

## 02B Solid Oxide Fuel Cells (SOFCs)

# Conversion of Chemical Energy into Electrical Energy

What are the units for the electrical work, as in a Fuel Cell or in a Lithium Ion Battery?

The of electrical energy is the eV

One eV is the work done in transporting a charge of one electron between two electrodes with a potential difference of one volt.

**Unit for energy is Joule.**

One Watt = One Joule s<sup>-1</sup>

Watt = Current \* Volts = Joule s<sup>-1</sup>

Current is Coulombs per second.

Watt = (C s<sup>-1</sup>) \* Volts = Joule s<sup>-1</sup>

Coulombs\*Volts = Joules

Conversion between Joules and eV, which we now understand to have energy in units of Joules

1eV=charge on one electron\*one volt

1 eV = 1.6\*10<sup>-19</sup> (Coulombs)\*1 (volt) Joules

Faraday (F) = Charge on one mole of electrons. = Charge on (one electron\* Avogadro's Number)

N<sub>A</sub>=6.02\*10<sup>23</sup> atoms/molecule per mole

F=1.6\*10<sup>-19</sup>\*N<sub>A</sub> = 96,500 Coulombs per mole

Conversion of kJ mol<sup>-1</sup> into eV

1 eV = 1.6\*10<sup>-19</sup> Joules

Equivalent in Joules per mole of electrons

1.6\*10<sup>-19</sup>\*N<sub>A</sub> energy per one mole of eV for one volt between electrodes = 96,500 J mol<sup>-1</sup>

or 96.5 kJ mol<sup>-1</sup>.

The conversion (easy to remember form) is the 1 eV (J/atom) is nearly equivalent to 100 kJ mol<sup>-1</sup>.

**Topics: Solid Oxide Fuel Cell (SOFC)**

What is the critical species (oxygen ion)?

What are the performance measures of the SOFC?

What are the properties of the electrolyte?

What are the properties of the anode and the cathode?

# Topics

- i. What are the critical species?  
 $O_2, H_2, H_2O, e, O^{2-}, H^+, OH^-$
- ii. The Nernst Potential: application of Gibbs Free Energy to relate chemistry to electrical engineering. What is open circuit voltage and its derivation?
- ii. Real electrical work on a resistive load and electrical losses - what is the energy conversion efficiency? Lumped parameters, and the lumped circuit model for SOFCs.
- iv. What is ASR: Area Specific Resistance
- v. Performance measures of SOFCs: voltage and power

## (i) The Nernst Potential: Equivalence of Chemical and Electrical Energy

### Derivation of the Nernst Potential: Method I

It is possible to derive the upper-bound for the electrical work by assuming that there are no losses within the cell (electrolyte resistance, interfacial resistance, etc.)

Meaning that no current flows through the fuel cell. Therefore the voltage measured across the cell is in "open circuit".

It is called the open circuit voltage.

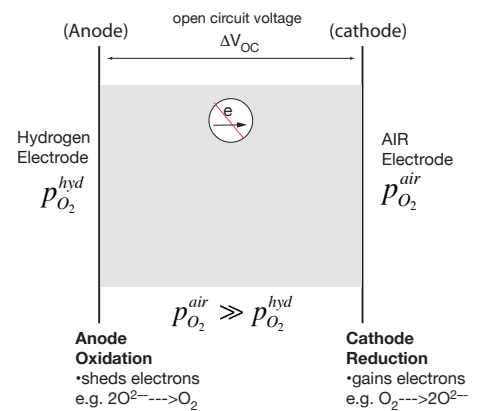
It is a thermodynamic quantity (called the Nernst Potential)

The chemical free energy (in units of Joule per mole - note that R has units of  $J mol^{-1}K^{-1}$ ) is given by

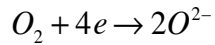
$$\Delta G = RT \ln \frac{P_{O_2}^{air}}{P_{O_2}^{hyd}} \quad (1)$$

energy available when one mole of  $O_2$  is transported through the electrolyte from air to the hydrogen electrode, in units of  $J mol^{-1}$ .

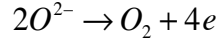
What is the electrical work that I can derive by transporting one mole of  $O_2$  from the cathode to the anode?



Reaction at the cathode (air electrode)



Reaction at the hydrogen electrode (the anode) is given by



The electrical work per mole of  $O_2$  transported through the electrolyte from the air to the hydrogen electrode,

$$\text{Electrical work} = \Delta V_{OCV} * 4eN_A \text{ J mol}^{-1} \text{ (of oxygen molecules)}$$

$$\text{Faraday constant } F = eN_A \text{ C mol}^{-1} = 96,500 \text{ C mol}^{-1}$$

$$\text{Electrical work} = \Delta V_{OCV} * 4F \quad (2)$$

this the upper-bound of electrical work that is available.

Equation (1) and (2) we are able to relate chemistry to electrical engineering.

$$\Delta V_{OCV} * 4F = RT \ln \frac{p_{O_2}^{air}}{p_{O_2}^{hyd}}$$

$$\Delta V_{Nernst} = \frac{RT}{4F} \ln \frac{p_{O_2}^{air}}{p_{O_2}^{hyd}} \quad (3)^*$$

Note the simplicity of the equation and also that it is accessible experimentally with a voltmeter. Indeed Eq. (3) can be used to measure the oxygen pressure at the hydrogen electrode.

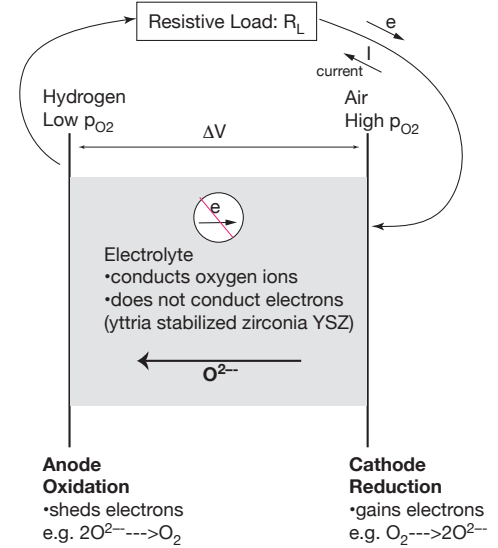
Eq. (3) is valid only if there is no current flow through the system, that is why it is called the open circuit voltage.

Typical values of the Nernst potential depends on the ratio of the hydrogen and the water vapor pressure at the anode (which depends on the  $2H_2 + O_2 = 2H_2O$  being in equilibrium). These values are around 0.8 volts.

$$\text{Then } p_{O_2}^{hyd} = 1.45E-17.$$

Remember that these are upper-bound calculations that is, the maximum work that can be derived from the fuel cell.

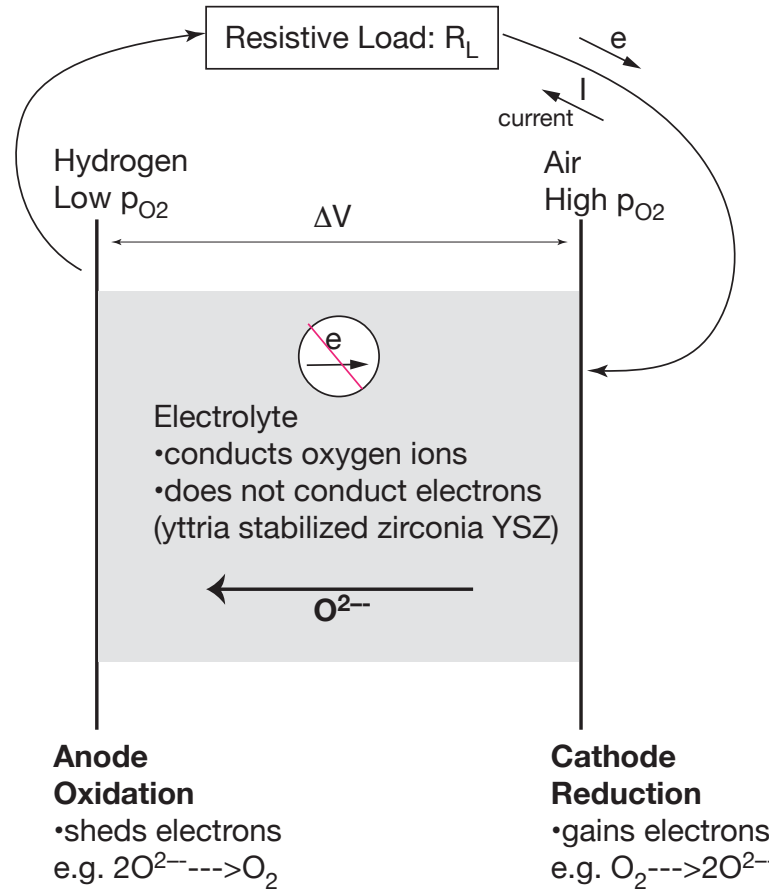
This upper-bound is calculated assuming there is no current flowing in the system.



We wish to calculate the oxygen partial pressure at the anode for a Nernst potential of 0.8V

R	8.31J/(mol*K)
T	1000K
F	96500C/mol
p_air	0.2
DEL_V	0.8V
FactorExp	37.2
p_O at hyd	1.5E-17atm.

## (ii) Another Method of Analyzing the Nernst Potential (using chemical potentials)



•The electrolyte is NOT an electronic conductor (otherwise the cell would discharge when not in use by self conduction of electrons)

\*The reaction at the air electrode (the cathode) is



\*This is a REDUCTION reaction, that is, electrons are ABSORBED in the reaction

\*The reaction at the hydrogen electrode (the anode) is



\*This is an OXIDATION reaction, that is, electrons are RELEASED in the reaction

\*The universal description

anode is the oxidizing electrode  
cathode is the reducing electrode



where  $\mu_e^C = eV_{cathode}$  and  $\mu_e^A = eV_{anode}$

Also as shown before

$$\mu_{O_2}^A = RT \ln(p_{O_2}^A)$$

and

$$\mu_{O_2}^C = RT \ln(p_{O_2}^C)$$

Take the difference between (6) and (7)

$$2\mu_{O_2}^A - 2\mu_{O_2}^C = \mu_{O_2}^A - \mu_{O_2}^C + 4\mu_e^A - 4\mu_e^C \quad (8)$$

$$4\mu_e^A - 4\mu_e^C = 4e(V_{anode} - V_{cathode}) = 4e\Delta V \quad (9)$$

$$\mu_{O_2}^A - \mu_{O_2}^C = RT \ln\left(\frac{p_{O_2}^A}{p_{O_2}^C}\right) \quad (10)$$

$$2\mu_{O_2}^A - 2\mu_{O_2}^C = 0 \quad (11)$$

•There is no current of oxygen ion; therefore the activity of oxygen ions in the electrolyte must be the same at both electrodes\*.

•The electrolyte is oxygen ion conductor

Inserting (9), (10) and (11) into (8):

$$4eN_A \Delta V = -RT \ln\left(\frac{p_{O_2}^A}{p_{O_2}^C}\right)$$

$$\Delta V = -\frac{RT}{4F} \ln\left(\frac{p_{O_2}^A}{p_{O_2}^C}\right) \quad (12), \text{ This is the open circuit voltage.}$$

•Note that in Eq. (9),  $4e\Delta V$  was replaced by  $4F\Delta V$  because the right hand side in EQ. (10) is written in terms of Joules mol<sup>-1</sup> (because we are using R instead of k<sub>B</sub>).

The conversion between k<sub>B</sub> and R can be a bit confusing but if the numbers do not work well you know that it is the Avogadro's number, that is  $R = N_A k_B$ . The Avogadro's number is a very large quantity which is easy to see where it may be missing.

\*Recall that the diffusional flux is driven by the gradient in the chemical potential, that is

$$J_{ion} = \frac{n_{O_2} D_{O_2}}{k_B T} \frac{d\mu_{O_2}}{dx}, \quad J_A = \frac{D_A}{\Omega_A k_B T} \frac{d\mu_A}{dx}$$

Note that the equations appear to be somewhat different (the first is related to ionic diffusion and the second to sintering). sintering workpiece). Here  $n_{O_2}$  is the concentration

in units of # m<sup>-3</sup>, which is also the units of  $\frac{1}{\Omega^3}$  since  $\Omega^{\frac{1}{3}}$  is the volume per atom.