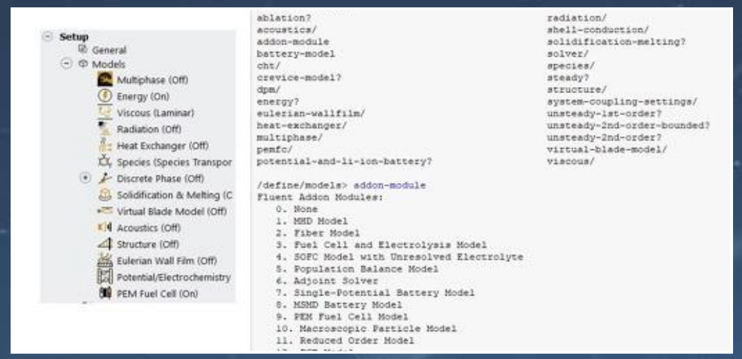




# CFD model






PEM Fuel Cell Model

Enable PEMFC

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

**Options**

- [x] Joule Heating
- [x] Reaction Heating
- [x] Electrochemistry Sources
- [x] Butler-Volmer Rate
- [x] Multicomponent Diffusion
- [ ] Anisotropic E-Cond. in GDL/MPL
- [ ] Effective P-Cond. in MEA
- [x] Use Half-Cell Potentials
- [x] Cathode Particle Model
- [x] Liquid Phase
- [ ] Compute Liquid in Channels
- [ ] Include Dynamic Head
- [ ] Knudsen Diffusion
- [x] Temperature Dependent Jref
- [ ] N2 Crossover

**W-Diff Model**

- (•) Wu
- ( ) Wang

**Automatic Settings**

- [x] F-Cycle for All Equations

**Electrical System Setup**

- (•) Set Up in B.C. Panels
- ( ) Specify Total Voltage
- ( ) Specify Total Current

**Under-Relaxation Factors**

Liq.-Vap. Source: 0.2

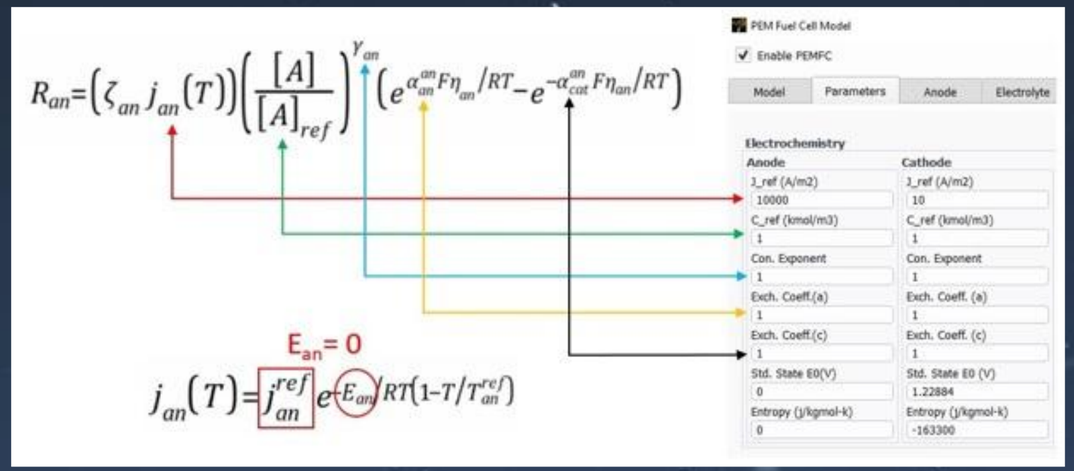
Disv'd-Vap./Liq. Source: 0.2

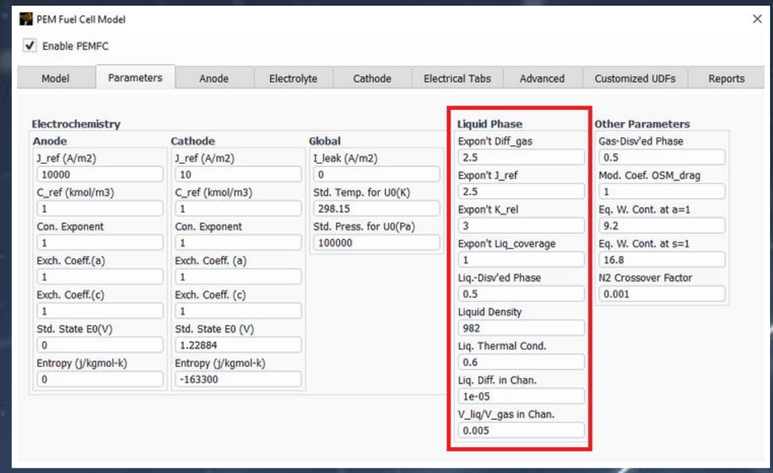
Osmotic Drag Source: 1

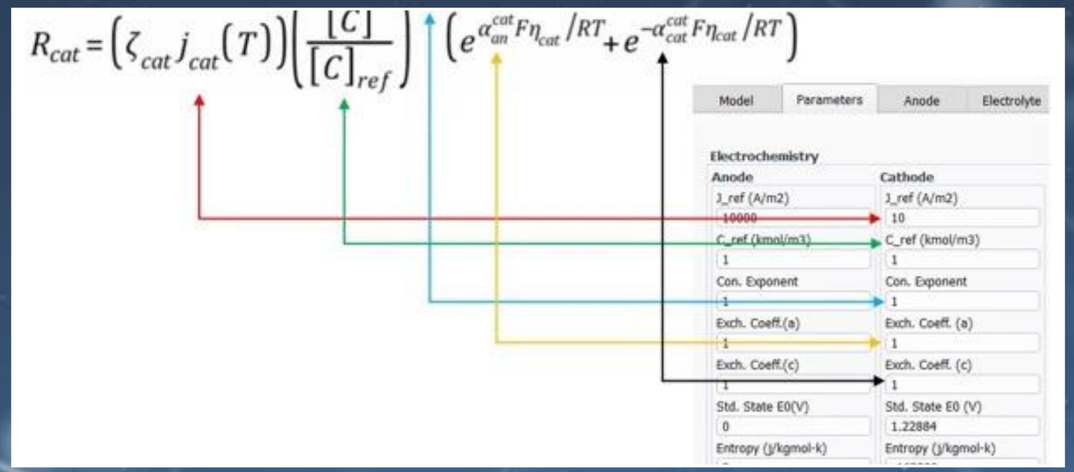
GDL Liquid Removal: 0.5

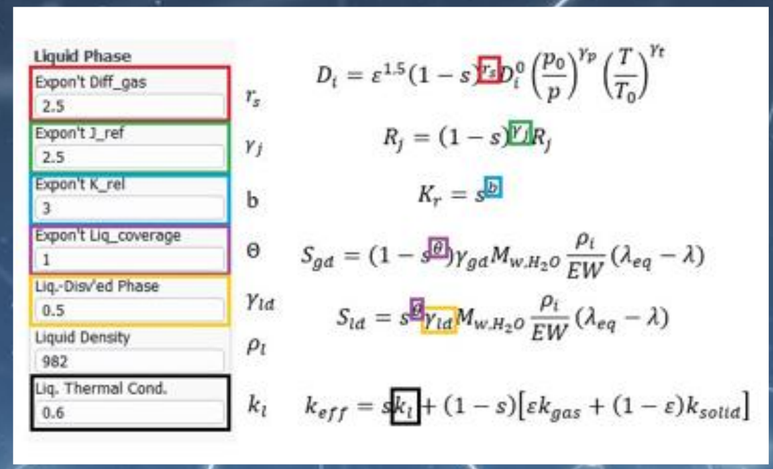
OK | Apply | Reset | Cancel | Help

# CFD model – equations of state



# CFD model – Input parameters



| 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 | $\zeta$ | 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 | $\theta_c$ | ° | 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 $J_{\mathrm{ref}}$ | $E_i$ | J/kmol | 5E+06, 8.314E+06, 1.2E+07 |
| 5 | Concentration exponent (anode) | $\gamma_{\mathrm{an}}$ | – | 0.3, 0.65, 1.0 | 43 | CL (anode) reference temperature for $J_{\mathrm{ref}}$ | $T_{0,\mathrm{an}}$ | K | 338 |
| 6 | Concentration exponent (cathode) | $\gamma_{\mathrm{cat}}$ | – | 0.3, 0.65, 1.0 | 44 | CL (anode) Leverett coeff. a | $a$ | – | 1.417 |
| 7 | Transfer coefficient (anode) | $\alpha_{\mathrm{an}}$ | – | 0.3, 0.65, 1.0 | 45 | CL (anode) Leverett coeff. b | $b$ | – | 2.12 |
| 8 | Transfer coefficient (anode) | $\alpha_{\mathrm{an}}$ | – | 0.3, 0.65, 1.0 | 46 | CL (anode) Leverett coeff. c | $c$ | – | 1.263 |
| 9 | Transfer coefficient (cathode) | $\alpha_{\mathrm{cat}}$ | – | 0.3, 0.65, 1.0 | 47 | CL (anode) condensation coeff. | $\gamma_c$ | – | 1E+06, 1E+08, 1E+10 |
| 10 | Transfer coefficient (cathode) | $\alpha_{\mathrm{cat}}$ | – | 0.3, 0.65, 1.0 | 48 | CL (anode) evaporation coeff. | $\gamma_e$ | – | 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. | $\beta_{mem}$ | – | 0.5, 1, 2 |
| 13 | Entropy (anode) | $\Delta S_{\mathrm{an}}$ | J/kmolK | -130000 | 51 | Membrane protonic conduction exponent | $\omega_i$ | – | 0.5, 1, 2 |
| 14 | Entropy (cathode) | $\Delta S_{\mathrm{cat}}$ | J/kmolK | -32660 | 52 | Membrane water diffusivity coeff. | $\eta_\lambda$ | – | 0.1, 1, 2 |
| 15 | Leakage current density | $I_{\mathrm{leak}}$ | 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 | $\epsilon$ | – | 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 | $\theta_c$ | ° | 90, 110, 135 |
| 19 | Exponent $J_{\mathrm{ref}}$ | $\gamma_j$ | – | 1.5, 2.5, 3.5 | 57 | GDL (cathode) water removal coef. | $\Theta$ | 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 | $\theta$ | – | 0.2, 1, 1.8 | 59 | GDL (cathode) Leverett coeff. b | $b$ | – | 2.12 |
| 22 | Liq.-Dissolved Phase | $\gamma_{ld}$ | – | 0.25, 0.5, 1, 1.5 | 60 | GDL (cathode) Leverett coeff. c | $c$ | – | 1.263 |
| 23 | Liquid density | $\rho_l$ | kg/m$^3$ | 982 | 61 | GDL (cathode) condensation coeff. | $\gamma_c$ | – | 1E+06, 1E+08, 1E+10 |
| 24 | Liquid thermal conductivity | $k_l$ | W/mK | 0.6 | 62 | GDL (cathode) evaporation coeff. | $\gamma_e$ | – | 1E+06, 1E+08, 1E+10 |
| 25 | Gas-dissolved Phase | $\gamma_{gd}$ | – | 0.25, 0.5, 0.75 | 63 | CL (cathode) porosity | $\epsilon$ | – | 0.4, 0.75, 0.9 |
| 26 | Osmotic drag coefficient | $\eta_{osm}$ | – | 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 | $\lambda_a$ | – | 9.2 | 65 | CL (cathode) surface/volume ratio | $\zeta$ | 1/m | 10000, 200000, 1000000 |
| 28 | Eq. water content at s=1 | $\lambda_s$ | – | 16.8 | 66 | CL (cathode) hydrophobic contact angle | $\theta_c$ | ° | 90, 110, 135 |
| 29 | GDL (anode) porosity | $\epsilon$ | – | 0.4, 0.75, 0.9 | 67 | CL (cathode) activation energy for $J_{\mathrm{ref}}$ | $E_i$ | 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 $J_{\mathrm{ref}}$ | $T_{0,\mathrm{cat}}$ | K | 343 |
| 31 | GDL (anode) hydrophobic contact angle | $\theta_c$ | ° | 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. | $\Theta$ | 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. | $\gamma_c$ | – | 1E+06, 1E+08, 1E+10 | 74 | CL (cathode) Leverett coeff. c | $c$ | – | 1.263 |
| 37 | GDL (anode) evaporation coeff. | $\gamma_e$ | – | 1E+06, 1E+08, 1E+10 | 75 | CL (cathode) condensation coeff. | $\gamma_c$ | – | 1E+06, 1E+08, 1E+10 |
| 38 | CL (anode) porosity | $\epsilon$ | – | 0.4, 0.75, 0.9 | 76 | CL (cathode) evaporation coeff. | $\gamma_e$ | – | 1E+06, 1E+08, 1E+10 |
| | | | | | 77 | Coolant density | $\rho_c$ | kg/m$^3$ | 998.2 |

| 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) | $\gamma_{\mathrm{an}}$ | – | 0.3, 0.65, 1.0 |
| 6 | Concentration exponent (cathode) | $\gamma_{\mathrm{cat}}$ | – | 0.3, 0.65, 1.0 |
| 7 | Transport coefficient (anode) | $\alpha_{\mathrm{anode}}$ | – | 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: $J_{\mathrm{ref}}$ | $\gamma_j$ | – | 1.5, 2.5, 3.5 |
| 11 | Exponent: relative permeability | $b$ | – | 2, 3, 4 |
| 12 | Exponent: liquid coverage | $\theta$ | – | 0.2, 1, 1.8 |
| 13 | Exponent: liquid–dissolved phase | $\gamma_{ld}$ | – | 0.25, 0.5, 1, 1.5 |
| 14 | Exponent: gas–dissolved phase | $\gamma_{gd}$ | – | 0.25, 0.5, 0.75 |
| 15 | Osmotic drag coefficient | $\eta_{osm}$ | – | 0.5, 1, 1.5 |
| 16 | GDL/CL porosity | $\varepsilon$ | – | 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 | $\theta_c$ | ° | 90, 110, 135 |
| 19 | Water removal coefficient (GDL/CL) | $\Theta$ | s/m | 1E-05, 5E-05, 1E-04 |
| 20 | Condensation rate coefficient (GDL/CL) | $\gamma_c$ | – | 1E+06, 1E+08, 1E+10 |
| 21 | Evaporation rate coefficient (GDL/CL) | $\gamma_e$ | – | 1E+06, 1E+08, 1E+10 |
| 22 | Catalyst layer surface-to-volume ratio (anode) | $\zeta$ | 1/m | 10000, 200000, 1000000 |
| 23 | Activation energy for $J_{\mathrm{ref}}$ | $E_i$ | 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 | $\beta_{\mathrm{mem}}$ | – | 0.5, 1, 2 |
| 26 | Membrane protonic conduction exponent | $\omega_i$ | – | 0.5, 1, 2 |
| 27 | Membrane water diffusivity coefficient | $\eta_\lambda$ | – | 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 | $R_{\mathrm{ion}}$ | s/m | 50, 100, 300 |

Variable

| 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) | $\Delta S_{\mathrm{an}}$ | J/kmolK | -130000 |
| 4 | Entropy (cathode) | $\Delta S_{\mathrm{cat}}$ | J/kmolK | -32660 |
| 5 | Leakage current density | $I_{\mathrm{leak}}$ | A/m$^2$ | 0 |
| 6 | Standard temperature | $T_0$ | K | 298.15 |
| 7 | Standard pressure | $p_0$ | Pa | 101325 |
| 8 | Liquid density | $\rho_l$ | kg/m$^3$ | 982 |
| 9 | Liquid thermal conductivity | $k_l$ | W/mK | 0.6 |
| 10 | Eq. water content at a = 1 | $\lambda_a$ | – | 9.2 |
| 11 | Eq. water content at s = 1 | $\lambda_s$ | – | 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 $J_{\mathrm{ref}}$ | $T_{0,\mathrm{an}}$ | 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 $J_{\mathrm{ref}}$ | $T_{0,\mathrm{cat}}$ | 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 | $\rho_c$ | kg/m$^3$ | 998.2 |

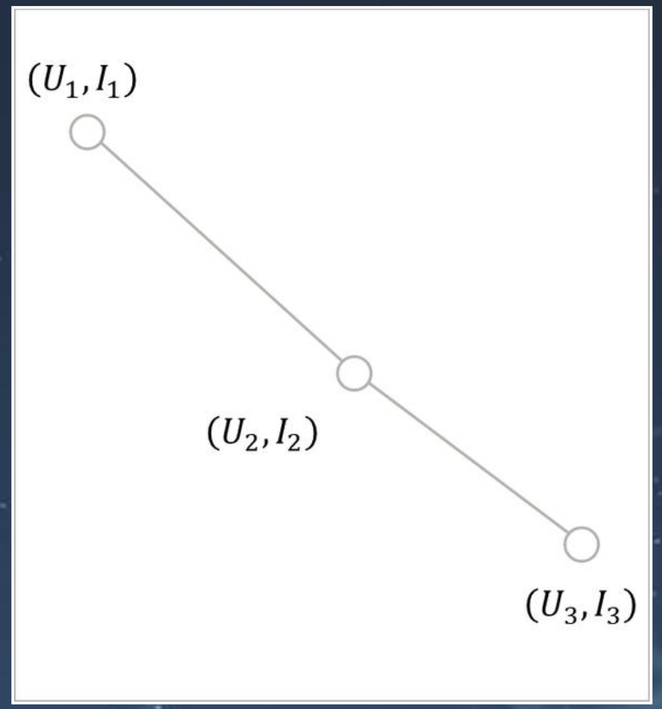
Fixed

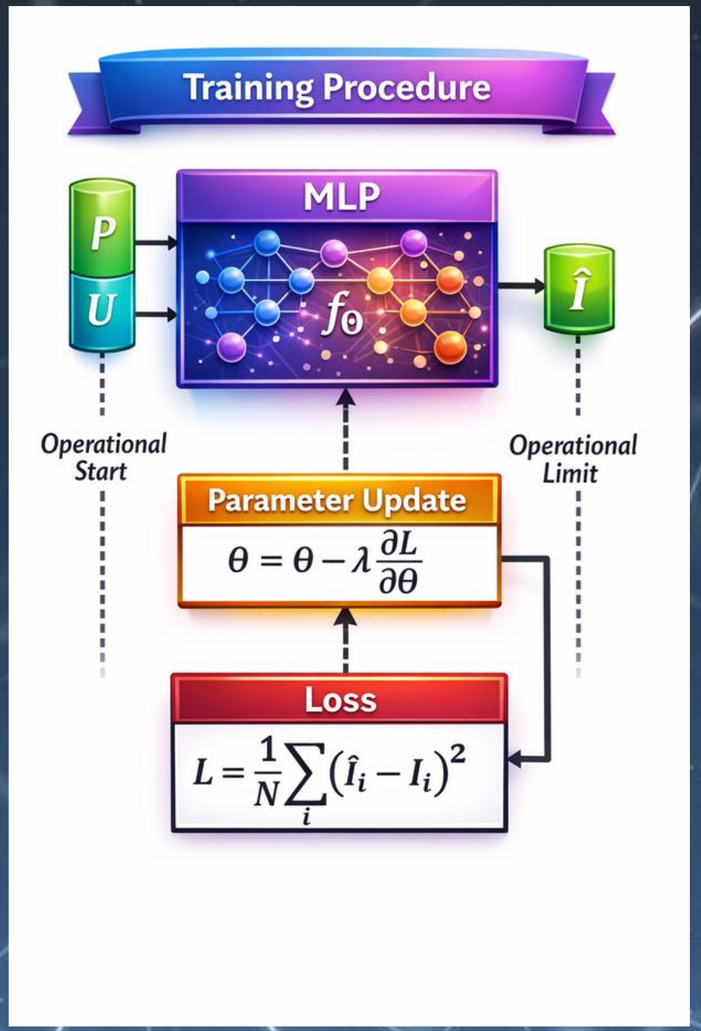
# Surrogate model of membrane

# AI model Problem description

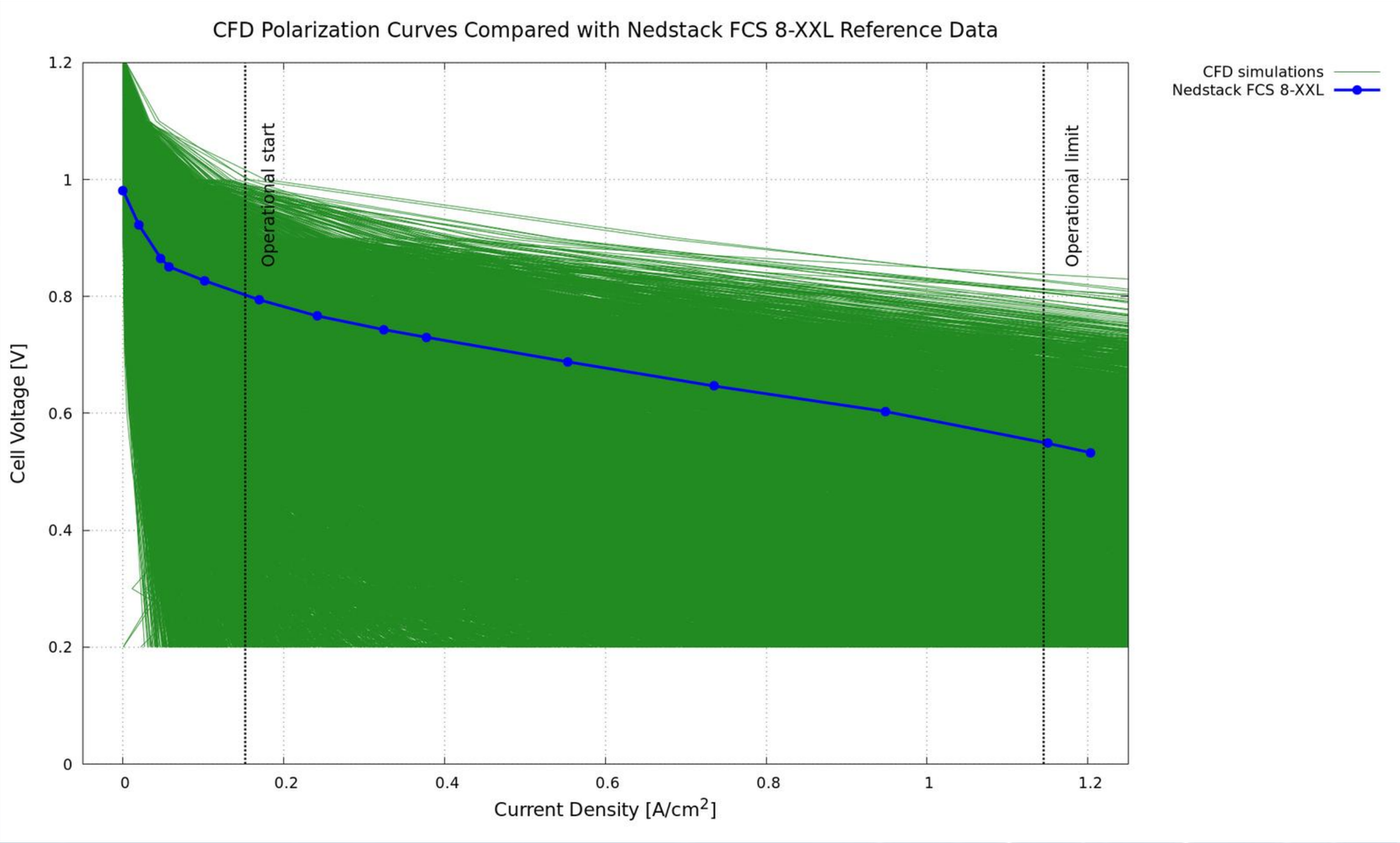
Find the set of parameters P corresponding to the volt-ampere characteristic.

{(Uj, Ij)}
for j∈{1, 2, 3}.

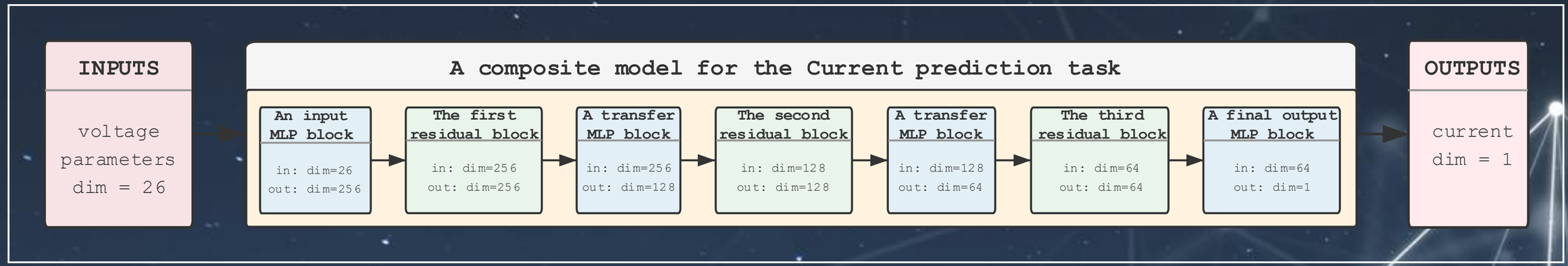


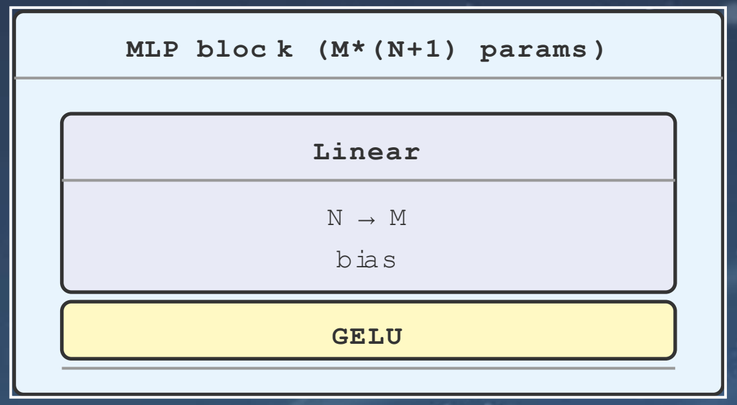



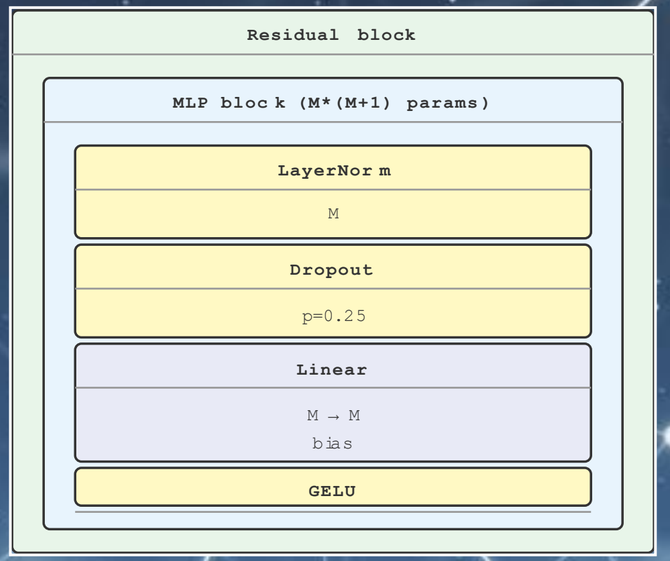
# CFD results: Polarization curves



# AI model architecture



# AI model Inference



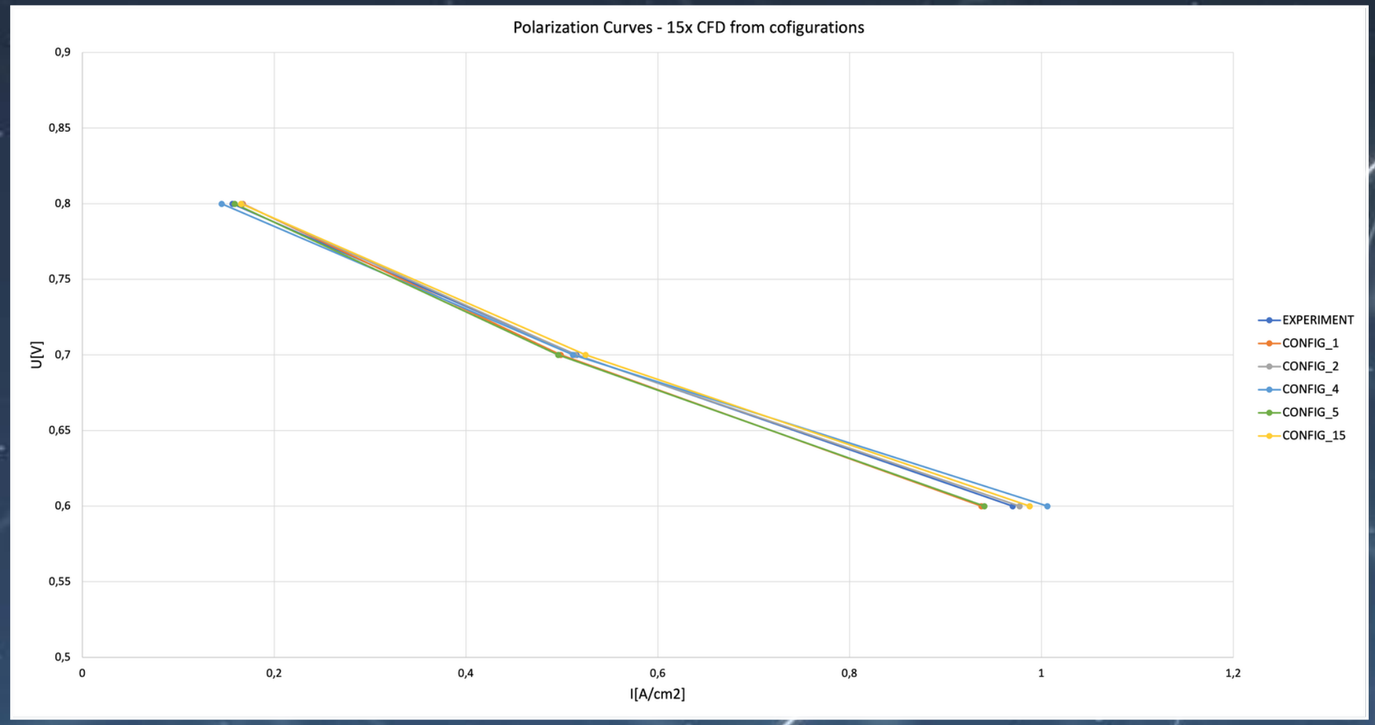
- Random initialisation of parameters P (50 configurations)
- Gradient optimisation method (Adam: learning rate 1e-3)
- Selected 15 best predictions
- Verification by CFD simulation (ANSYS)
  - 2 divergent configurations
  - 2 non-acceptable configurations
  - 3 acceptable configurations (difference < 3%)

# CFD simulation: Validation

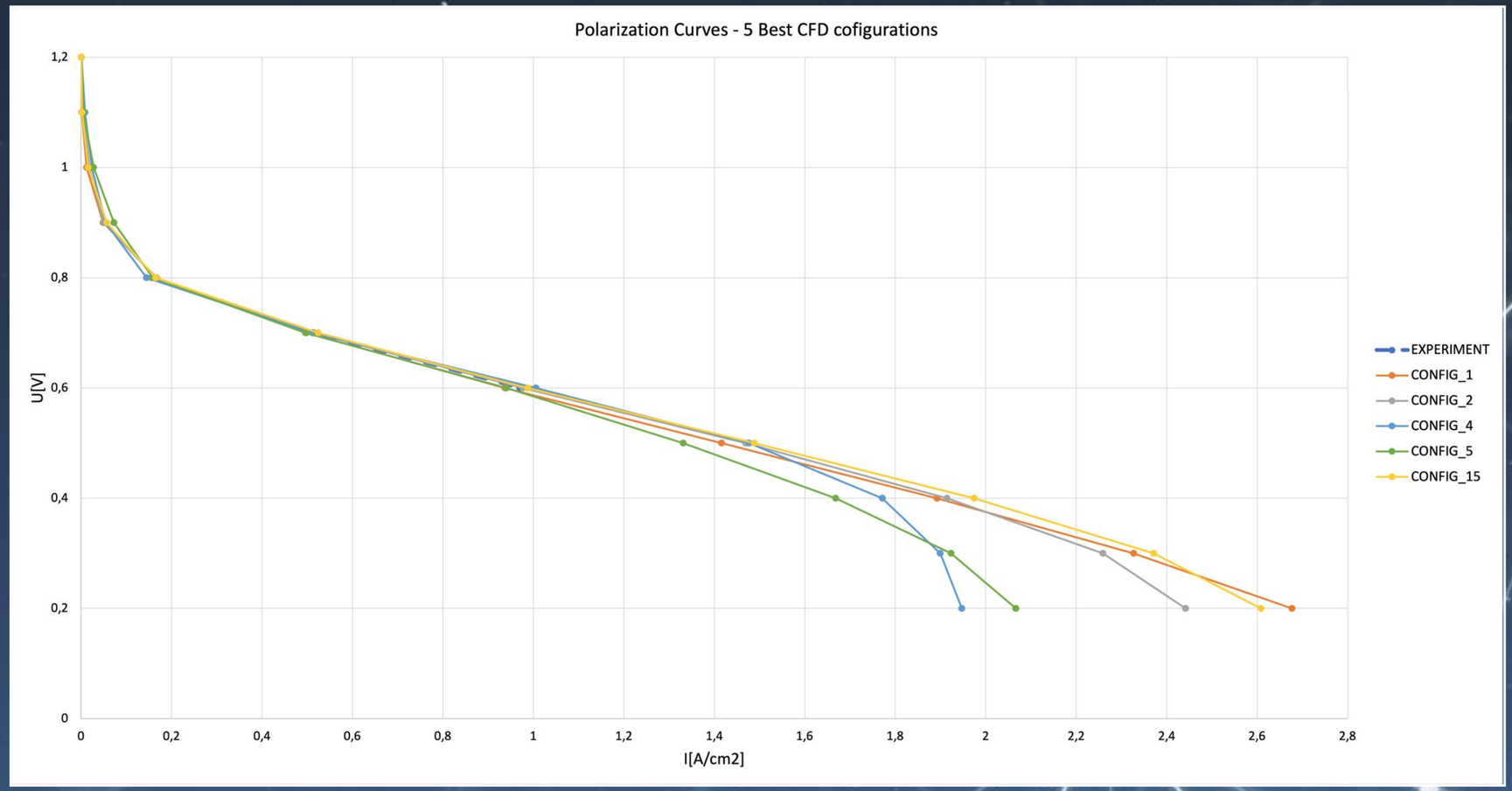
| RANK | CONFIGURATION | ERROR[%] |
|---|---|---|
| 1 | CONFIG_2 | 2,37 |
| 2 | CONFIG_5 | 2,74 |
| 3 | CONFIG_15 | 3,12 |
| 4 | CONFIG_4 | 3,88 |
| 5 | CONFIG_1 | 4,46 |
| 6 | CONFIG_8 | 5,11 |
| 7 | CONFIG_14 | 5,29 |
| 8 | CONFIG_11 | 5,90 |
| 9 | CONFIG_7 | 5,95 |
| 10 | CONFIG_13 | 8,01 |
| 11 | CONFIG_9 | 12,25 |
| 12 | CONFIG_12 | 43,98 |
| 13 | CONFIG_3 | 52,70 |
| 14 | CONFIG_10 | 53,96 |
| 15 | CONFIG_6 | 105,91 |

DIVERGENT SOLUTION

| RANK | CONFIGURATION | ERROR[%] |
|---|---|---|
| 12 | CONFIG_12 | 43,98 |
| 15 | CONFIG_6 | 105,91 |



# CFD simulation: Validation



REFRESH

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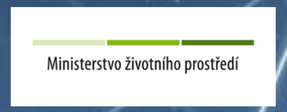


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