

# Fuel cell system fundamentals

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# Agenda

- Basic introduction to different fuel cell technologies
- Describe main components of a Galvani and Electrolytic cell
- Basic fuel cell thermodynamics and performance
- Describe main voltage losses affecting the fuel cell

## Good references:

- Fuel cell handbook <https://www.netl.doe.gov/sites/default/files/netl-file/FCHandbook7.pdf>
- Fuel cell fundamentals by Ryan O'Hayre, Suk-Won Cha, Whitney Colella, and Fritz B. Prinz



# Chemical reaction vs electrochemical reaction

- A chemical reaction is a process in which reactants rearrange in the products
- Electrochemical reaction is characterized by a transfer of electrons, in other words, some substances will gain electrons and some will lose them. This class of reactions it is also called redox.

- **Oxidation**

It is called Oxidation because the reactant loses electrons



- **Reduction**

In a reduction process the reactants acquire an electron



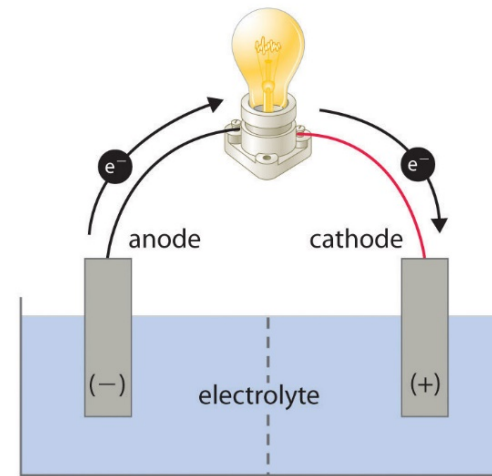
# Galvanic Cells: A simple fuel cell

- A **galvanic cell** (or voltaic cell) transforms the energy in the reactants generating an electrical current or *electromotive force*
- The **electrolytic cell** convert the electrical current into chemical energy (i.e. gasses)
- In both cases there is a redox reaction involved, however it operates in the opposite direction.

- A cell consists of:

2 electrodes: they collect the electrons

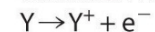
Electrolyte: it transport charges (protons; anions)



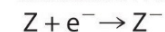
**GALVANIC CELL**

Energy released by spontaneous redox reaction is converted to electrical energy.

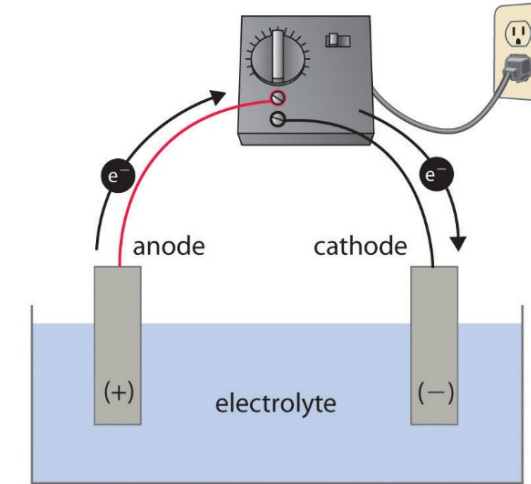
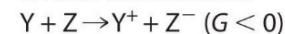
Oxidation half-reaction:



Reduction half-reaction:



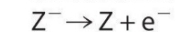
Overall cell reaction:



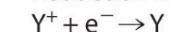
**ELECTROLYTIC CELL**

Electrical energy is used to drive nonspontaneous redox reaction.

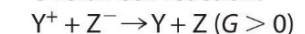
Oxidation half-reaction:



Reduction half-reaction:



Overall cell reaction:

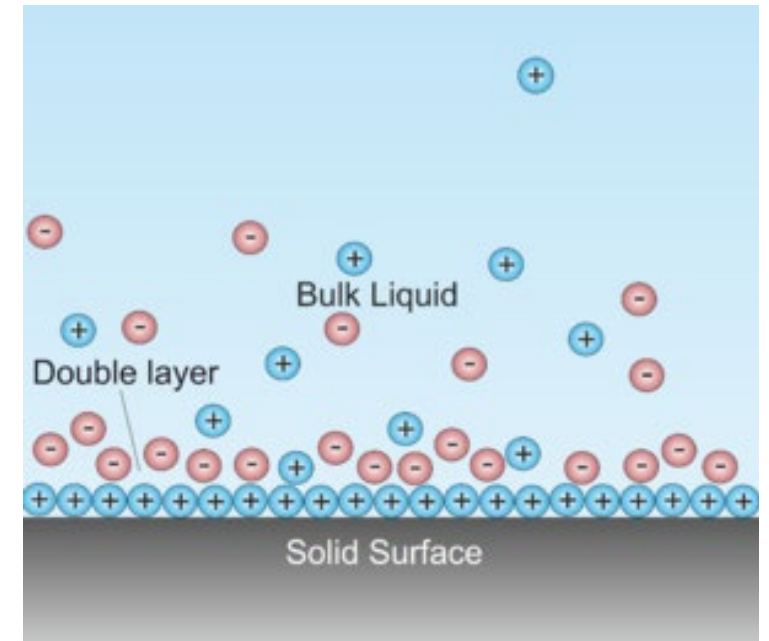


[https://chem.libretexts.org/Core/Analytical\\_Chemistry/Electrochemistry/Electrolytic\\_Cells](https://chem.libretexts.org/Core/Analytical_Chemistry/Electrochemistry/Electrolytic_Cells)



# Electric double layer

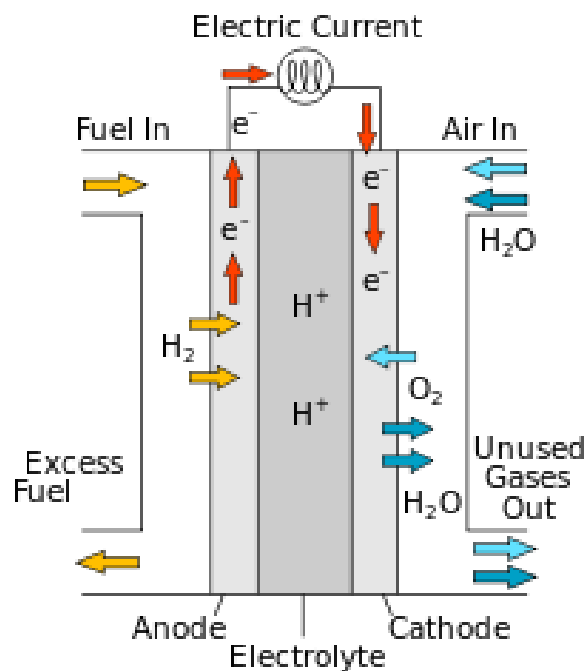
- A phenomena that happen at the **electrode/electrolyte interface**
- Transition region between 2 phases in which there is an **imbalance of charges which strongly interact.**
- It is the area of the electrode where electrochemical reaction occurs like for instance a metal immersed in a solution. It will be a thin layer between the metal and the solution.
- We should remind that in nature a **bulk is characterized by neutral charged unless electrically perturbed**



SOURCE: Wikipedia Larryisgood



# Fuel cell basic configuration



What will be the overall cell potential?

Table 3.1: Standard Electrode Potentials at 298 K

Ions are present as aqueous species and H<sub>2</sub>O as liquid; gases and solids are shown by g and

Reaction (Oxidised form + n e <sup>-</sup> )	→ Reduced form	E <sup>0</sup> /V
F <sub>2</sub> (g) + 2e <sup>-</sup>	→ 2F <sup>-</sup>	2.87
Co <sup>3+</sup> + e <sup>-</sup>	→ Co <sup>2+</sup>	1.81
H <sub>2</sub> O <sub>2</sub> + 2H <sup>+</sup> + 2e <sup>-</sup>	→ 2H <sub>2</sub> O	1.78
MnO <sub>4</sub> <sup>-</sup> + 8H <sup>+</sup> + 5e <sup>-</sup>	→ Mn <sup>2+</sup> + 4H <sub>2</sub> O	1.51
Au <sup>3+</sup> + 3e <sup>-</sup>	→ Au(s)	1.40
Cl <sub>2</sub> (g) + 2e <sup>-</sup>	→ 2Cl <sup>-</sup>	1.36
Cr <sub>2</sub> O <sub>7</sub> <sup>2-</sup> + 14H <sup>+</sup> + 6e <sup>-</sup>	→ 2Cr <sup>3+</sup> + 7H <sub>2</sub> O	1.33
O <sub>2</sub> (g) + 4H <sup>+</sup> + 4e <sup>-</sup>	→ 2H <sub>2</sub> O	1.23
MnO <sub>2</sub> (s) + 4H <sup>+</sup> + 2e <sup>-</sup>	→ Mn <sup>2+</sup> + 2H <sub>2</sub> O	1.23
Br <sub>2</sub> + 2e <sup>-</sup>	→ 2Br <sup>-</sup>	1.09
NO <sub>3</sub> <sup>-</sup> + 4H <sup>+</sup> + 3e <sup>-</sup>	→ NO(g) + 2H <sub>2</sub> O	0.97
2Hg <sup>2+</sup> + 2e <sup>-</sup>	→ Hg <sub>2</sub> <sup>2+</sup>	0.92
Ag <sup>+</sup> + e <sup>-</sup>	→ Ag(s)	0.80
Fe <sup>3+</sup> + e <sup>-</sup>	→ Fe <sup>2+</sup>	0.77
O <sub>2</sub> (g) + 2H <sup>+</sup> + 2e <sup>-</sup>	→ H <sub>2</sub> O <sub>2</sub>	0.68
I <sub>2</sub> + 2e <sup>-</sup>	→ 2I <sup>-</sup>	0.54
Cu <sup>+</sup> + e <sup>-</sup>	→ Cu(s)	0.52
Cu <sup>2+</sup> + 2e <sup>-</sup>	→ Cu(s)	0.34
AgCl(s) + e <sup>-</sup>	→ Ag(s) + Cl <sup>-</sup>	0.22
AgBr(s) + e <sup>-</sup>	→ Ag(s) + Br <sup>-</sup>	0.10
2H <sup>+</sup> + 2e <sup>-</sup>	→ H <sub>2</sub> (g)	0.00
Pb <sup>2+</sup> + 2e <sup>-</sup>	→ Pb(s)	-0.13
Sn <sup>2+</sup> + 2e <sup>-</sup>	→ Sn(s)	-0.14
Ni <sup>2+</sup> + 2e <sup>-</sup>	→ Ni(s)	-0.25
Fe <sup>2+</sup> + 2e <sup>-</sup>	→ Fe(s)	-0.44
Cr <sup>3+</sup> + 3e <sup>-</sup>	→ Cr(s)	-0.74
Zn <sup>2+</sup> + 2e <sup>-</sup>	→ Zn(s)	-0.76
2H <sub>2</sub> O + 2e <sup>-</sup>	→ H <sub>2</sub> (g) + 2OH <sup>-</sup> (aq)	-0.83
Al <sup>3+</sup> + 3e <sup>-</sup>	→ Al(s)	-1.66
Mg <sup>2+</sup> + 2e <sup>-</sup>	→ Mg(s)	-2.36
Na <sup>+</sup> + e <sup>-</sup>	→ Na(s)	-2.71
Ca <sup>2+</sup> + 2e <sup>-</sup>	→ Ca(s)	-2.87
K <sup>+</sup> + e <sup>-</sup>	→ K(s)	-2.93
Li <sup>+</sup> + e <sup>-</sup>	→ Li(s)	-3.05

# Fuel cell types

Fuel cell are divided according to electrolyte material

Note the different ions crossing the electrolyte, different temperature of operations and material.

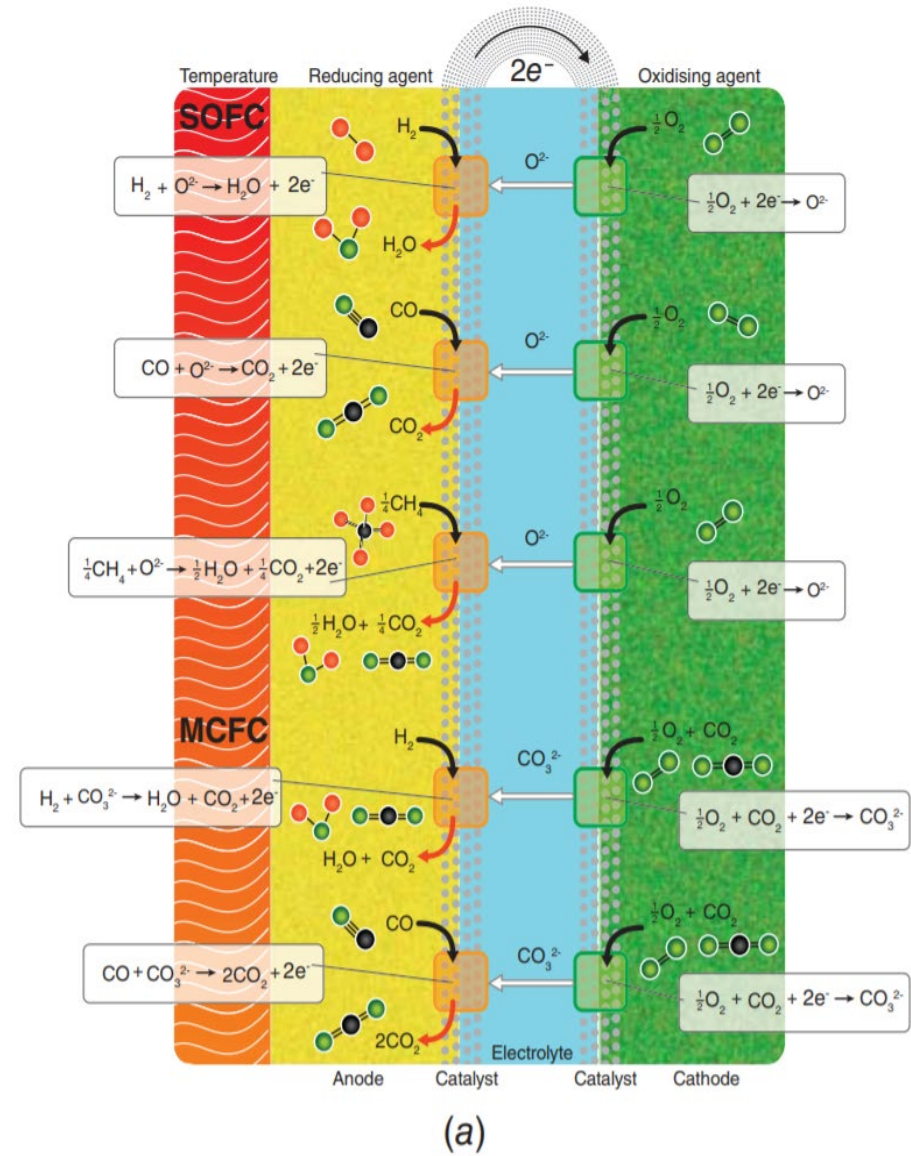
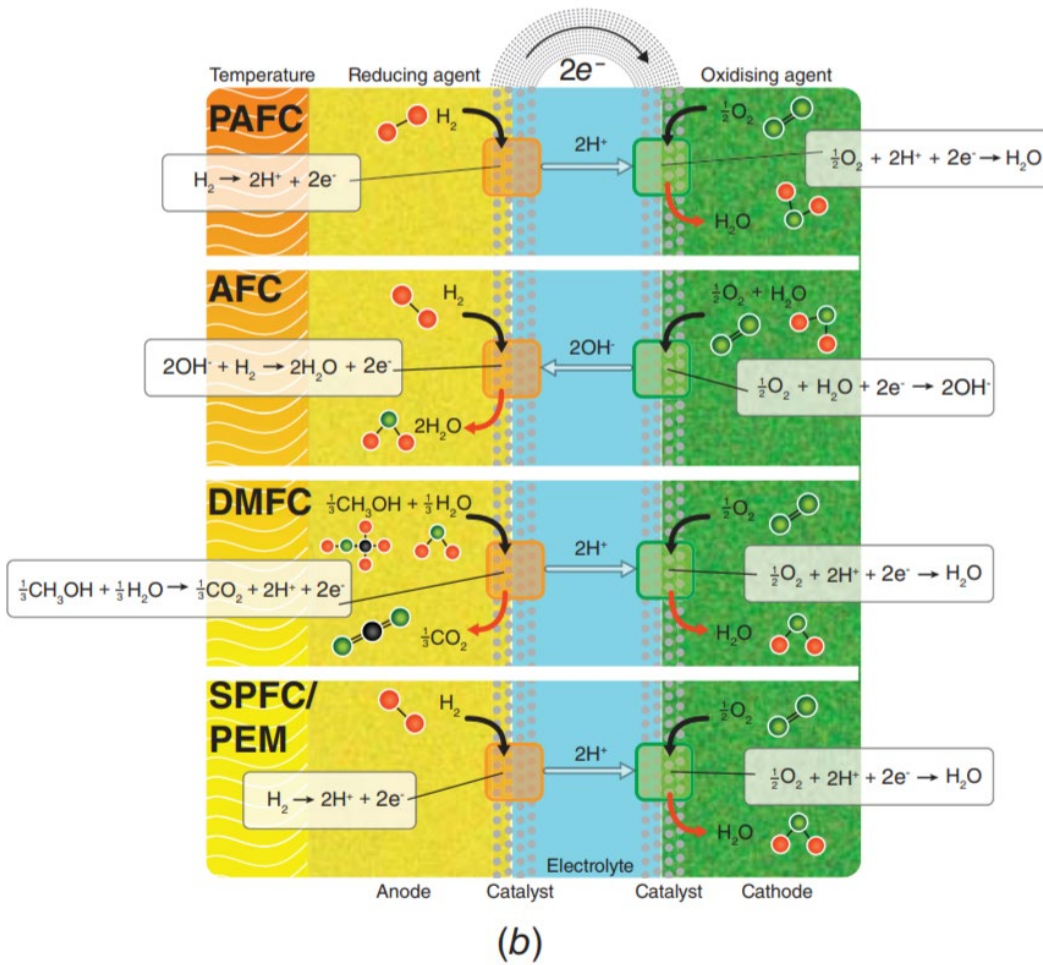
There are 5 main fuel cell types.

1. Phosphoric acid fuel cell (PAFC)
2. Polymer electrolyte membrane fuel cell (PEMFC)
3. Alkaline fuel cell (AFC)
4. Molten carbonate fuel cell (MCFC)
5. Solid-oxide fuel cell (SOFC)

PS the classification of FC is provided in Chapter 8 of Fuel cell fundamentals



# Classification of Fuel cells





# Summary of electrochemical reaction if different type of Fuel cell

## Comparison of Fuel Cell Technologies

Fuel Cell Type	Common Electrolyte	Operating Temperature	Typical Stack Size	Efficiency	Applications	Advantages	Disadvantages
Polymer Electrolyte Membrane (PEM)	Perfluoro sulfonic acid	50-100°C 122-212° typically 80°C	< 1kW-100kW	60% transportation 35% stationary	<ul style="list-style-type: none"> <li>Backup power</li> <li>Portable power</li> <li>Distributed generation</li> <li>Transportation</li> <li>Specialty vehicles</li> </ul>	<ul style="list-style-type: none"> <li>Solid electrolyte reduces corrosion &amp; electrolyte management problems</li> <li>Low temperature</li> <li>Quick start-up</li> </ul>	<ul style="list-style-type: none"> <li>Expensive catalysts</li> <li>Sensitive to fuel impurities</li> <li>Low temperature waste heat</li> </ul>
Alkaline (AFC)	Aqueous solution of potassium hydroxide soaked in a matrix	90-100°C 194-212°F	10-100 kW	60%	<ul style="list-style-type: none"> <li>Military</li> <li>Space</li> </ul>	<ul style="list-style-type: none"> <li>Cathode reaction faster in alkaline electrolyte, leads to high performance</li> <li>Low cost components</li> </ul>	<ul style="list-style-type: none"> <li>Sensitive to CO<sub>2</sub> in fuel and air</li> <li>Electrolyte management</li> </ul>
Phosphoric Acid (PAFC)	Phosphoric acid soaked in a matrix	150-200°C 302-392°F	400 kW 100 kW module	40%	<ul style="list-style-type: none"> <li>Distributed generation</li> </ul>	<ul style="list-style-type: none"> <li>Higher temperature enables CHP</li> <li>Increased tolerance to fuel impurities</li> </ul>	<ul style="list-style-type: none"> <li>Pt catalyst</li> <li>Long start up time</li> <li>Low current and power</li> </ul>
Molten Carbonate (MCFC)	Solution of lithium, sodium, and/or potassium carbonates, soaked in a matrix	600-700°C 1112-1292°F	300 kW-3 MW 300 kW module	45-50%	<ul style="list-style-type: none"> <li>Electric utility</li> <li>Distributed generation</li> </ul>	<ul style="list-style-type: none"> <li>High efficiency</li> <li>Fuel flexibility</li> <li>Can use a variety of catalysts</li> <li>Suitable for CHP</li> </ul>	<ul style="list-style-type: none"> <li>High temperature corrosion and breakdown of cell components</li> <li>Long start up time</li> <li>Low power density</li> </ul>
Solid Oxide (SOFC)	Yttria stabilized zirconia	700-1000°C 1202-1832°F	1 kW-2 MW	60%	<ul style="list-style-type: none"> <li>Auxiliary power</li> <li>Electric utility</li> <li>Distributed generation</li> </ul>	<ul style="list-style-type: none"> <li>High efficiency</li> <li>Fuel flexibility</li> <li>Can use a variety of catalysts</li> <li>Solid electrolyte</li> <li>Suitable for CHP &amp; CHHP</li> <li>Hybrid/GT cycle</li> </ul>	<ul style="list-style-type: none"> <li>High temperature corrosion and breakdown of cell components</li> <li>High temperature operation requires long start up time and limits</li> </ul>

### For More Information

More information on the Fuel Cell Technologies Program is available at <http://www.hydrogenandfuelcells.energy.gov>.



- The table from the US department of Energy provide a comparison between different type of fuel cells

# Stationary Fuel Cell Power Systems



**Fuel Cell Energy  
2 MW MCFC**



**Plug Power 7kW  
Residential PEFC**



**Siemens-Westinghouse  
100kW SOFC**



**UTC Fuel Cells  
200kW PAFC**



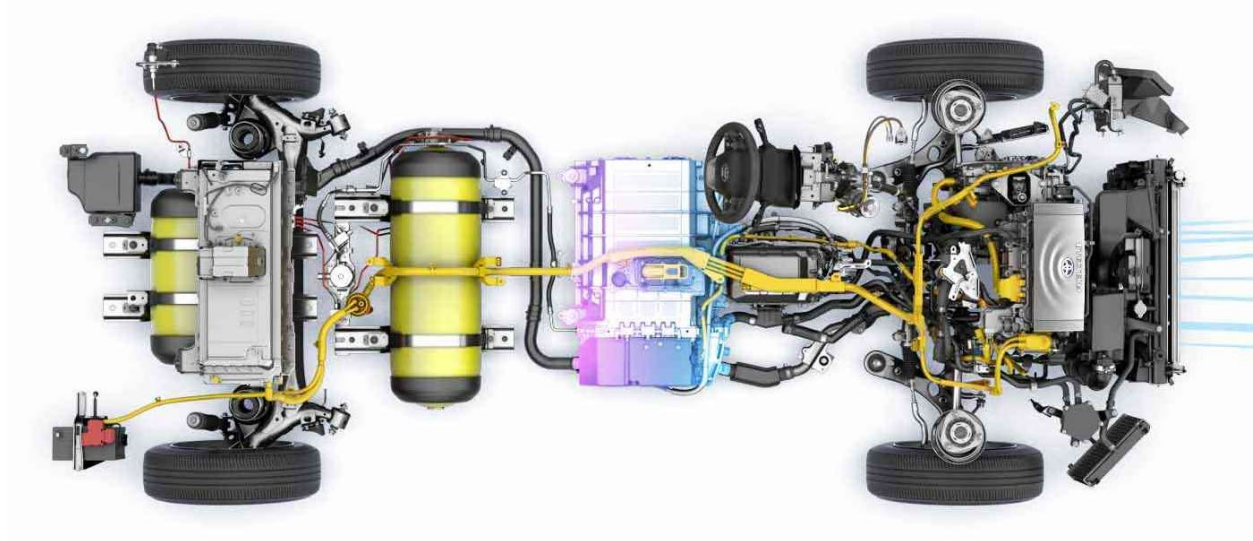
**Ballard 250kW  
PEFC**



**Plug Power 10 kW  
Residential unit**



# Fuel cell system In the car



# Fuel cell system In the car

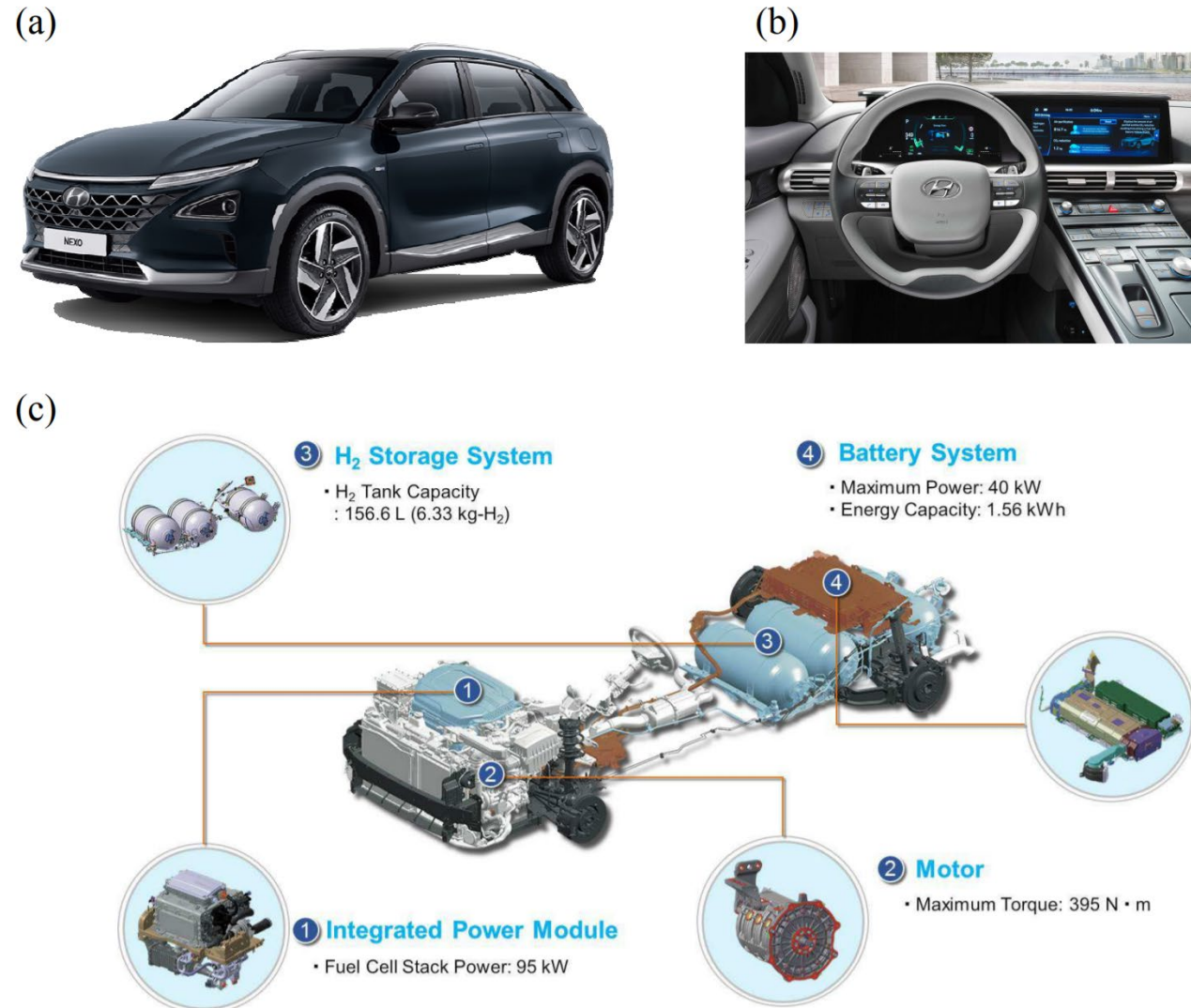
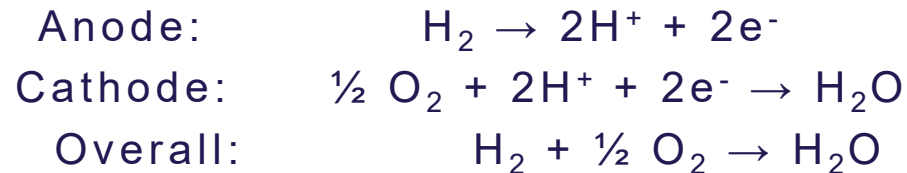


Figure 3. An overview of the Nexo FCEV: (a) exterior; (b) interior; (c) vehicle layout.



# Gibbs free energy and voltage

The FC reactions are:



The standard free energy of an electrochemical reaction

$$\Delta G = -nFE = 2 \text{ mol e}^-/\text{mol reactant} * 96485 \text{ C/mol} * 1.23 \text{ V} = -237000 \text{ J/mol}$$

$E$ : Reversible potential at equilibrium or ideal potential 1.23V

$F$ : Faraday constant(i.e. magnitude of the electric charge for moles of electrons)

$n$ : nr of electrons exchanged in the electrochemical reaction  $\text{H}_2 + \frac{1}{2} \text{O}_2 \rightarrow \text{H}_2\text{O}$



# Relationship between Gibbs Free energy and equilibrium

- For a general reaction  $aA + bB \rightarrow cC + dD$  the equilibrium constant is defined:

$$K = \frac{[C]^c [D]^d}{[A]^a [B]^b}$$

- Where A;B;C;D are the concentrations and a;b;c;d are the stoichiometric coefficient of the reaction
- The relationship between the eq constant and the Gibbs free energy of reaction is given below:

$$\Delta G = -RT \ln(K)$$



# Nernst Equation

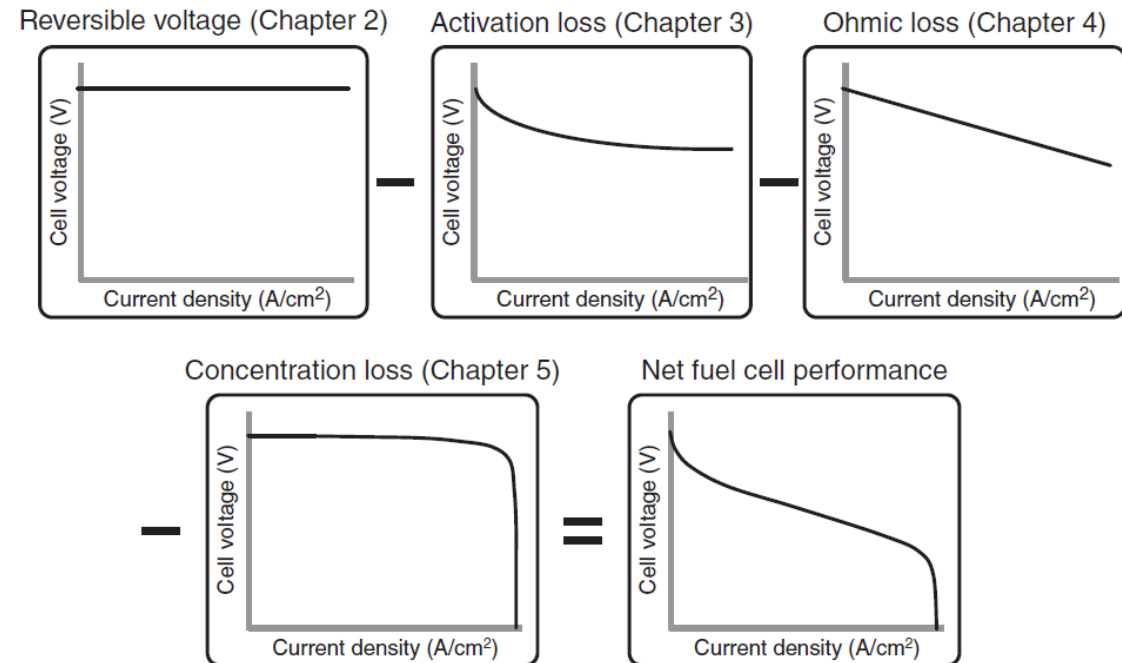
- The relationship accounts for the effect of pressure and temperature when calculating the cell electrical potential  $E$
- $E^\circ$  represents the ideal standard potential at standard condition
- If pressure and temperature of the reactants  $H_2$  and  $O_2$  is increased the equilibrium potential  $E$  will also increase.
- For a cell reaction  $H_2 + O_2 \rightarrow H_2O$  the Nernst eq is:

$$E = E^\circ + \frac{RT}{nF} \ln \left( \frac{P_{H_2} \cdot P_{O_2}^{1/2}}{P_{H_2O}} \right)$$



# Fuel cell performance

We can assume the fuel cell curve as the algebraic sum of the reversible cell voltage

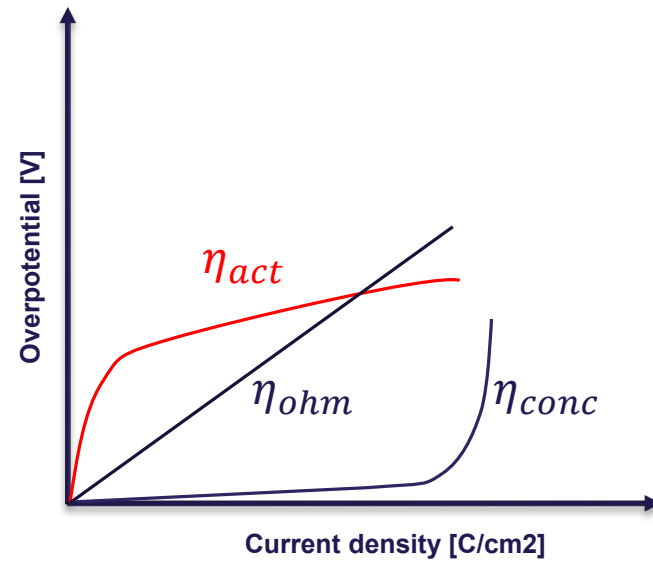


Fuel cell Fundamentals





# Activation overvoltage

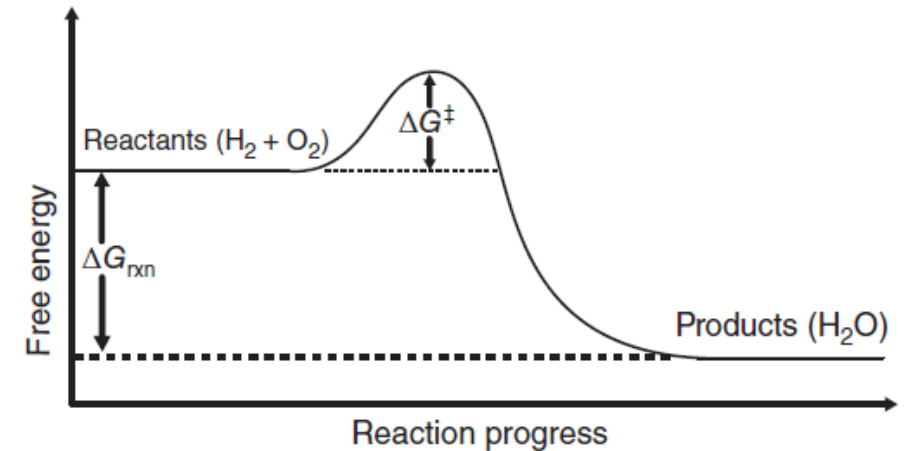


Can you come with an example of Activation energy?



# Rate of the electrochemical reaction

- Reactions happen spontaneously when the reactants free energy is larger than products free energy
- The activation energy is represented by the energy “barrier” that the reaction has to overcome to convert reactants into products.
- The activation energy limits the rate of reaction



Source: Fuel cell fundamentals Chapter 3



# Net rate of reaction

- In the **forward reaction**, hydrogen releases one electron the metal catalyst (i.e. platinum)
- In the **backward reaction**, the hydrogen ion gain an electron from the metal.
- At equilibrium both this reactions must balance; although both reactions are taking place the net rate is 0

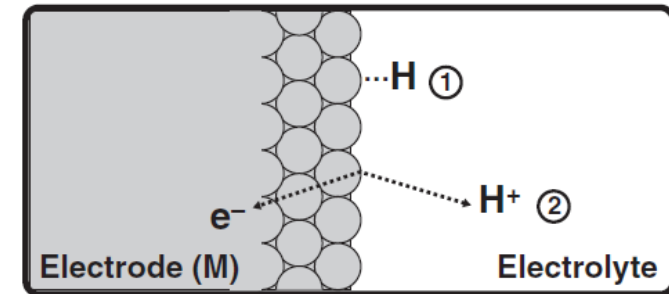
$$J = C_R^* f_1 e^{-\Delta G_1/RT} - C_P^* f_2 e^{-\Delta G_2/RT}$$

Forward reaction
Backward reaction

J: net reaction rate

C\_R/P: reactant/product surface concentration

f\_1/2: decay rate to product/reactant (i.e. likelihood that the reaction will convert to product/reactant)



**Figure 3.4.** Schematic of chemisorbed hydrogen charge transfer reaction. The reactant state, a chemisorbed hydrogen atom ( $M \cdots H$ ), is shown at 1. Completion of the charge transfer reaction, as shown at 2, liberates a free electron into the metal and a free proton into the electrolyte ( $(M + e^-) + H^+$ ).



Chemisorbed  
Hydrogen

Source: Fuel cell fundamentals Chapter 3



# Net rate of reaction

- We can restate the rate of reaction as a function of  $\Delta G$  of reaction

$$J = \underbrace{C_R^* f_1 e^{-\Delta G_1/RT}}_{\text{Forward reaction}} - \underbrace{C_P^* f_2 e^{-\Delta G_2/RT}}_{\text{Backward reaction}}$$

- The activation barrier for the overall reaction can be calculated as the difference between the activation barrier for forward and backward reaction.

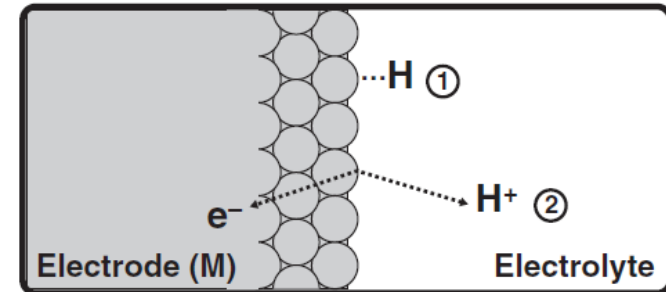
$$\Delta G_{react} = \Delta G_1 - \Delta G_2$$

- Therefore  $\Delta G_2$  can be expressed as a function of  $\Delta G_{react}$  and  $\Delta G_1$

$$J = C_R^* f_1 e^{-\Delta G_1/RT} - C_P^* f_2 e^{-(\Delta G_{react} - \Delta G_1)/RT}$$

- At equilibrium the reaction rate of reaction is 0

$$J = 0$$



**Figure 3.4.** Schematic of chemisorbed hydrogen charge transfer reaction. The reactant state, a chemisorbed hydrogen atom ( $M \cdots H$ ), is shown at 1. Completion of the charge transfer reaction, as shown at 2, liberates a free electron into the metal and a free proton into the electrolyte ( $(M + e^-) + H^+$ ).



Chemisorbed  
Hydrogen

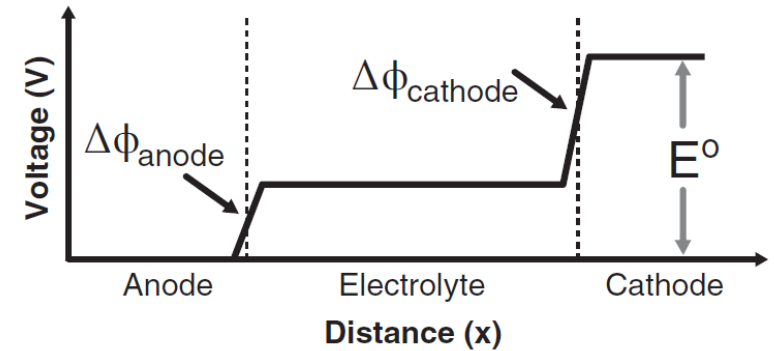
Source: Fuel cell fundamentals Chapter 3



# Potential of reaction at equilibrium in a fuel cell

- In a fuel cell we have 2 electrodes, electrochemical reactions occurs both at anode and cathode, hence generating 2 electrical potentials.
- The overall cell voltage,  $E^0$ , will be the sum of the 2 electrode potentials.

$$E^0 = \Delta\phi_{Anode} + \Delta\phi_{Cathode}$$



# Butler Volmer equation

- Current density and reaction rate are related by the relationship:

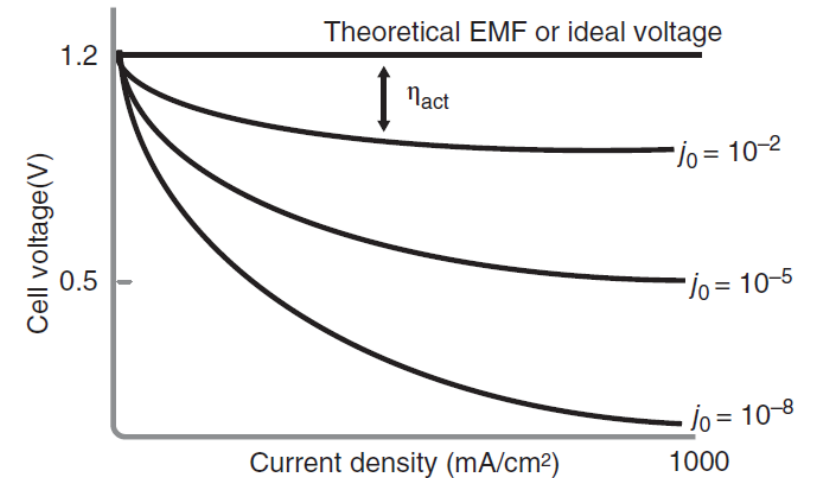
$$j = nFJ$$

Lower case    Capital case

- The current density is defined as (Butler Volmer eq.):

$$j = j_0 \left( \frac{C_R^*}{C_R^{0*}} e^{\alpha n F \eta / (RT)} - \frac{C_P^*}{C_P^{0*}} e^{-(1-\alpha) n F \eta / (RT)} \right)$$

- $\eta$ : activation voltage loss
  - $n$ : number of electron transferred by the electrochemical reaction
  - $\alpha$ : charge transfer coefficient (proportional to the energy “barrier”)
  - $C_R^*$ ,  $C_P^*$ : actual reactant and product concentration
  - $C_R^{0*}$ ,  $C_P^{0*}$ : reference reactant and product concentration
  - $j_0$ : reference current density
- Current density increases exponentially with activation overvoltage



Source: Fuel cell fundamentals Chapter 3



# Butler Volmer equation

- Based on this equation we can say that there are different ways increase cell performance.
  - Increase reactant concentration (e.g. increase reactant flow rate and pressure)
  - Reduce the activation barrier (e.g. better catalyst material)
  - Increase temperature ( i.e. higher temperature will cause a larger moments in the gas and a higher probability to engage in reactions )
  - Increase the reaction sites ( i.e. more sites available for electrochemical reactions)

$$j = j_0 \left( \frac{C_R^*}{C_R^{0*}} e^{\alpha n F \eta / (RT)} - \frac{C_P^*}{C_P^{0*}} e^{-(1-\alpha) n F \eta / (RT)} \right)$$



# Tafel equation

- If voltage is larger than 50-mV the forward reactions in the Butler Volmer equation dominate, so that the rate of reverse reaction is negligible

$$j = j_0 \left( \frac{C_R^*}{C_R^{0*}} e^{\alpha n F \eta / (RT)} - \frac{C_P^*}{C_P^{0*}} e^{-(1-\alpha) n F \eta / (RT)} \right)$$

$\cong 1$  (pointing to  $\frac{C_R^*}{C_R^{0*}}$ )       $= 0$  (pointing to  $-\frac{C_P^*}{C_P^{0*}} e^{-(1-\alpha) n F \eta / (RT)}$ )

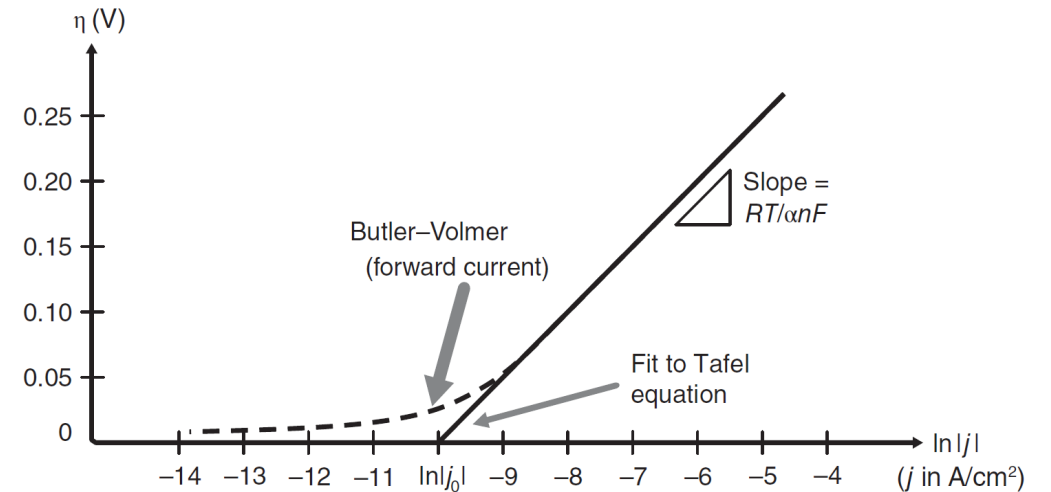
- We can rewrite the current density as:

$$j = j_0 e^{\alpha n F \eta / (RT)}$$

- We can rewrite the equation solving for the activation voltage loss (TAFEL EQUATION)

$$\eta_{Act} = - \frac{RT}{\alpha n F} \ln j_0 + \frac{RT}{\alpha n F} \ln j$$

Const      Tafel slope

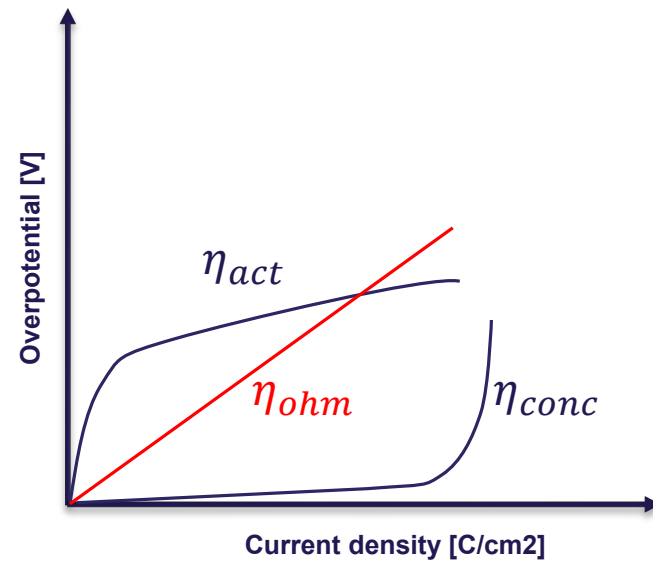


Source: Fuel cell fundamentals Chapter 3





# Ohmic overvoltage



Examples?



# Fuel cell charge transport

- The current density can be related to charge transport via a relationship with voltage and conductivity,  $\sigma$

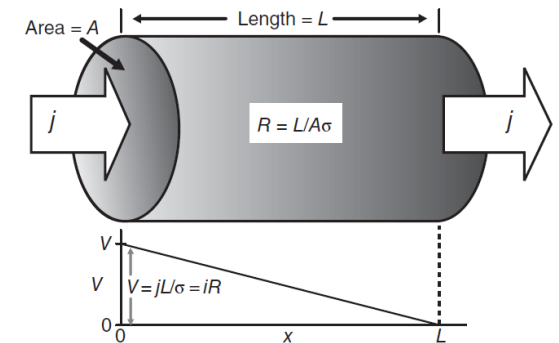
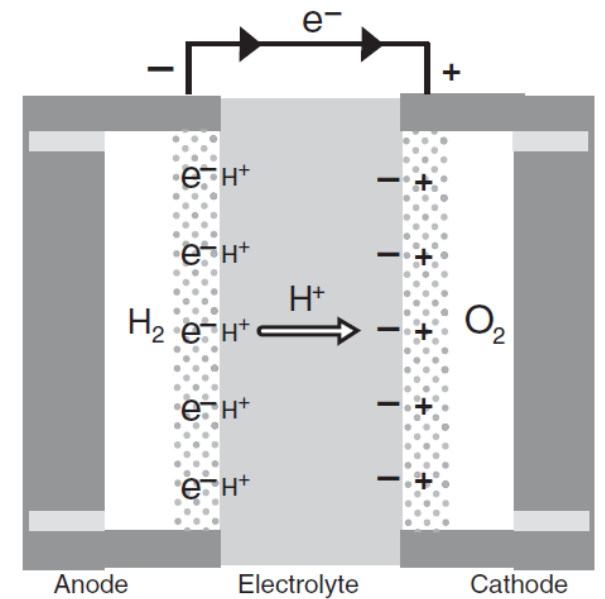
$$j = \sigma \frac{dV}{dx}$$

- We can deduce the voltage as a function of current and resistance:

$$j = \sigma \frac{V}{L}$$

$$V = j \frac{L}{\sigma} = i \left( \frac{L}{A\sigma} \right) = iR$$

$i = jA$       $R: \text{resistance}$



Source: Fuel cell fundamentals Chapter 4



# Charge transport

- Charge transport is linear and is evident in the electrolyte where there is a reduction of voltage from anode to cathode due to resistance of the electrolyte to the hydrogen ion

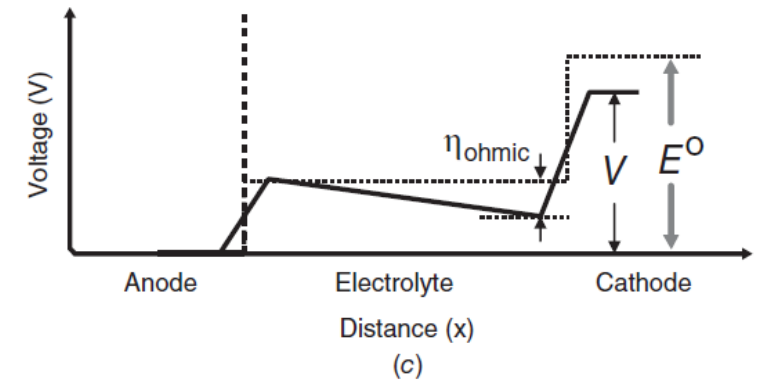
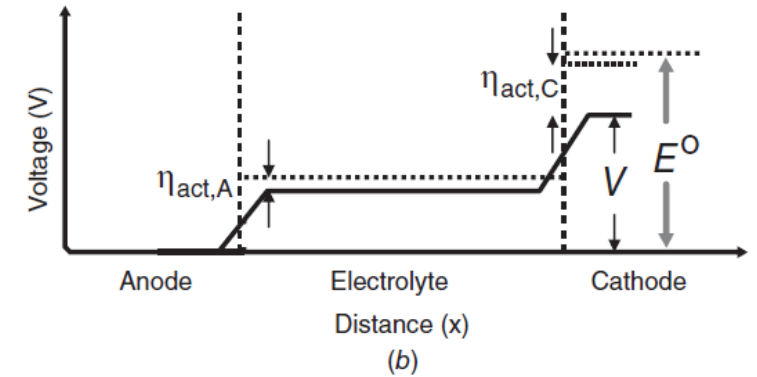
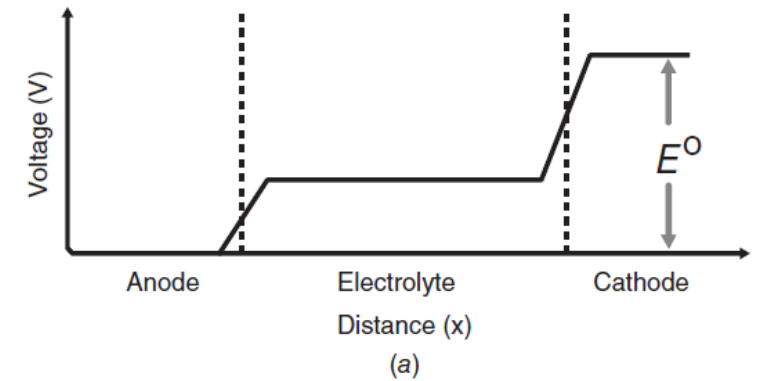
$$\eta_{ohm} = i \cdot R_{ohm} = i(R_{Elec} + R_{Ionic})$$

$$R_{Ionic} \gg R_{Elec}$$

$$\eta_{ohm} = j \cdot ASR$$

ASR: Area specific resistance [ $\Omega \cdot cm^2$ ]

$$ASR = A_{FC} R_{ohmic} = \frac{L}{\sigma}$$

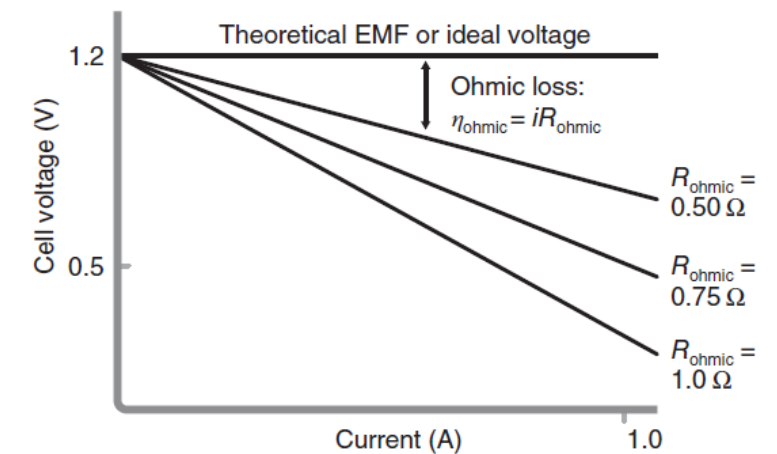
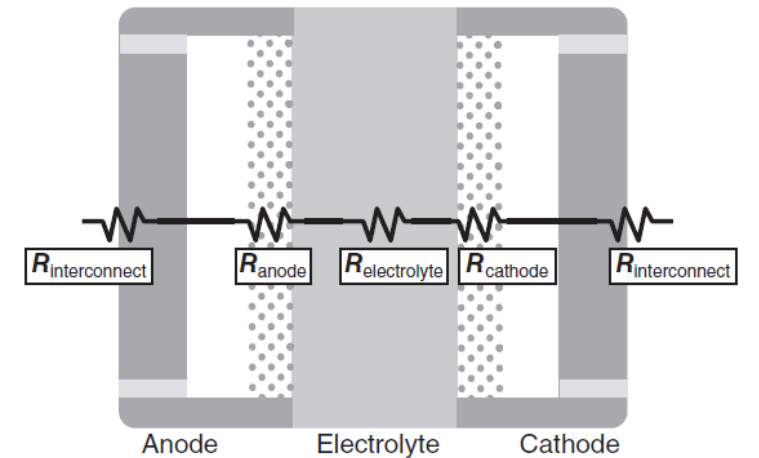


Source: Fuel cell fundamentals Chapter 3



# Charge transfer

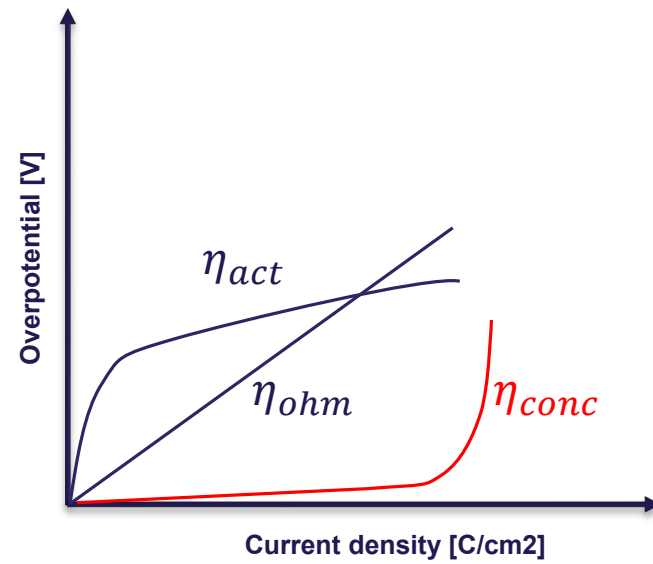
- Resistances in different stacked components can be summed
- The electrolyte accounts for most of the resistance
- Charge transfer reduces cell voltage



Source: Fuel cell fundamentals Chapter 4



# Concentration overvoltage



Examples?



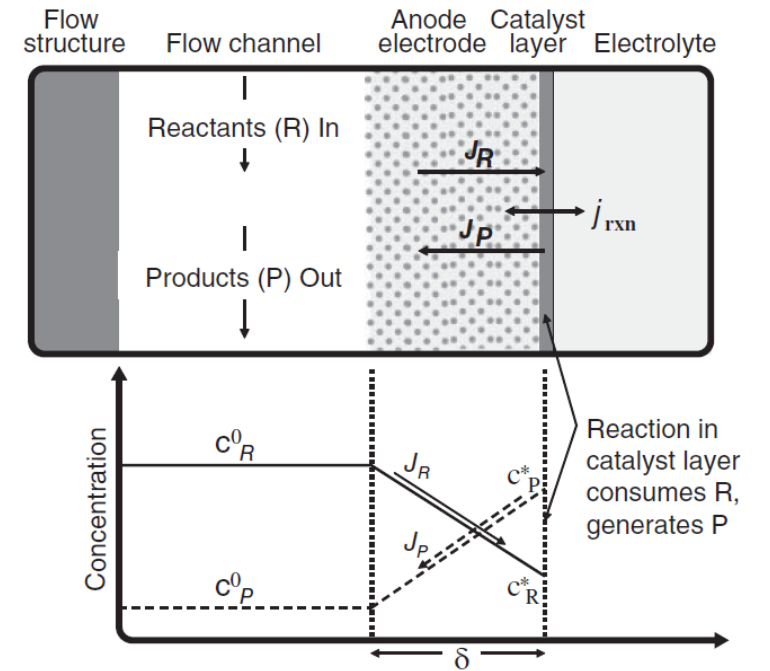
# Mass transport in FC

Combination of:

**(1) Nerstian losses:** Due to depletion of reactants (and their activity) in the channel

$$E = E^0 - \frac{RT}{2F} \ln \frac{a_{H_2O}}{a_{H_2} a_{O_2}^{1/2}}$$

**(2) Reaction losses:** Activation losses increases due depletion of reactants ( $J_R$  reduces along the gas diffusion layer)



Source: Fuel cell fundamentals

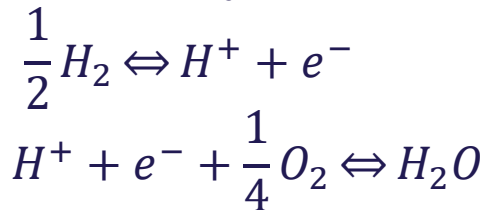


# Gas depletion along the channel

- Reactants are consumed along the channel
- In the right figure we consider mass transport by diffusion along the GDL and convection along the channel

- The oxygen mass flux is depending on current density produced at the fuel cell electrolyte (Faraday Law):

$$J_{O_2}^{RXN} = M_{O_2} \frac{j(x)}{4F}$$



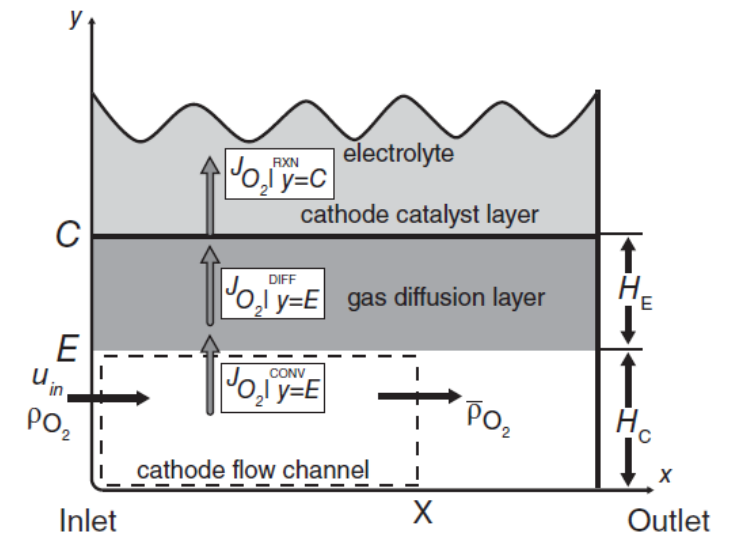
- Oxygen gas consumed by the electrochemical reaction has to be provided by diffusion across the gdl (Fick law):

$$J_{O_2}^{Diff} = -D_{O_2}^{Eff} \frac{\rho_{O_2}^C - \rho_{O_2}^E}{H_E}$$

- Convective mass transport across the channel

$$J_{O_2}^{Conv} = -h_m (\rho_{O_2}^E - \hat{\rho}_{O_2}^{Channel})$$

Steady state  $J_{O_2}^{RXN} = J_{O_2}^{DIFF} = J_{O_2}^{CONV}$



Source: Fuel cell fundamentals



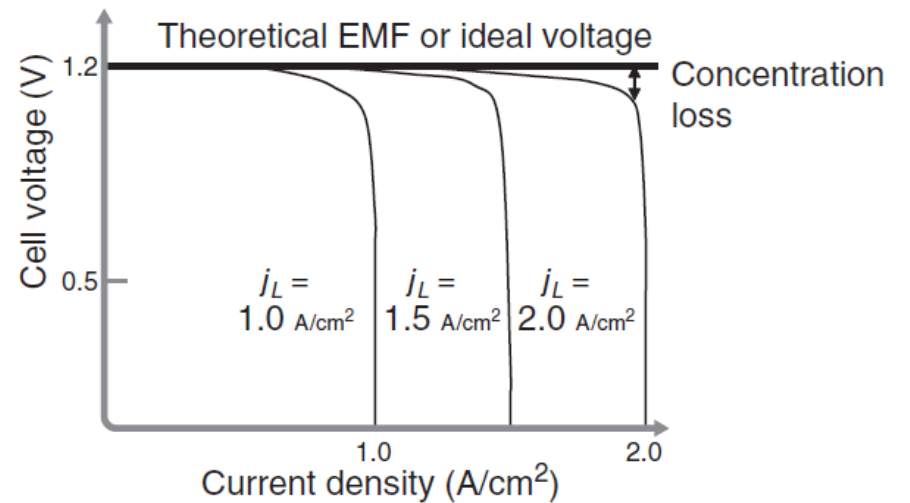
# Limiting current density

- When reactants concentration drops to is very low, current cannot produced. We call this instance “Limit current density”:

$$j_L = nFD^{eff} \frac{C_R^0}{\delta} \leftarrow \text{Gas diffusion layer thickness}$$

- In a fuel cell where hydrogen and oxygen are the reactants

The conversion rate is 0



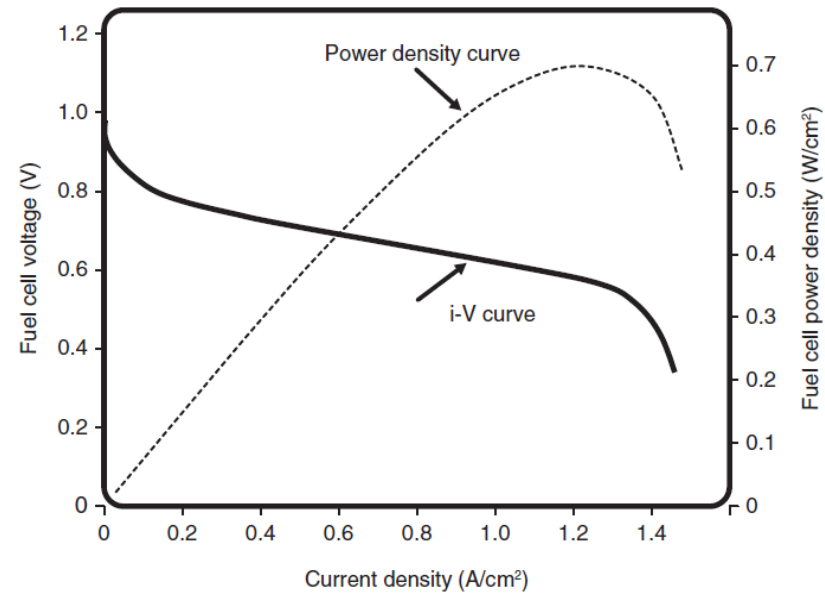
Source: Fuel cell fundamentals





# Fuel cell power

$$\text{Power} = I * V$$



From: Fuel cell fundamentals, Chapt.1



# Cell performance

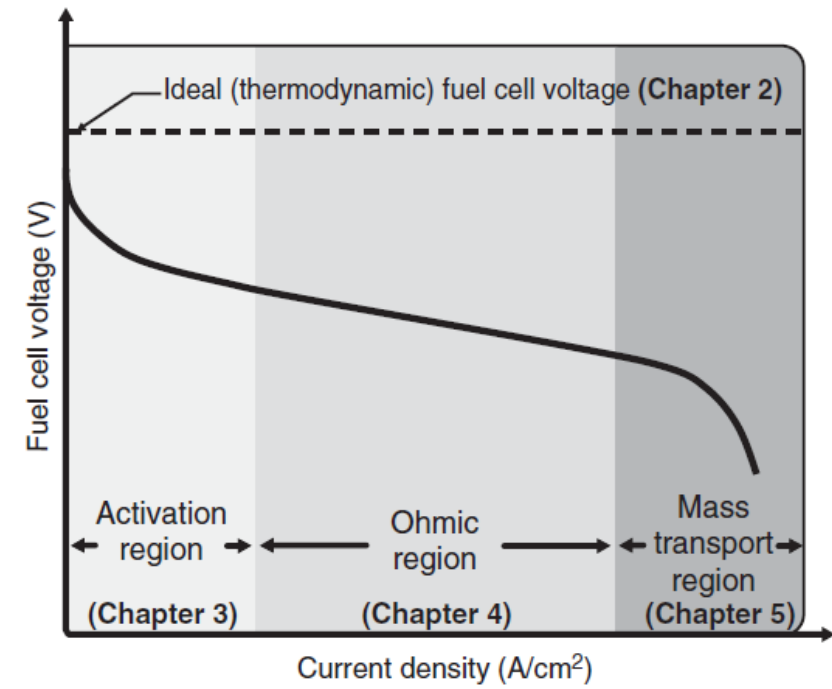
Under load a decrease of cell voltage is experienced

$$V = E - \eta_{act} - \eta_{ohm} - \eta_{conc}$$

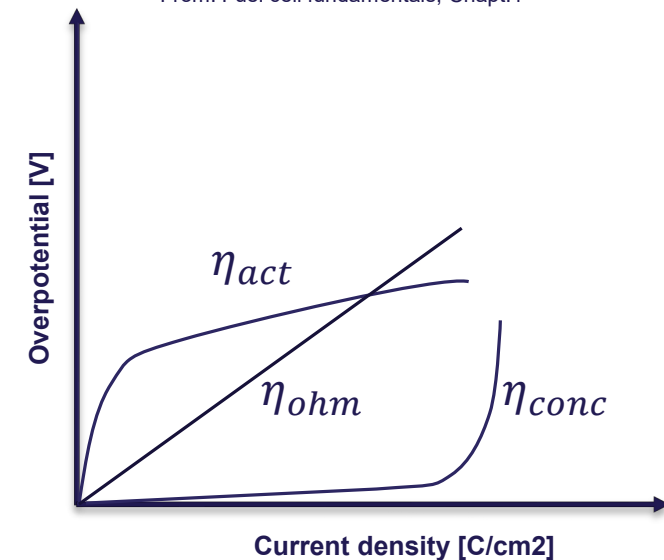
$\eta_{act}$ : **Activation overvoltage** due to kinetics of reaction. It occurs at all current densities but is dominant at low current density and is associated with sluggish electrode reaction kinetics

$\eta_{ohm}$ : **Ohmic resistance** due to Ohmic resistance. Resistances to charge conduction through the various cell components demonstrate a linear dependence with current.

$\eta_{conc}$ : due to mass transport. The cell is essentially "starved" of reactants as they cannot be supplied at the rate at which the electrode reactions demand.



From: Fuel cell fundamentals, Chapt.1



Thanks for your attention



**AALBORG UNIVERSITY**  
DENMARK

# Simple mathematical model of a Fuel Cell in Matlab

Cell voltage can be expressed a difference between open circuit voltage and voltage losses:

$$V_{Cell} = V_{OCV} - V_{loss}$$

The open circuit voltage can be expressed using the Nenrst Equation:

$$V_{OCV} = V_{Rev} = \frac{-\Delta G^\circ}{n_e F} + \frac{RT_{FC}}{n_e F} \ln \left( \frac{P_{H2} \sqrt{P_{O2}}}{P_{H2O}^{Sat}} \right)$$

The activation losses can be expressed using the Tafel equation:

$$\eta_{act} = \frac{RT}{\alpha n_e F} \cdot \ln \left( \frac{i}{i_o} \right) = \underbrace{-\frac{RT}{\alpha n_e F} \cdot \ln i_o}_{Const} + \underbrace{\frac{RT}{\alpha n_e F} \cdot \ln i}_{Tafel Slope}$$

$\alpha$ : Simmetry factor (It measure the direction of the reaction)

$i_o$ : exchange current density (Material parameter which depend the ability of the cell to exchange current)



# Simple mathematical model of a Fuel Cell in Matlab

The Ohmic losses are depending on Ohmic resistance  $R_{ohm}$

$$\eta_{ohm} = i \cdot R_{ohm}$$

The Ohmic losses are function of the Limiting current density which is the max current a fuel cell can exchange

$$\eta_{conc} = \frac{RT}{\alpha n_e F} \ln \frac{j_L}{j_L - j}$$



# Matlab model (1)

```
clc;
close all;
clear all;

%Fuel cell reaction H2 + 0.5*O2 => H2O Gibbs Free energy [Source FC Explained fig2.4]

%Liquid H2O
T_tab_liq = [25 80];
T_q1 = 25:5:80;
DeltaG_tab1 = [-247.2 -228.2]; %kJ/mol
DeltaG_l = interp1(T_tab_liq,DeltaG_tab1,T_q1); %kJ/mol
%Gas H2O
T_tabg = [100 200 400 600 800 1000];
T_qg = 100:10:1000;
DeltaG_tabg = [-225.2 -220.4 -210.3 -199.6 -188.6 -177.4]; %kJ/mol
DeltaG_g = interp1(T_tabg,DeltaG_tabg,T_qg); %kJ/mol

DeltaG0 = interp1(T_tab_liq,DeltaG_tab1,70)*1000; % [J/mol of H2] standard Gibbs free energy of reaction with liquid water as bioproduct at 70C
Tcell = 70+273.15; %[k] Cell temperature
n = 2; %[-] Number of electrons involved in the electrochemical reaction
F = 96485; %[C] Charge of 1 mole of electrones
R = 8.314; %[J/mol] Universal gas constant

P_an = 101325; %[Pa] Anode pressure
P_cat = 101325; %[Pa] Cathode press

P_sat = exp(23.1963-3816.44./(Tcell-46.13)); % [Pa] Saturation pressure of water vapor
p_H2 = (P_an-P_sat)/P_an; %[-] H2 partial pressure with RH100%
p_O2 = (P_cat-P_sat)*0.21/P_cat; %[-] O2 partial pressure
p_H2O = 1; %Water partial pressure assuming liquid water
```



# Matlab model (2)

```
j_cell = 0.01:0.01:1; %[A/cm^2] Cell current density
%Reversible voltage [V]
E = -DeltaG0/(n*F);
%Open circuit voltage (OCV)
p_RATIO = (p_H2*p_O2^0.5)/p_H2O;
Vocv = E + (R*Tcell)/(n*F)*log(p_RATIO); %[V] open circuit voltage
%Activation overvoltage
alpha = 0.2; %[-] Symmetry factor
j_0 = 0.01; %[-]
S_Tafel = (R*Tcell)/(alpha*n*F);%Tafel slope
Vact = S_Tafel*log((j_cell)/j_0);%[V]
%Ohmic overvoltage
ASR = 0.1; %[Ohm*cm^2]
Vohm = j_cell*ASR;%[V]
%Concentration overvoltage
c = 0.032;
j_cell_L = 1;%[A/cm^2]
Vcon = c*log(j_cell_L./(j_cell_L-j_cell));%[V]
%Cell voltage
V = Vocv-Vact-Vohm-Vcon;%[V]
A_cell = 10*10;%cm2
ncell = 50;
P_cellcm2 = j_cell.*V;
I_cell = j_cell*A_cell;
V_stack = A_cell*ncell*V;
P_cell = A_cell*j_cell.*V;
P_stack = P_cell*ncell;

%Plotting results
figure(1)
plot(j_cell,V,j_cell,Vact,j_cell,Vohm,j_cell,Vcon,j_cell,P_cellcm2),legend('Vcell','Vact','Vohm','Vcon','P_cell')
xlabel('Current Density [A/cm2]')
ylabel('Voltage [volt] // Power [watt]')
figure(2)
plot(T_ql,DeltaG1,T_qg,DeltaGg),legend('DeltaG(g)','DeltaG(l)')
xlabel('Temperature [degreeC]')
ylabel('DeltaG')
figure(3)
plot(I_cell,V_stack,I_cell,P_stack),legend('V_{stack}','P_{stack}')
xlabel('Current [A]')
ylabel('Voltage [volt] (Blue) // Power [watt] (red)')
```

