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Efficient Time-Stepping/Spectral Methods for the Navier-Stokes-Nernst-Planck-Poisson Equations

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Abstract. This paper is concerned with numerical methods for the Navier-Stokes-Nernst-Planck-Poisson equation system. The main goal is to construct and analyze some stable time stepping schemes for the time discretization and use a spectral method for the spatial discretization. The main contribution of the paper includes: 1) an useful stability inequality for the weak solution is derived; 2) a first order time stepping scheme is constructed, and the non-negativity of the concentration components of the discrete solution is proved. This is an important property since the exact solution shares the same property. Moreover, the stability of the scheme is established, together with a stability condition on the time step size; 3) a modified first order scheme is proposed in order to decouple the calculation of the velocity and pressure in the fluid field. This new scheme equally preserves the non-negativity of the discrete concentration solution, and is stable under a similar stability condition; 4) a stabilization technique is introduced to make the above mentioned schemes stable without restriction condition on the time step size; 5) finally we construct a second order finite difference scheme in time and spectral discretization in space. The numerical tests carried out in the paper show that all the proposed schemes possess some desirable properties, such as conditionally/unconditionally stability, first/second order convergence, non-negativity of the discrete concentrations, and so on.

AMS subject classifications: 76M10, 76M22, 65M12

Key words: Navier-Stokes-Nernst-Planck-Poisson equations, stabilized finite difference schemes, spectral method.

1 Introduction

The Navier-Stokes-Nernst-Planck-Poisson (NSNPP) equations play role in both physical chemical modelling and electrohydrodynamic model. It has been frequently used to

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model the interactive behavior of charged colloidal particles, electro-hydro, and micro-/nano-fluidic dynamics. In collochemistry, precise description of the aggregation, separation, and sedimentation of charged colloidal particles is needed. In some application fields, there is need to design micro-/nano-fluidic devices to control the separation, mixing and pumping of some specific substances. Suitable computational models can be useful in a better understanding of the electrokinetic phenomena occurring in such applications, and thus helpful to improve the design of related devices.

Electrokinetic phenomena are a family of several different effects that occur in heterogeneous fluids, or in porous bodies filled with fluid, or in a fast flow over a flat surface. These phenomena were first observed by Reuss [12] in 1809, which is now known as electroosmosis or electrophoresis, depending on different generation mechanism of electrokinetic flows. The electric double layer (EDL) is the common source of the two phenomena. For the detail of the phenomena, one can refer to [8,9]. Applying the electrokinetic effect, the movement of fluid and dispersed particles can be controlled by electric field without other moving parts. The results of these theories have many applications in industry, such as dehydration and purification of certain materials, isolation and identification of enzyme, protein and virus, drug delivery, desalination, and membrane filtration. In addition, it can also be used to improve the performance and service life of lithium cell and other fuel cell.

Several models describing the electrokinetic flows have been used in the past. Poisson-Boltzmann equation describes the EDL system for the net charge distribution. Applying the thin double layer limit by asymptotic analysis, the EDL can also be modelled by the Nernst-Planck-Poisson equation [1]. As compared to the above two models, the incompressible Navier-Stokes-Nernst-Planck-Poisson equation set (NSNPP) is a more general model to describe the electrokinetic flows [9, 14]. It combines three parts: (1) Navier-Stokes equations modelling the movement of the fluid field under the action of the internal and external electric fields; (2) Nernst-Planck equations for the positive and negative ionic-densities; (3) Poisson equation for the internal potential. Schmuck [13] analyzed the well-posedness of the NSNPP system, and proved the existence and uniqueness of the solution when the domain is open bounded and convex in $\mathbb{R}^d$ for $d=2,3$. Deng et al. [3] established the well-posedness of the NSNPP system in spatio-temporal unbounded domain. In recent years, several numerical methods have been proposed to solve this couple system. Yang et al. [18] applied artificial compressibility method and approximated the system by a finite difference/alternative direction method. Tsai et al. [16] employed this method in capillary electrophoresis microchips, and tested some injection systems with different configurations. Valencia et al. [17] combined the operator-splitting and finite element method for the numerical solution in some limit cases. Prohl and Schmuck [10] used finite element method for spatial discretization and an implicit temporal discrete scheme which preserves non-negativity of the ionic concentrations. They also considered a Chorin's type projection method, which is easier-to-implement, but does not preserve physically relevant properties.

In this paper, we aim at proposing and analyzing some efficient methods for numer-