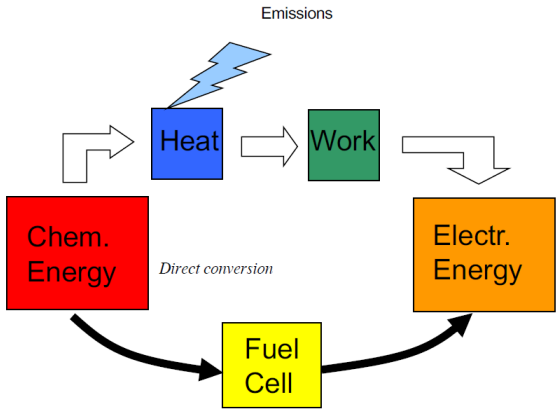
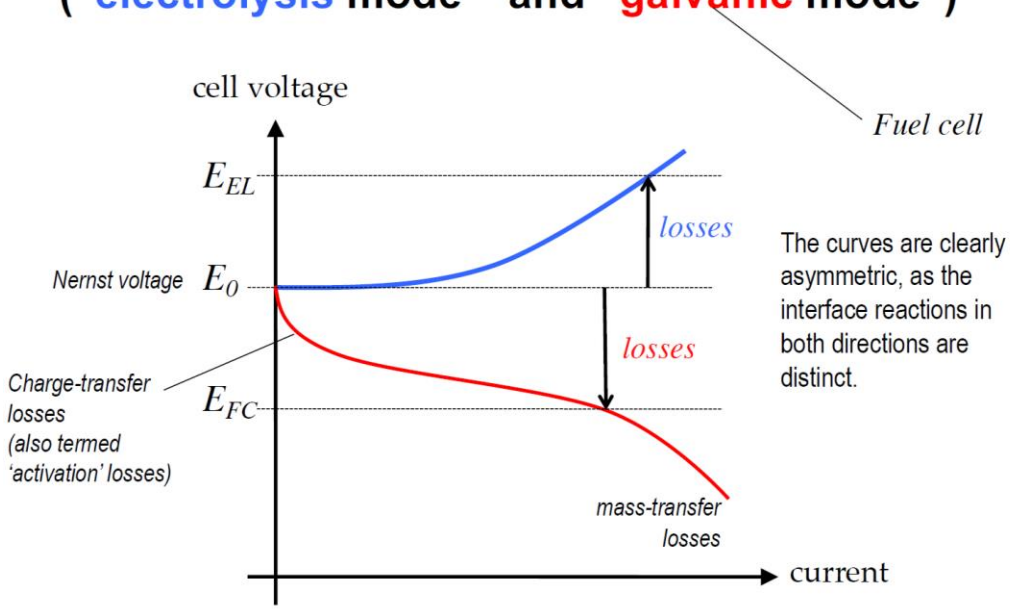
Formula memento
Fuel Cells

1. Refresher

A fuel cell bypasses the mechanical cycle



Characteristic i-V (current-voltage curve) ("electrolysis mode " and "galvanic mode")



Materials in fuel cells: low vs high T (Pt vs Ni)

Type	Electrolyte	Temperature	Fuel
AFC	Alcaline solution	20-100° C	H_2
PEFC DMFC	Polymère membrane	20-100° C	H_2 methanol
PAFC	liquid acide	20° C	H_2 (nat. gas)
MCFC	Molten salt	650° C	C_xH_y
SOFC	Solid ceramic	600-1000° C	C_xH_y

Type	Electrolyte	Cathode	Anode	Interconnect	Dimensions
AFC	KOH	Ag	Ni	steel	flat,50-400cm²
PEFC	« Nafion » (=« sulfonate de teflon »)	Pt on C	Pt(-Ru)	graphite	flat, 5-400 cm²
PAFC	H_3PO_4	Pt on C	Pt on C	graphite	flat, 1 m²
MCFC	$(Na,K,Li)_2$-CO_3	NiO or $LiCoO_2$	Ni	inox	flat, 1 m²
SOFC	90% ZrO_2 + 10% Y_2O_3	$LaSrMnO_3$	Ni	Steel Cr or ferritic	flat / 100 cm² tubes / (2 m long * 2 cm diam.)

2. Fuel Cell Energy Balance and Thermodynamics

1. Available Chemical Energy = Liberated Heat ΔH_r of reaction

Anode: $H_2 \Rightarrow 2H^+ + 2e^-$

Cathode: $\frac{1}{2}O_2 + 2H^+ + 2e^- \Rightarrow H_2O$

p = 1 atm, stoechiometric reaction of 1 mole

$\Delta H_r^o(298K)$ = 241.83 kJ/mol (LHV)
= 285.84 kJ/mol (HHV)

Overall: $H_2 + \frac{1}{2}O_2 \Rightarrow H_2O$ (Gas or Liquid)

$CH_4 + 2O_2 \rightarrow 2H_2O + CO_2$

2. Theoretical Mechanical Work= Theoretical Work given by Gibbs Free energy

$$\Delta G_r(T) = \Delta H_r(T) - T.\Delta S_r(T)$$

$$\Delta G = -nFE$$

(n = number of electrons exchanged per molecule of fuel)

(F = Faraday constant, 96484 C/mol)

n=2 for H_2, CO..

n=8 for CH_4

Fuel @25°C 1 atm	LHV [kJ mol^{-1}]	HHV [kJ mol^{-1}]	LHV [MJ kg^{-1}]	HHV [MJ kg^{-1}]
H_2	241.83	285.84	119.96	141.8
CH_4	802	890	50.00	55.50

ΔH_{fuel}^o

Loss $T\Delta S_r$

ΔG_{fuel}

Transformation Joule to Volts

E_{Nernst}

Voltage loss

U_{cell}

H_2 vs. hydrocarbons: properties

	H_2	Natural gas (CH_4)	Gasoline
Boiling point	-252.7 ° C	-160° C	40-200° C
Melting point	-259 ° C	-182° C	-40° C
Gas density	0.089 kg/m^3	0.707 kg /m^3	4 kg /m^3
Liquid density	0.071 kg/L	0.41-0.5 kg/L	0.72-0.78 kg/L
Lower HV	120.2 MJ/kg, 8.6 MJ/L as liquid	47 MJ/kg 21 MJ/L as liquid	42 MJ/kg
Higher HV	142 MJ/kg, 12.7 MJ/m^3 10.1 MJ/L as liquid	53 MJ/kg, 40 MJ/m^3 24 MJ/L as liquid	46 MJ/kg 36 MJ/L
Autoignition	585° C	632° C	220° C
Flammability in air	4-75%	5-15%	1-7.6%
Flame Temperature	2045° C	1875° C	2200° C

2. Fuel Cell Energy Balance and Thermodynamics

3. Equilibrium Voltage= Includes effect of concentration

All species at 1 atm

$$\Delta G_r(p,T) = \Delta G_r^0(T) + \frac{RT}{nF}\ln(Q_r)$$

Equilibrium constant

$$E^{SOFC} = E^0 + \frac{RT}{2F}\ln\left(\frac{x_{H_2}^{anode}\sqrt{x_{O_2}^{cathode}}}{x_{H_2O}^{anode}}\right)\left[\frac{P^{cathode}}{p^0}\right]^{\frac{1}{2}}$$

$$E^{PEFC} = E^0 + \frac{RT}{2F}\ln\left(\frac{x_{H_2}^{anode}\sqrt{x_{O_2}^{cathode}}}{x_{H_2O}^{cathode}}\right)\left[\frac{P^{anode}}{p^0}\right]\left[\frac{P^{cathode}}{p^0}\right]^{-\frac{1}{2}}$$

$(=1 \text{ if liquid } H_2O)$

$$E^o = \frac{\Delta G_r^0}{nF}$$

$x_{H_2}^{anode}$: Anode Hydrogen molar fraction

$x_{O_2}^{Cathode}$: Oxygen Cathode molar fraction

$x_{H_2O}^{Cathode}$: Steam Cathode molar fraction

$x_{H_2O}^{anode}$: Anode steam molar fraction

$P^{Cathode}$: Cathode total pressure

P^{Anode}: Anode total pressure

P^o: Reference Pressure 1atm

$\Delta H_{fuel}{}^o$

$Loss\ T\Delta S_r$ ↓

ΔG_{fuel}

Transformation Joule to Volts ↓

E_{Nernst}

Voltage losses ↓

U_{cell}

4. Useful Cell Power

$$U_{cell} = E_{Nernst}(p,T) - (i.R_{ohmique} + |\eta_{cathode}| + \eta_{anode})$$

U_{cell}: Voltage – operating point

Ohmic Loss

Cathode total polarization loss

Anode total polarization loss

i: Current – operating point

$i.R_{ohmique} + |\eta_{cathode}| + \eta_{anode}$: Voltage Losses

3. Key Values

$V = Operating\ Voltage$

$J = Current\ Density$

$\Delta H_{293K}[J/mol]$ = Fuel LHV or HHV

f – molar fuel flowrate

F = 96485.332 C mol^{-1}

η_{cell} = LHV or HHV efficiency

- Operating Map

$$Power\ P[W] = V\ [V] \times I\ [A]$$

$$Power\ Density\ P\ [W\ cm^{-2}] = V\ [V] \times J\ [A\ cm^{-2}]$$

- Efficiency

$$\eta_{cell} = \frac{P[W]}{\dot{f}[mol/s] \bullet \Delta H_{293K}[J/mol]}$$

$$\eta_{cell} = \frac{I[A]}{\dot{f}[mol/s] \bullet nF[C/mol]} \cdot \frac{E_{cell}\ [V]}{E_{Nernst}[V]} \cdot \frac{\Delta G(p,T)[J/mol]}{\Delta H_{293K}[J/mol]}$$

$$\eta_{cell} = \eta_I \bullet \eta_V \bullet \eta_{THDYN}$$

current efficiency, "fuel utilisation"

voltage efficiency

thermodynamic efficiency

Electrical efficiency as *fct*(power size)