Notes Thursday March 3rd – NPRE 470

**The Butler-Volmer Equation:**

* Equation gives current as a function of over potential, η
* The over potential is given as equal potential minus voltage
* BV equation allows for plots of Voltage vs. j (current density) to be constructed in order to calculate the activation over potential, ηact (see page 86 in fuel cell fundamentals for graphs)
* BV equation has three unknown constants
  + j0 – equilibrium exchange current
  + c – concentrations
  + α – transfer coefficient
* α is a value from 0 – 1
  + Where 1 is no activation barrier for reaction (see figures on page 84)
* At equilibrium j0 = 0 because the net exchange current is zero.
  + Does not mean no current exists just that the forward and reverse exchange currents are equal.
* Important notes about over potential
  + It is an experimental value
  + Helps to decrease activation barriers to reaction
  + Reverse activation barriers are still larger than forward activation barriers
* The BV equation becomes more complicated when both electrodes (anode and cathode) are taken into account.

**Comparing the Nernst and BV equations:**

* Nernst equation relates equilibrium voltage to concentration
* BV is the non-equilibrium equation for fuel cell calculations and is considered to be the “master equation”

**Tafel Equation:**

* When j << j0, current and over potential are linear for small changes in equilibrium voltage.
* Tafel equation describes this linear relationship
* Allows for exchange current and transfer coefficient to be experimentally determined.
* See example 3.3 for sample calculations
* Tafel equation shows that small changes in exchange current can have profound effects on the activation over potential ηact.

**Ways to improve kinetic performance:**

* Increase the reactant concentrations
* Decrease activation barrier, ΔG+1
  + Change the catalyst, hard to compete with platinum
* Increase the Temperature
* Increase the number of reaction sites
  + Increase surface area and roughness
  + Put more catalyst in
* Reactions are commonly dominated by the cathode activation potential
* Exchange current densities are dependent on surface and electrolyte
  + Table 3.1 summarizes this
* Table 3.2 shows values that explicitly prove the limitations of oxygen when calculating exchange current densities
  + Compared to hydrogen in Table 3.1, oxygen is at best seven orders of magnitude smaller

**Catalyst Electrode Design:**

* Three key attributes
  + High Mechanical Strength
  + High electrical conductivity
  + Low corrosion
* Putting catalyst on surface
  + Catalyst hot pressed onto membranes (ex: ironing on t-shirt designs)
* Hydrogen-oxygen bonding with Pt catalyst
  + Hydrogen bond completely separates and has lower energy when splitting into two atoms
  + Oxygen does not completely separate when bonding with Pt. Thus having higher energy when compared the bonded hydrogen.