Bob Eisenberg <bob.eisenberg@gmail.com>

Treatment of finite size ions

Bob Eisenberg <beisenbe@rush.edu> **Tue, Nov 1, 2011 at 8:31 AM**
Reply-To: beisenbe@rush.edu
To: Weishi Liu <wliu@math.ku.edu>
Cc: Chun Liu <liu@math.psu.edu>, YunKyong Hyon <hyon@ima.umn.edu>, Bob Eisenberg <beisenbe@rush.edu>
Bcc: Yoichiro Mori <ymori@umn.edu>

Dear Weishi

I realized that I should write a little more.
First, I think it would be very useful indeed
for you to get hold of the wonderful book
on biomath

Gabbiani, F. and S. J. Cox (2010). Mathematics for Neuroscientists. New York, Academic Press.

This puts the channel work into a good biological context.
It has lots of well thought through membrane and cell biology in it.

I should also add that it would be a mistake for you to use DFT PNP as a description of the finite size of ions.

DFT PNP was our first attempt and was a lot better than nothing (and does quite well for the ryanodine receptor) but

a) it leaves out many of the physical effects THAT ARE KNOWN FOR SURE
to be important in ionic solutions. It turns out that DFT PNP assumes that the shape of the ionic atmosphere is the same at equilibrium and during flow. This is probably a decent approximation in the inside of the channel (because

most of the ionic atmosphere is the protein!) but it is DEFINITELY SERIOUSLY
WRONG in the antechambers and in bulk.

Fuoss, R. M. and F. Accascina (1959). Electrolytic Conductance. New York, Interscience.
Fuoss, R. M. and L. Onsager (1955). "Conductance of Strong Electrolytes at Finite Dilutions." Proc Natl Acad Sci U S A 41(5): 274-83.
Fuoss, R. M. and L. Onsager (1961). "Thermodynamic Potentials of Symmetrical Electrolytes." Proc Natl Acad Sci U S A 47(6): 818-25.

The definitive review (that I know about) is

Justice, J.-C. (1983). Conductance of Electrolyte Solutions. Comprehensive Treatise of Electrochemistry Volume 5 Thermondynbamic and Transport Properties of Aqueous and Molten Electrolytes. B. E. Conway, J. O. M. Bockris and E. Yaeger. New York, Plenum: 223-338.

It is hard to find so I include a copy for you.

b) It is "jury rigged" with complex integral formulas
that are not well defined mathematical approximations
and cannot be easily generalized. Rosenfeld (who created
this approach) explained this to me at length, before he
sadly passed away, and Chun has worked at length on
this, so I copy him on this email.

c) It is not the solution of a general physical model. In particular,
the minimization involved is not general for equilibrium systems
and is not applicable at all to nonequlibrium systems

d) The attached papers that Chun, YunKyong, and I have written
have a specific Lennard Jones model that fixes all this and is the
best known basis for dealing with finite diameter ions, as far as I
know (I say rather immodestly....) See eq 40-45 of the JCP EnVarA
paper and BEST OF ALL Section 3.2 of Hyon's Communications
paper, where things are more clear and succinct.

All questions, comments, and criticisms of this email are VERY

welcome!!

As ever
Bob

PS I also include some of the introductory papers on EnVarA by Chun and YunKyong which I think are helpful.

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6 attachments

Justice ComprehenTreatiseElectrochem optimized CHAP2-3.pdf

7826K

As Published EnVara J. Chem. Phys. 133, 104104 (2010).pdf
513K

Communications Mathematical Sciences May 2011 Hyon Eisenberg Chun.pdf
463K

Hyon Introduction to EnVarA Hyon March 2 2010.pdf
1205K

Introductiuon to EnVarA Chun Liu.pdf
755K

Hyon Kwak Liu Variational approach Dissipation Principle.pdf
846K
