

## Assignment 5 Nernst-Planck and Goldman Equations

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The Nernst-Planck equation describes the steady state balance between current flux of an ion due to the combined effect of diffusion (random walk) and drift (in the electrostatic field of a voltage gradient). We can use this equation to try to gain some insight into how ionic currents might flow through a membrane. So, we will examine the Nernst-Planck equation describing the current flow inside the membrane, representing the (inside) of the membrane as the interval  $[0, a]$  (0 is on the intra-cellular side of the (inside) of the membrane, and  $a$  is on the extra-cellular side (of the inside of the membrane). Note that there is a problem for us here, since we can't measure anything "inside" the membrane— the ionic concentrations are known "outside" the membrane — in other words on the wall of the membrane facing the intra and extra-cellular components. So, we are going to have a problem specifying boundary conditions. Another problem is that we don't know the functional forms of  $c_S(x)$  or  $V(x)$  "inside the membrane", but these are what will govern the current flow "inside" the membrane. Goldman dealt with these problems by assuming that the concentration and voltage gradients are linear – therefore this is called the "constant field" approximation, since the electric field in the membrane, under the linear voltage gradient, is constant, i.e.  $E = -\frac{\partial V(x)}{\partial x}$  is taken to be, by linearity,  $E = \frac{V_m}{a}$ . The voltage difference across the membrane is  $V_m = V_i - V_e$ , so this is measurable (known). The problem of specifying the concentrations on the "inside" of the membrane, is handled by Goldman, by assuming that the measured concentrations  $c_i$  and  $c_e$  are "partitioned" by a constant  $\beta_S$  called the partition constant. This is motivated by the idea that the solubility of ions in "membrane" might be described by a partition constant which tells us how much of the molarity of the ion solution is able to exist in the membrane. So, if the partition constant for  $Na$  ions was 0.01, we would think that the concentration of  $Na$  ions on the "inside" of the membrane was  $\beta_S c_i$  at the intracellular side and was  $\beta_S c_e$  at the extracellular side. Since we can measure or know the concentrations in the intra and extra cellular solutions, we can use this simple partition idea to estimate the concentrations "inside" the membrane from their values immediately "outside", where we can measure them. So, we make the assumption that the concentration gradient across the (inside) of the membrane is linear, so  $c(x) = \beta_S \frac{c_i - c_e}{a} x$  Using these simplifications, we

can integrate the Nernst-Planck equation across the membrane, since it is an ODE and there is a simple method of integrating this type of ODE, by constructing an integrating factor to multiply all the terms of the equation, to make it an “exact differential”. In this assignment, we’ll examine how to integrate the Nernst-Planck equation, and next week, we’ll put in the approximations of linear concentration and voltage gradient.

**Problem 1 Integrating Factor for ODE solution** Given a differential equation in the form  $y' + P(x)y(x) = Q(x)$  defined on a domain  $[s_0, s_a]$ ; We showed in class that if we multiply through with a function  $M(x) = e^{\int_{s_0}^x P(s)ds}$  ( the “integrating factor”), then we are left with a problem of the form  $\frac{d(M(x)y(x))}{dx} = M(x)Q(x)$  which can be immediately integrated as  $M(x)y(x) = \int_{t_0}^x M(t)Q(t)dt + C$ .

1. Show

$$M(x)y(x) = \int_{t_0}^x M(t)Q(t)dt + C$$

where  $M(t)$  is the integrating factor described above – in other words, that the integrating factor method works as claimed.

2. Use this method to solve the ODE  $y' - \frac{2y}{x} = 0$  . Plug your solution back into the ODE and show that the solution is correct.

**Problem 2: Integrate the Nernst-Planck equation** Now use this method to solve the problem of integrating the Nernst-Planck equation for an ion S, which is

$$J_s = -z_s F D_S (\nabla c_S(x) + z_s c_S \frac{F}{RT} \nabla V(x))$$

where  $J_S$  is current density in  $\frac{\text{Amperes}}{\text{cm}^2}$ . Regroup and relabel the constants in the form of  $\alpha, \gamma$  as done in class. In other words, re-write the Nernst-Planck Equation in one dimension as

$$\frac{J}{\alpha} = \frac{\partial c_S(x)}{\partial x} + \gamma c_S(x) \frac{\partial V(x)}{\partial x}$$

The point is to simplify writing the various constants.

1. Find the integrating factor for the Nernst-Planck equation, and re-write the Nernst-Planck Equation (using the integrating factor) as

$$\frac{d(c_S(x)e^{\gamma V(x)})}{dx} = \frac{e^{\gamma V(x)}}{\alpha} J_S$$

**Problem 3** Show that the Nernst-Planck equation reduces to the Nernst Equation when the current flux  $J_s$  is zero, in other words, at conditions of “steady-state”. The Nernst-Equation is a valid for equilibrium – comment on how equilibrium differs from steady state.