International Journal of Mathematics Trends and Technology
ISSN: 2231 – 5373 / https://doi.org/10.14445/22315373/IJMTT-V68I4P515
Volume 68 Issue 4, 94-101, April 2022
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Original Article

Stabilized Finite Element Method for Poisson Nernst-Planck Equations with Steric Effects for Ion Transport

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Received Date: 19 March 2022
Revised Date: 21 April 2022
Accepted Date: 26 April 2022

Abstract *- In this paper, Nernst-Planck(NP) equation for ion fluxes that uses Lennard Jones(LJ) potential to incorporate finite-size effects in terms of hard sphere repulsion was coupled with Poisson equations to form modified PNP(mPNP) system of equations. These coupled equations were then discretized using Galerkin finite element Method(GFEM) approach based on Taylor-hood elements with regular rectangular sub-domains. However, this method resulted into numerical oscillations in the approximate solution, necessitating stabilization to obtain desired results. Consequently, Stream-Upwind Petrov-Galerkin(SUPG)method which adds a mesh dependent term to the FEM together with iterative linearization was adopted resulting into a stable numerical scheme. The resulting linear system of equations was solved iteratively using preconditioned conjugate gradient(PCG) scheme to speed up convergence, where potential consistently updated the concentration components. Concentration profiles of two ion species under varied steric effects for mPNP and PNP were compared and analyzed.*

Keywords *- Modified PNP, Lennard Jones, Hard-sphere, SUPG, Finite-size effects.*

I. INTRODUCTION

Ion channels are proteins with pores down their middle, found in the membranes of biological cells [9]. These channels control access to the interior of cells enabling them to perform biological functions such as; signal transfers in the nervous system, regulation of secretion of hormones among others. The mechanisms of ionic flow within a channel as a function of ionic concentration, membrane potential and the structure of the channel is a central problem in molecular biophysics such as in[26].

Poisson-Nernst Planck (PNP) theory is a mean-field continuum model widely applied for describing ion flow in areas such as physics and chemistry. PNP treats electrostatic potential, concentration and ion fluxes in a consistent manner capable of providing accurate prediction for ion channels flows. Hence, the model have been extensively used for nano-fluidic systems, electrochemical diffusion and ion channel applications. Numerous numerical techniques have been applied to solve PNP equations, among them Finite Element method(FEM) is granted as most suitable for simulation of ion channels, due to the inbuilt and unmatched capabilities which enables them to adequately handle irregular geometries and nonuniform boundaries[3, 14, 15, 16, 20, 24]. Recently, FEM have undergone several modifications to improve accuracy, convergence rate and degrees of freedom. However, when computing approximate solution, system of PNP equations present several challenges using Galerkin FEM, attributed to non linearity calling for linearization. In addition, fluxes in PNP equations are convection-dominated hence introducing instabilities which may result into negative concentration in the approximate solution, see [11, 18]. Recently, robust approaches have been successfully applied to eradicate such difficulties, and stabilize the schemes, such as Stream-upwind Petrov-Galerkin (SUPG) methods[5, 10, 22] and Galerkin Least Square methods which adds mesh dependent terms to FEM.

SUPG method was considered by [18] for solving unsteady Naiver-Stokes equations in 2D, which besides eliminating oscillations it also incorporated small time increments to obtain stable solutions. Equally, [4] developed stabilized schemes for simulation of ion transport. SUPG methods and the Pseudo Residual free bubble function was introduced to enhance the robustness and convergence performance of the finite element algorithm in the ion channel. The two schemes gave reasonable results which are in agreement with experimental data and Brownian motion. [12] solved 3D PNP model using SUPG and interior penalty(IP) method which adds a penalizing term corresponding to gradient jumps across element boundaries to enforce smooth solution. The scheme was successfully applied to KcsA ion channel and the results showed numerical stability and robustness of SUPG.

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Transformation using slotboom variable[21, 6] or quasi-fermi variable approach [17, 7] was also utilized to address numerical difficulties of the nonlinear systems. An efficient numerical algorithm of finite difference for solving 3D steady state PNP equation using excess chemical potential of mobile ions described by classical density function theory was developed in [13]. In these algorithms, the Nernst Planck equations were transformed into the Laplace equation through the slotboom transformation. The algebraic multigrid method was applied to efficiently solve the system and excess chemical potentials were calculated through fast Fourier transforms to reduce computational complexity. The numerical results were established to be in agreement with experimental data. [8] presented an efficient nonlinear FE solver for solving PNP ion channel model with Neumann boundary conditions and membrane surface charge density. In some instances, slotboom variables transformation was introduced for each NP equations together with modified Newton iterative scheme to improve accuracy. Subsequently, [25] developed mathematical model for finite size effects using a regularized Lennard Jones (LJ) repulsive potential and Density function theory under energy variational framework enabling numerical verification to recover layering behaviour. This resulted into development and application of Edge Average finite element method to solve systems of mPNP coupled with convex iteration scheme ensuring self-consistency between ionic concentrations and electrostatic potentials.

Building up from our previous study that demonstrated existence of approximate solution for system of mPNP [1]and numerical simulation of mPNP equation [2], we now use SUPG approach to stabilize GFEM to solve 2D steady PNP with LJ potential for hard-sphere repulsion accounting for the steric effects. Approximate solutions are then compared with those obtained using Galerkin FEM. Iterative linearization was also adopted for nonlinear terms and an efficient preconditioned-conjugate gradient method for iteration of the resulting linear system of equation to improve convergence and stability of the schemes. Main aim of this study was to derive an effective modified PNP(mPNP)model which describes ion interaction based on hard-sphere repulsion. The emerging LJ potential in the energy functional for modeling hard-sphere repulsion using band limit function which cut-off higher frequencies and preserve spatial frequencies in Fourier modes,is derived in [19].

This paper is organized as follows:In section two we discuss ion transport models with finite size effects. We also demonstrate modification of the Nernst-Planck equation using LJ potential to in-cooperate hard sphere repulsion and the imposed boundary conditions. Section three explains the numerical techniques used to solve the nonlinear system of mPNP equations. Whereas, in section four, we present the numerical results and discussions. Then make concluding remarks and recommendation for future study in section five.

II. MATHEMATICAL MODEL

A. Poisson Nernst-Planck equation with Steric effects

Consider a continuum flow in two dimensional rectangular domain, $\Omega \in \mathbb{R}$ of unit thickness representing a channel in cell membrane. The PNP equations are given by;

$$\frac{\partial c_i}{\partial t} = \nabla . D_i(\nabla c_i + \frac{c_i}{K_B T} z_i e \nabla \Phi), \quad i = 1, \dots N \tag{2.1a}$$

$$-\nabla . (\varepsilon \nabla \Phi) = \sum_{i=1}^{N} z_i e c_i \tag{2.1b}$$

with (2.1a) and (2.1b) representing Nernst-Planck (NP) equation the Poisson equations respectively. Where c_i and z_i are concentration and valence for the ith ion species, φ is the electrostatic potential, K_B is the Boltzmann constant, T is the absolute temperature, N is the number of ions, e is the unit charge and D_i is the diffusion coefficient of ion species, and ε is the coupling energy constant.

The modified form of the PNP equation is obtained by adding a nonlinear term comprising of the Lennard Jones repulsive potential to the NP equation. The repulsive potential accounts for finite size effects of ions by incorporating the ion interaction which are modeled as infinitesimal hard spheres in a rectangular space with unit thickness. Contribution of the potential to the total free energy functional is given by

$$E = \int (K_B T \sum_{i=1}^{N} c_i \ln c_i + \frac{1}{2} \sum_{i=1}^{N} z_i e c_i \Phi) dx + \sum_{i,j=1}^{N} \iint \frac{\varepsilon_{ij}}{2} \frac{(a_i + a_j)^{12}}{|x-y|^{12}} c_i(x) c_j(y) dx dy \tag{2.2}$$

a_i and a_j are the radii of the i^{th} and j^{th} and ε_{ij} becomes their coupling energy constant, in which we assume $\varepsilon_{ij} = \varepsilon_{ji}$. Variational derivative with respect to each ion $\delta E / \delta c_i$, we obtain repulsive energy term into the system of equations resulting into a Nernst-Planck equation for charge densities as

$$\frac{\partial c_i}{\partial t} = \nabla . D_i \left(\nabla c_i + \frac{c_i}{K_B T} z_i e \nabla \Phi + \frac{c_i}{K_B T} \sum_{i=1}^{N} \nabla \int_{\Omega} \varepsilon_{ij} \frac{(a_i + a_j)^{12}}{|x-y|^{12}} c_j(y) dy\right) \tag{2.3}$$

where the first, second and third terms in (2.3) are respectively, diffusion, drift driven by electrostatic potential in the field and the hard sphere potential that characterizes finite size of ions depending on the ion species.

Major computational challenge arises when solving equations (2.2)-(2.3) due to inefficiency in simulation occasioned by the effects of high frequencies. To address the problem and the resultant inaccuracy, we employ a band-limit function which depends on a cut-off length σ to eliminate the high spatial frequencies and preserve the bounded spatial frequencies, see [19, 23]. The cut-off length is a parameter whose value tends to zero for better approximation. Using band-limit function and fourier analysis, an approximate energy functional is derived which reduces the numerical complexity of the repulsive term in the LJ potential describing ion interaction represented as [19]

$$E_\sigma = \int (K_B T \sum_{i=1}^{N} c_i \ln c_i + \frac{1}{2} \sum_{i=1}^{N} z_i e c_i \Phi) dx + \sum_{i,j=1}^{N} \iint \frac{\varepsilon_{ij}}{2} (a_i + a_j)^{12} c_i(x) c_j(y) dx dy \tag{2.4}$$

where $S_\sigma \approx \sigma^{d-12}$, the dimensional space $d \leq 3$.

Applying variational derivative in equation (2.4) for each charge density we obtain reorganized mathematical model given by

$$\frac{\partial c_i}{\partial t} = \nabla . D_i \left(\nabla c_i + \frac{c_i}{K_B T} z_i e \nabla \Phi + \frac{c_i}{K_B T} \sum_{i=1}^{N} \nabla S_\sigma \varepsilon_{ij} (a_i + a_j)^{12}\right) \tag{2.5}$$

Decomposing the model for the two ion species, c_n (negative) and c_p (positive) in steady state, equation (2.5) is simplified to obtain diffusive rates of ion concentrations given by

$$D_n \left[\nabla . \left(\nabla c_n + \frac{z_n}{K_B T} c_n \nabla \Phi\right) + S_\sigma \nabla . (g_{nn} c_n \nabla c_n + g_{np} c_n \nabla c_p)\right] = 0 \tag{2.6a}$$

$$D_p \left[\nabla . \left(\nabla c_p + \frac{z_p}{K_B T} c_p \nabla \Phi\right) + S_\sigma \nabla . (g_{pp} c_p \nabla c_p + g_{np} c_p \nabla c_n)\right] = 0 \tag{2.6b}$$

where $g_{nn} = \varepsilon_{11}(2a_1)^{12}$, $g_{np} = \varepsilon_{12}(a_1 + a_2)^{12}$ and $g_{pp} = \varepsilon_{22}(2a_2)^{12}$. Coupling equation (2.6a) and(2.6b) with (2.1b), we obtain the nonlinear system of mPNP equations.

1.1 Boundary and initial conditions

Then imposing Dirichlet boundary conditions by specifying ion concentrations and potential at the channel inlet and outlet for the domain as

$$\begin{gathered} c_n(x,0) = c_p(x,0) = H_1 \\ c_n(x,0.1) = c_p(x,0.1) = 0 \\ \Phi(x,0) = H_2, \ \Phi(x,1) = 0, \qquad x, y \in \partial\Omega \end{gathered} \tag{2.7}$$

where $H_1 > 0$ and $H_2 > 0$ are constants. For completeness, we prescribe Neumann boundary condition at the channel walls for both concentration and potential, representing no flux conditions and given by

$$\begin{gathered} \left[(\nabla c_n + \frac{z_n e}{K_B T} c_n \nabla \Phi) + S_\sigma \nabla . (g_{nn} c_n \nabla c_n + g_{np} c_n \nabla c_p)\right] . n = 0 \\ (\varepsilon \nabla \Phi) . n = 0 \end{gathered} \tag{2.8}$$

where electro-neutrality condition is assumed for the charge densities

$$\lim_{x \to \infty} c_n(x,0) = c_p(x,0) \tag{2.9}$$

III. NUMERICAL METHOD

This section reduces the model to a two dimensional systems of modified PNP equations given by equation (2.6) and (2.1b), redefine numerically the boundary conditions in section 2.2. We then consider two ion species denoted by n and p, with valencies taken to be $z_n = -1$ and $z_p = 1$, and radii $a_1 = 1.5$Å and $a_2 = 2.0$Å, respectively. Diffusion coefficients were taken to be $D_n = 2.0305 \times 10^{-5}$and $D_p = 1.335 \times 10^{-5}$ for negative and positive ions respectively and flow assumed to be in the y-axis and normal to the x-axis.

A. Galerkin Finite Element Method

The study examined use of Taylor-hood rectangular discretization of the systems of mPNP and PNP equations with 9 nodes for concentration and 4 nodes for potential variables. Shape functions were derived using local co-ordinates(η,ξ) to

express the components in form of 4-noded bilinear elements and 9-noded quadratic element denoted by M_j for $j = 1,\ldots 4$ and N_i for $i = 1,\ldots 9$ respectively. The resulting quadratic interpolation functions are used for concentration components, c_n and c_p while bilinear interpolation functions for potential component, Φ. Resulting into 22 unknown variables for each subdomain are applied to uniform partition of the whole domain, Ω. To overcome non linearity in the equations, the unknown was expressed in iterative form as

$$c_n^{k+1} = c_n^k + \widehat{c_n}, \quad c_p^{k+1} = c_p^k + \widehat{c_p}, \quad \Phi^{k+1} = \Phi^k + \widehat{\Phi}, \tag{3.1}$$

where c_i^k and Φ^k are the previous known values while $\widehat{c_i}$ and $\widehat{\Phi}$ are the corrected values.

For novelty purposes we let $S_1 = S_\sigma g_{nn}$, $S_2 = S_\sigma g_{np}$ and $S_3 = S_\sigma g_{pp}$ and ${}^{e}/_{K_B T} = q$ in equation (2.6), hence obtaining

$$D_n \nabla.(\nabla c_n - q c_n \nabla\Phi + S_1 c_n \nabla c_n + S_2 c_n \nabla c_p) = 0 \tag{3.2a}$$
$$D_p \nabla.(\nabla c_p - q c_p \nabla\Phi + S_1 c_p \nabla c_p + S_2 c_p \nabla c_n) = 0 \tag{3.2b}$$

To express components of equation (3.1) in terms of shape functions we have

where c_{nj}, c_{pj} and Φ_j are the parameter measurements at the nodes. Consequently, employing Galerkin weighted residual approach and weight function to the coupled constitutive equations(3.2)and (2.1b) results into a set of algebraic linear system of equations. Subsequently, we seek a solutions of the form $c_i \in [H_0^1]^2$ and $\Phi \in L_2(\Omega)$ satisfying the boundary conditions in section 2.1. At this instance concentration and potential equations (3.2) and (2.1b) are reduced into weak forms with help of divergence theorem to obtain

$$R(c_i, w) = D_i \int_\Omega (\nabla c_i - q c_i \nabla\Phi + S_j c_i \nabla c_i).\nabla w \, \partial\Omega = \int_\Omega f_i \, . w \, d\Omega, \quad j = 1,2 \text{ or } 3 \tag{3.3a}$$

$$\int_\Omega \varepsilon \nabla\Phi.\nabla\varphi \, d\Omega = \int \sum_{i=1}^{N} z_i \, e c_i \varphi \, d\Omega - \oint_\Gamma \varepsilon \frac{\partial\Phi}{\partial\eta} \varphi d\Gamma, \quad i = n, p \tag{3.3b}$$

wherew $\in H_0^1(\Omega)$ and $\varphi \in L_2(\Omega)$ are the weight function and η is the unit outward normal for each control volume.

B. Stabilized Finite Element Method

Since application of the standard Galerkin FEM in NP equation (3.3a) results into oscillations in the computed numerical solutions, need for stabilization of the numerical scheme arises. Stream Upwind Petrov-Galerkin(SUPG) mesh dependent stabilization term is added to the weak form of NP equation to improve the results and redefining of the Peclet number as strength of convection intensity and given by

$$pe_T = 0.33 \frac{\|b_i\|_2 h_T}{2D_I} \tag{3.4}$$

Where $b_i = -\frac{D_i \nabla\varphi}{K_B T}$ and h_T is the diameter of the element,T. Stabilization parameter is given by

$$T_k = \frac{h_T}{2\|b_i\|_2} \psi(pe_T) \quad \text{and} \quad \psi(pe_T) = \begin{cases} 1, & if\ pe_T > 1 \\ pe_T, & otherwise \end{cases} \tag{3.5}$$

Then the notations are used we regenerate improved NP equations containing the weak form and SUPG stabilization term as

$$R(c_i, w) + \sum_T \int_T D_i \nabla \cdot (\nabla c_i - \square c_i \nabla\Phi) + S_j c_i \nabla c_i) \, . w_{supg} \square\square = \int_\Omega f_i w d\Omega + \int_T f_i w_{supg} dT. \tag{3.6}$$

where $w_{supg} = T_k b_i . \nabla w$ is the stabilization parameter. The SUPG scheme helps to stabilize the mPNP equation, however it is very costly to implement the scheme due to the strong form of the nonlinear SUPG term in equation (3.6), since integration by parts is not applied to reduce the order. Therefore, equation (3.6) and (3.3b) are decoupled and solved iteratively for potential with initial concentration values, the updated potential values are then imposed on the NP equations, which are solved using preconditioned conjugate gradient method to improve convergence of the numerical scheme. The process is repeated until accepted tolerance is achieved.

IV. NUMERICAL RESULTS AND DISCUSSION

Now, we consider two monovalent ion species in closed domain, Ω to describe the effects of steric components S_1, S_2 and S_3 on dynamics of concentration for mPNP and compare with PNP model using stabilized FEM and standard Galerkin FEM. We take $\varepsilon = 1$, $q = 1$, $e = 1$ and $T_{kn} = 3.059 \times 10^{-3}$ and $T_{kp} = 4.015 \times 10^{-2}$ stabilization parameters for c_n and c_p, respectively. Figures 2, 3 and 4 illustrates the results obtained for mPNP using Galerkin FEM, whereas Figures 5, 6 and 7 are results obtained using SUPG method. We end up determining the effects of variation of the steric components on ion concentration for mPNP system.

Upon varying S_1 when S_2 and S_3 are held constant increases the repulsive forces between anions allowing upsurge in penetration and flow of cations in the channel. The changes in flow of the ions did not synchronize with changes in steric component, some steric values displayed negative concentration as demonstrated in Figure 2. Increase in the positive steric component, S_3 creates increase in the repulsive forces between cation, permitting more anions to be adsorbed and accumulated than cations in the ion channel, see Figure 4. The minimal change in flow of cations noted upon varying S_3 values, is attributed to frequent collision and competition between them. Finally, a slight increase in the attractive steric component, S_2 is observed to induce increase in flow of both ions as illustrated in Figure 3. However the adsorption of anions was observed to be higher than cations.

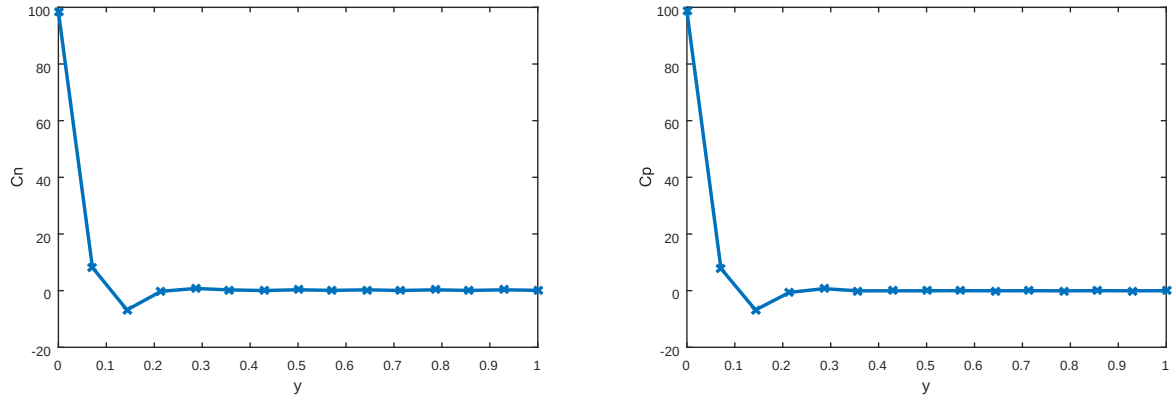

Fig. 1 PNP for Ions concentration c_n and c_p

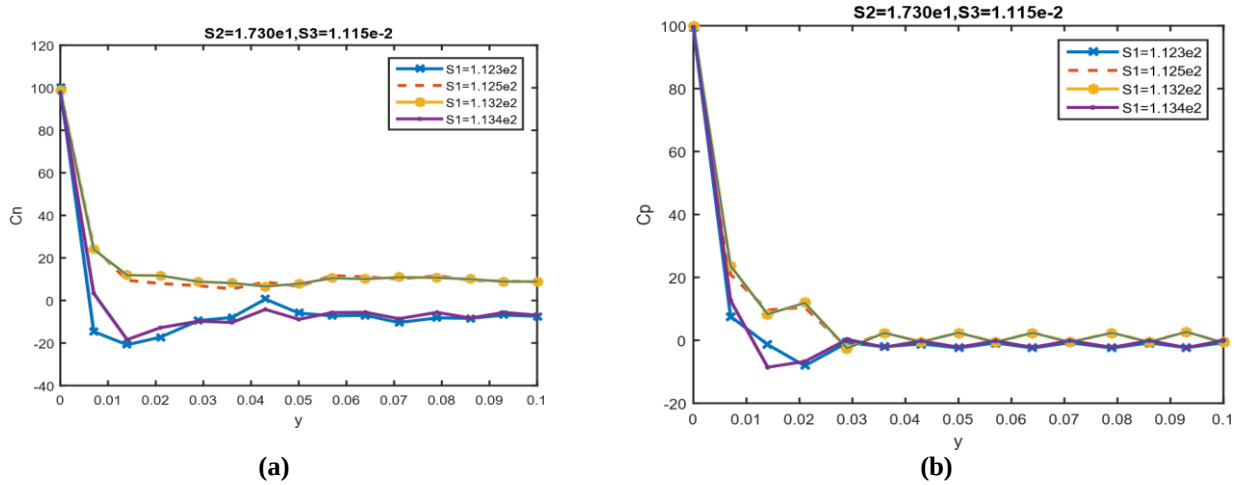

Fig. 2 Galerkin FEM for Ions concentration with varying negative steric values S_1

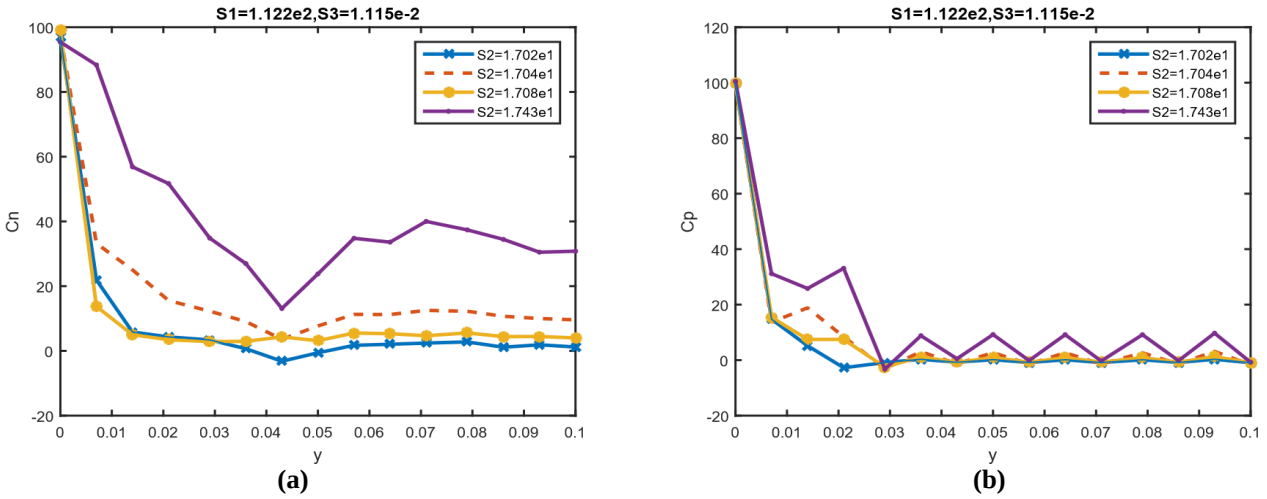

Fig. 3 Galerkin FEM for Ions concentration with varying attractive steric values, S_2

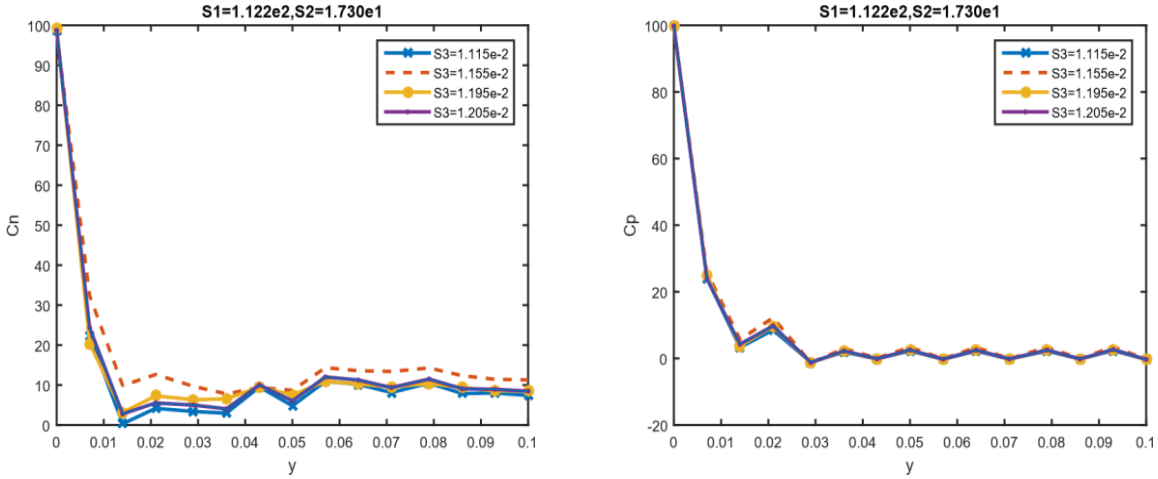

Fig. 4 Galerkin FEM for Ions concentration with varying positive steric values, S_3

The SUPG scheme was utilized to stabilize the numerical scheme and results displayed in Figures 5, 6 and 7. Comparing these results with Galerkin FEM scheme for solving the mPNP system we obtain better and improved results. It is observed that sight increase in steric components S_1, S_2 and S_3 resulted in increase of concentration for both cation and anions. However, the flow was much faster for anions, see Figure 5-7. The variation of repulsive forces of anions, S_1 holding S_2 and S_3 constants and repulsive forces of cations S_3 taking S_1 and S_2 to be constants, resulted into increase in flow of both ion species corresponding to insignificant increase in steric values. The flow in cations was shown to be minimal compared to anions and this may be due to larger size of cations, increase in repulsive forces between them leads to frequent collisions preventing their flow. Whereas, the anion have smaller radius size allowing more penetration when they interact. Varying the attractive forces between the ions, S_2, resulted in minimal flow for both anions and cations, see Figure 6.

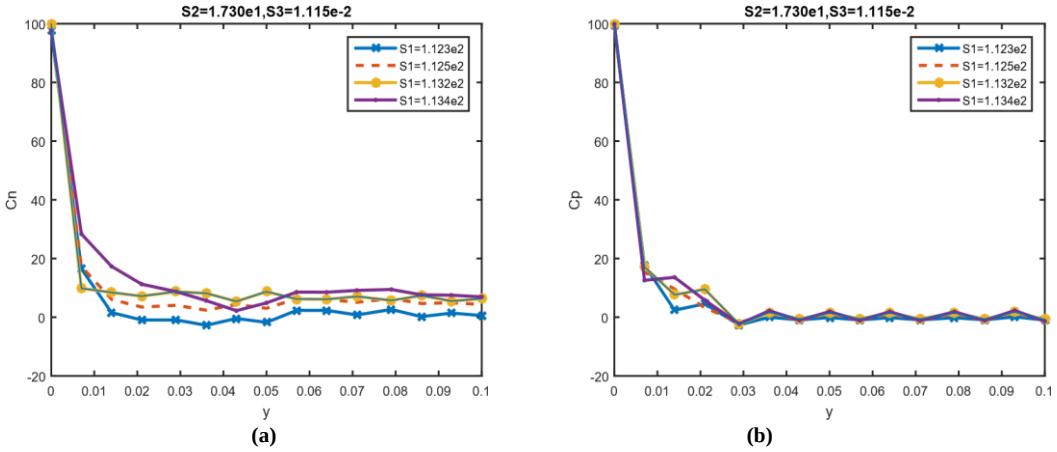

Fig. 5 SUPG stabilization for Ions concentration with varying steric component, S_1

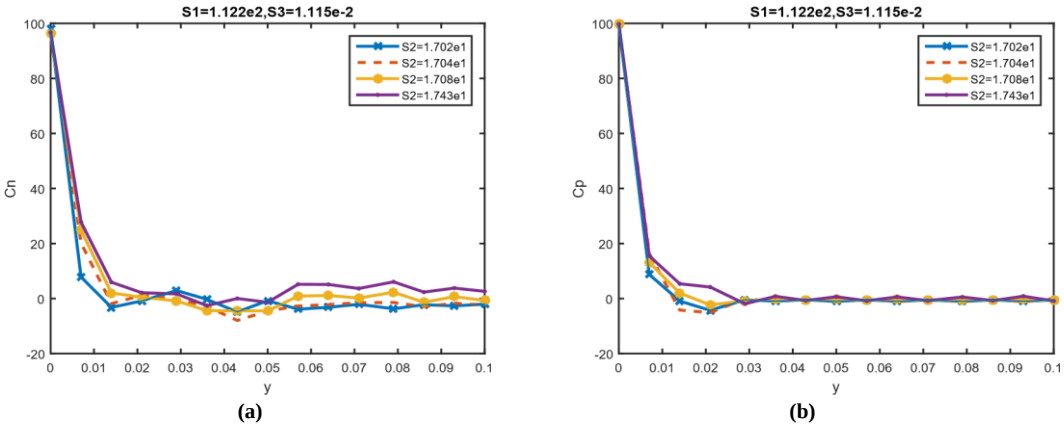

Fig. 6 SUPG stabilization for Ions concentration with varying steric component, S_2

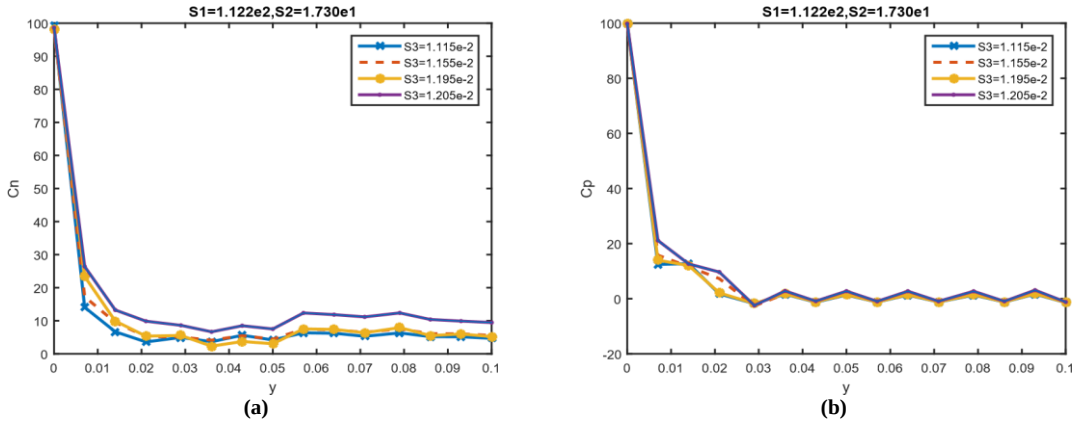

Fig. 7 SUPG stabilization for Ions concentration with varying steric component, S_3

It can be deduced that SUPG method gave stable approximate solution showing the dynamics of concentration with varying steric components compared to the Galerkin FEM for mPNP and PNP equations in Figure 1. From the results presented in Figures 2 and 3 it is evident that finite size of ions plays a crucial role in the flow and accumulation of ions in the ion channel. The diffusion of anions is also observed to be faster than cations in all the variations, this may be as a result of bulk mobility of the anions which is higher than the cations in the channel caused by larger radius size of cation compared to anions.

Table 1. Mesh refinement for number of elements, N to determine the convergence after I iterations

Iterations (I)	Absolute errors in c_i for N elements			
	N = 36	N = 49	N = 100	N = 144
I = 10	0.0700	0.0579	0.1507	0.2825
I = 40	0.0063	0.0088	0.0067	0.0079
I = 70	0.0028	0.0041	0.0036	0.0042
I = 100	0.0018	0.0028	0.0027	0.0032

The stability is demonstrated by convergence of our numerical scheme in Table 1, which enlists the number of iterations and corresponding to the absolute global error in concentration. The error was found to reduce as iteration increases.

V. CONCLUSION

This paper presents approximate solutions for PNP with hard-sphere repulsion for Galerkin FEM, SUPG with stabilization. SUPG stabilization of GFEM eliminates inconsistency in the computed solution enabling establishment of distinction between the flow in relation to steric components qualitatively. It is observed that finite size effects impacted on the flow of ion, evident by changes in ion flow as a result of insignificant increase in all steric components. The anions were particularly, observed to flow faster and accumulate more than cations. Mesh refinement and increase in the number of iterations resulted in error reduction demonstrating stability and convergence of the numerical scheme. We were able to undo the main challenge in using the SUPG scheme which is the choice of optimum stabilization parameter crucial in obtaining stable solutions, and compare results against those obtained using Galerkin FEM. The impact of the steric effects and extension to multiple ion species competition in unsteady mPNP model forms an integral future area of study.

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