A THEORETICAL STUDY OF THE EFFECTS OF INHOMOGENIOUS RF FIELDS IN THE VICINITY OF MEMBRANES

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ABSTRACT:
In this paper we show that the gradients of an RF field at the boundary between fluids and cell membranes may be large enough to increase the average ion currents by amounts that are on the same order of magnitude as the diffusion currents. We this is one of two mechanism that could lead to biological effects by RF fields that are bellow the level that will lead to significant changes in temperature.

INTRODUCTION:

The increased use of cell phones make it of considerable interest to explore the possibilities that exposure to low levels of RF fields can cause changes in biological systems. It is well documented that power levels sufficient to cause temperature rises of a degree or more can be biological active, however, at power levels that lead to heating of less than a tenth of degree centigrade a generally accepted theoretical bases biological effects has not been established. We that believe that two of the mostly likely ways that low level fields could effect biological systems are chemical reaction rates by means spin flips from a singlet to triplet state as a free radicals and by means of dielectrophoresis. In this paper we will treat only the second of these or the dielectrophoric forces that are associated with the gradient of the RF as means of changing the flow of ions and molecules in the vicinity of an ion channel.

It has been shown that continuum theories break down when we are looking at details of the currents near a channel. [**??**] Currently molecular dynamics, MD, and Brownian dynamics, BD, are being use to model the behavior ion channels. Brownian dynamics takes substantially less computing power and this approach that we are using to estimate the changes in the current that will strike a membrane in a one dimensional model.

A BROWNING DYNAMICS MODEL

A. D Brownian Dynamics Simulation

1. Langevin Equation

$$\ddot{r} = -y\dot{r} + \frac{R}{m} + \frac{F}{m} \tag{1}$$

where y^{-1}: relaxation constant, R: random force and F : structured force.

2. Forces

   a. Random force: random thermal force, with standard distribution,
   δt: time-step

$$variance < R^2 >= 2mykT/\delta t \tag{2}$$

   b. Structured forces

$$F = qE - \alpha VE\nabla E + \sum_{j\neq i}\left[\frac{-1}{4\Pi E}\frac{q^2 e^{-x_{ji}/k_d}}{x_{ji}^2} + \frac{AR^3}{x_{ji}^4}\right] \tag{3}$$

   2^{nd} term: dialectropheretic force
   3^{rd} term: screened coulomb force ()k_d:Debye constant)
   4^{th} term: Van der Waals force (A: Hammaker constant)

B. Position update equations ([**?**])

$$\begin{aligned} x(t_{n+1}) &= x(t_n)(1+e^{-r}) - x(t_{n+1})e^{-r} + \frac{F(t_n)}{my^2} r(1-e^{-r}) \\ x(t_{n+1}) &= x(t_{n+1}) + \frac{\dot{F}(t_n)}{my^3}\tau(\tau(1+e^{-r})/2 - 1 + e^{-r}) + X_n(\delta t) + X_n(-\delta t)e^{-r} \end{aligned} \tag{4}$$

where, $x_n(\delta t) = \frac{1}{\gamma}\int_{t_n}^{n+1}[1-e^{\gamma(t-t_n-\delta t)}]R(t)dt$

initial conditions : well-distributed ions at $x_i(0)$ and $dx_i/dt = 0$

C. Calculation Flow

Set-up linear positions $[0 \sim 10nm]$
Set-up primitivity profile

$0nm$ $5nm$ $6nm$ $10nm$

Solve Poisson Equation using FEM
Using equations in (**??**), calculate the positions
Calculate average current J through set point $(x = 8nm)$

D. Electric field and gradient profile $(V = 1\text{Volt at} x = 10\text{nm}, \text{horizontal axis} = \text{position})$

Gradient E: only strong at the edges (dx $\sim$ 0.2nm) around 5nm and 6nm

E. No electric field, No gradient $\rightarrow$ only thermal motion $+$ Van der Walls force (Redlines show the dielectric discontinuities)

$\rightarrow$ Average current $J = 0$nA measured at 8nm and 7nm

F. No electric field, Gradient (applied $V = 0.1$ Volt at $x = 10$nm) plus thermal motion + Van der Walls force (Red lines show the dielectric discontinuities)

$\rightarrow$ Average <u>current$J = 0.799$nA</u> measured at 8nm and 7nm

Important note

Current simulation uses dt$=$ 100fsec and computer speed limits to maximum time scale to 200psec $\sim$ 1nsec depending on configurations. But we need to run the simulation over 10 nsec to find the VALID current values considering ion current $\sim 10^8$ ions/sec (16pA). For current simulation, initial ion distance of 0.5nm was used which is equivalent to $n \sim 10^{27}$ ions/m^3 and about 100 times higher value than nominal ion concentration (n $\sim 10^{26}$ ions/$m^3 \leftarrow$ 0.15 mole). This may give higher current in shorter time frame (799 pA compared to 16 pA).

The life time of water molecule in hydrated ion is K $\sim$ 1nsec, Na $\sim 2-4$nsec, Ca $\sim$ 10nsec and Mg $\sim$ 10microsec. So for $f > 1$GHz, it may be considered water-ion compound as a double-layered ion cloud of radius R. This model is used here to simulate the dielectrophretic force.

Also we need to run 3D simulations (or 2D for cylindrical symmetry) to see the ion motions in 3D (2D) space.

OBJECTIVE: To explore possible theoretical models for the effects of highly in-homogeneous radio frequency fields on biological systems.

BACKGROUND: One of the open questions in the study of possible health effects of the electromagnetic fields from cell phones is “Are their theoretical reasons to believe that the fields from cell phones can effect biological systems by mechanism other than heating?” There are experimental results that are not as yet explained as effects of heating in spite of the fact that some experimental results that were first thought to be non-thermal have now been shown to depend on the rate of temperature rise.[**?**]

However, experimental measurements have failed to show rectification by way of a shift in the voltage across a cell membrane upon exposure to RF fields at frequencies above about 10*mhz*. [**?**] This thought to be the result of limitations of the distance an ion can be moved in half a cycle at higher frequencies. At this time mechanisms other than heating have no been confirmed.

METHOD: A theoretical model has been constructed of the various forces that affect the motion of both charged and uncharged molecules in the vicinity of the surface of a membrane. These forces include Van der Waals forces, Coulomb forces, solvent effects, diffusion of osmotic forces and dielectrophoric forces. Numerical methods are used to calculate the effect of these forces.

RESULTS: The calculations show that under the assumption that we have made that the fields in the low dielectric materials such as the membranes are approximately 30 times higher than the electric fields in high dielectric fluids such as the intra cellular and inter-cellular fluids. As the separation of membranes are often only a few nanometers and large protein molecules are known to project well beyond the average position of the lipid membrane surface fields are expected to vary rapidly in space when examined on the scale of nanometers. Under these condition we estimate the forces that are most likely to be effected by the application of RF fields at cell phone frequencies of 900MHz and 2GHz are the dielectrophoric forces and that these forces could lead to changes in the rate at which both charged and uncharged molecules move to the surface of the membrane. See Figures 1-x. The currents generated by these forces will be compared to those are expected from the background biological fields and diffusion.

DISCUSSION: It is expected that the currents of either ions or neutral molecules such as neural transmitters that are generated by the applied RF fields will have to be on same order as the natural currents if they are to be biologically significant. Among the biological studies that this theoretical work suggests are of interest are those looking for changes in growth rates and signaling such as might effect stress reactions and the immune system.