**Well Posed PNP**

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Now, to equations.

Here is a version of PNP in which Maxwell’s version of the continuity equation ***for charge***[[1]](#footnote-1) is used so the resulting flux equation for the flux  of charge (i.e., flux of total electric current) always involves the permittivity (i.e., dielectric coefficient).

 

This is eq. 6.4 of Jackson, p. 238, expanded, see p. 154. I follow Jackson’s notation exactly and use  for the permittivity (that has units. It is not the dielectric ‘constant’).

The variable  is the net charge, related to the concentration of ions through

 

where we use chemical units (Faradays) because we are dealing with a macroscopic system.

 Now we introduce the Nernst Planck equations for the flux of individual ions (NOT the flux of ionic current, rather the flux of the number of ions). Remember ions of different valence *zi* are very important in biology (calcium ions have charge +2; chloride ions have charge -1; sodium and potassium ions have charge +1). They all have significantly different diffusion coefficients. It is NEVER permissible to treat all ions as having the same diffusion coefficient or the same (magnitude let alone sign) of charge if one wants to deal with biology.

 

I use the diffusion coefficient and not mobility to avoid the confusion between the two definitions of mobility (absolute and electrical) in the literature. Obviously if the Einstein approximation fails and enough information is available to distinguish mobility from diffusion coefficient, the mobility should be used explicitly, and the choice of definition should be made explicitly.

Now, we sum over all the ions to get total flux of charge

 

Maxwell Continuity eq. gives the equation for continuity of electric charge, i.e., current

 

I leave the permittivity inside the brackets so we never forget the assumption that is involved in moving it outside! And then the classical continuity equation for the flux of charge  (remember  is the flux of charge, not the flux of ions).

 

 

It is very important that no attempt be made to compute the sum on the right hand side of eq.  from the concentrations . The sum  is ill posed. Rather, one must compute  the net charge and its time derivative directly without summing concentrations or there rate of change.

Note the different form of the continuity of mass for each species

 

and the different form for the continuity equation of total ‘mass’.

 

The mass continuity equations are ***not*** equivalent to the Maxwell continuity equation. They do not involve the charge  at all For example, the sum  is well posed and easy to compute because all its terms are positive while the corresponding terms in the sum in eq.  can be positive or negative, and must be nearly equal, because of the enormous strength of electrical forces, summarized by the (approximate) physical principle of electroneutrality. In order to avoid confusion we do not even have a symbol for the flux of total mass .

**Boundary Conditions**. We now have difficulty when we set boundary conditions. We need to set boundary conditions on the electrical current  but the usual formulation of PNP sets boundary conditions on all *N* of the ionic species. This obviously over-specifies the problem.

This apparent paradoxical situation is resolved when we realize that to make the system well posed (i.e., to reach steady state when concentrations and potentials on the boundaries are constants independent of time), we must ***relax our boundary conditions on concentration. We must allow one of the concentrations  (say) to ‘float’, i.e., to be determined by the rest of the problem.***

We introduce an artificial additional pathway for this ion we call the leak pathway, e.g., an  flux equation added to the set described in eq. .

We now have two flux equations for the same ionic species, one the real one and the other the leak. We choose parameters for the leak so the system is not perturbed in the time domain we study. The leak ensures that at infinite time the system will be stable.

 **Set Of Equations Including Leak Conductance** are then

1. The Maxwell Continuity Equation for the total flux of charge

 

1. The mass continuity equations for the (mass) flux of  species. This set excludes ion *m*:

  ion *m* is excluded

1. Dirichlet boundary conditions on the concentrations of  species, ion is excluded, imposed at time zero, and maintained from then on.
2. Some initial condition on ion *m* which is not maintained in time so the system starts in a well-defined state close to electrical neutrality We will discuss what ‘close to electrical neutrality’ means next.

In this document do not discuss the stray and ‘membrane’ capacitances in the setup. That goes as I wrote earlier and can be added if there is some reason I do not perceive right now. Note the discussion of capacitance to ground (found in earlier versions of this paper) has been replaced by (what I hope) is an exact mathematical statement of the role of permittivity, arising from polarization (see p. 152-154 of Jackson). The electricians’ formulation of ‘capacitance to ground’ used in my previous discussion is easy to understand from eq. .

 

suggesting a formula close to the electricians’ capacitance to ground idea

 

as well as the strange looking formulae. I suspect something is here that I do not understand.

 

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1. See p. 238 of J. D. Jackson, *Classical Electrodynamics*, Third Edition (1999), attached to this document. [↑](#footnote-ref-1)