EDLSim: Simulations of Electrical Double Layer at

Graphene SGFET-Electrolyte Interface

Technical Documentation and Theoretical Background

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**1D:** Simulate EDL properties in one dimension (x) representing distance away from one point on graphene

**Directory: EDLSim/1D/**

*Electrical Potential Profile (as function of distance x from graphene surface)*

1. A Boundary Value Problem with boundary conditions:

V(x = 0) = V0

V(x = D) = 0

where V0 is potential applied to graphene and D is a distance far enough away to not be unaffected by charges in graphene (~ 20 nm).

2. Shape of potential function with respect to x is determined by the Modified Poisson-Boltzmann equation (Kilic, Bazant, & Ajdari, 2007):



: permittivity

a: effective ion size

zi: valence of ion i

c0i: bulk concentration of ion i

3. Second derivative of V(x) is also given by the three-point formula:



4. We discretize V(x) as a set of points along the x-axis initialized along the line:



5. And solve for the equilibrium condition through an iterative process. Use equations in (2) and (3) to compute update step to minimize the objective error.

Repeat until max step size smaller than our convergence criterion:

For each point x except endpoints x = 0 and x = D:

Compute Vcalc(x) from:



Then relax V(x) toward Vcalc(x) with update function:



6. MATLAB Implementation:

The above algorithm is fully contained in the MATLAB function EDLSim/1D/potential\_1d.m.

In the code, ‘P’ stands for potential and is equivalent to ‘V’ as specified in the mathematical definitions above.

Specify all parameters of simulation in the function call. The signature is:

[X, P, R] = potential\_1d(P\_0, Zi, Ci, E\_R, EFF, MPB)

Input Parameters:

P\_0: applied potential

Zi: array of ion valence values (array size = # of ions)

Ci: array of ion bulk concentration values (array indices correspond with Zi)

E\_R: *relative* permittivity value (78.3 for H2O)

MPB: Set to **1** to use Modified Poisson Boltzmann formula.

Setting to **0** will implement regular Poisson Boltzmann without modification for steric effect of ion size

Outputs:

X: x-axis values of points

P: electric potential at all x points

R: second derivative of potential at all x points

Advanced parameters like resolution along x-axis and convergence criteria can be edited in first section of code labeled “Constants”

*+/- Ion Concentration (as function of distance x from graphene surface)*

Ion concentration distribution can be computed from potential function (P) returned by potential\_1d, according to the Boltzmann equation:



*Total EDL Charge (as a function of applied voltage V0)*

The charge distribution of the electrical double layer that forms at a given applied voltage can be calculated from the second derivative of potential (R) returned by potential\_1d, according to the Poisson equation:



Then integrate over all values x = 0 to x = D to get total charge in EDL.

This is repeated over a range of V0 values (first compute potential by passing in V0 to potential\_1d, then do computation above) to obtain charge as a function of applied voltage.

*Capacitance and Differential Capacitance (as a function of applied voltage V0)*

These follow directly from EDL charge v. V0, as calculated above.

 

**2D:** Simulate EDL properties in two dimensions – away from the graphene interface (x) and along the graphene channel from source to drain (y).

**Directory EDLSim/2D/**

**See README file**

*Electrical Potential Along Channel*

1. The following equation describes charge carrier density in graphene (Meric et al., 2008):



n0 : minimum sheet carrier density

Ctop : top gate capacitance

Vgs,top : top gate bias

with 

 and  are voltages at the Dirac point.

1. Source-drain current is described as:  
     
   

We characterize the drift velocity by a velocity saturation model:



 : ion mobility

E : electric field

vsat : saturation velocity of the charge carriers

From substituting –dV/dt for E and integrating both sides of the above, we derive the following form of the equation for source-drain current:



W: channel width

L: channel length