CHALMERS

TITLE OF PROJECT

Master's Thesis in ...

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Abstract

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Acknowledgements

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The Authors, Location 11/9/11

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Introduction

Short intro for this section

1.1 Background

Historically - LBM and modelling of electrohydrodynamics. Development til today.

1.2 General problem description

Description of problem + what we want to achieve in this work.

1.3 Outline

How is this report structured?

2

Electrohydrodynamics in microchannels

In this chapter some fundamental physics behind electrokinetic flow, important for later discussions, will be presented. Also a modelling approach based on the coupling of Navier-Stokes, Nernst-Planck and Poission's equations is given.

2.1 Electrical double layers

Consider an electrically neutral liquid, i.e. a liquid containing the same amount of positive and negative ions. When this liquid is introduced to, for example, a negatively charged surface, this even charge distribution is disturbed in an area close to the surface. Due to the introduced electrostatic forces, positive ions will be attracted to the surface leaving a positive net charge in the vicinity of the surface. It is possible to divide this positively charged region in the liquid into two different layers. In the direct vicinity of the surface, positive ions will adsorb onto the surface making them less mobile than the others in the positively net charged area closer to the bulk liquid. The two layers are often referred to as the Stern layer (adsorbed) and the diffusive layer (mobile). This is also illustrated in fig. **??** [**?**]

The interface between the Stern and the diffusive layer is often called the shear plane. Due to the difficulty of measuring the potential at the true surface, i.e. the one in contact with the Stern layer of the liquid, most models in the field of electrokinetics use the shear plane as the boundary for which it exists accurate methods to measure the potential [**?**]. The potential at the shear plane will, from heron, be referred to as the ζ-potential.

To be able to model the flow dynamics of liquids in a channel with present EDLs, the potential and charge distribution in the channel must be determined. These quantities are mutually related through Poisson's equation for electrostatics:

$$\nabla^2\psi = -\frac{\rho_e}{\epsilon_r\epsilon_0} \tag{2.1}$$

where ψ is the electrical potential, ρ_e the electrical charge density, ϵ_r is the relative permittivity and ϵ_0 the vacuum permittivity. Under certain assumptions, the charge density may be explicitly determined as a function of the potential distribution, one such result is the so called Poisson-Boltzmann equation.

2.2 Poisson-Boltzmann equation

A simple and commonly used approach for determining potentials (and charge distributions) in systems with present EDLs is by solving eq. (2.1) with a charge distribution of Boltzmann type. Here follows a brief derivation of this term together with some discussion on the assumptions made.

The fundamental assumption that the derivation of the charge distribution is based on, is the fact that the system is assumed to be under thermodynamical equilibrium. I.e. forces, acting on the ions, due to chemical diffusion from concentration gradients and from the electrical field are therefore balancing each other. In one dimension:

$$\frac{d\mu_i}{dx} = -z_i q_e \frac{d\psi}{dx} \tag{2.2}$$

where μ_i is the chemical potential for species i, z_i is the relative charge of species i, q_e the fundamental charge and ψ is the EDL potential. The chemical potential is given by [**?**]:

$$\mu_i = \mu_i^\infty + k_B T \ln n_i \tag{2.3}$$

where μ_i^∞ is a reference value for the chemical potential, here the potential value far from the charged wall is used, $k_B T$ is the thermal energy and n_i is the ion concentration of species i. This expression plugged into eq. (2.2) gives

$$\frac{d\ln(n_i)}{dx} = -\frac{z_i q_e}{k_B T}\frac{d\psi}{dx}. \tag{2.4}$$

The charge density is determined by solving eq. (2.4) for n_i, i.e. integrating the equation. In order to avoid introducing additional unknown quantities, the equation is integrated to far away from the wall where the potential from the EDL has decreased to zero and where the concentrations, n_i^∞, of the ions are known.

$$\int_x^\infty d\ln(ni(x')) = -\frac{zq_e}{k_B T}\int_x^\infty d\psi(x') \tag{2.5}$$

This finally gives an expression for $n_i(x)$:

$$n_i(x) = n_i^\infty \exp\left(-\frac{z_i q_e \psi(x)}{k_B T}\right). \tag{2.6}$$

and ρ_e is given by

$$\rho_e = q_e \sum_i z_i n_i. \tag{2.7}$$

Summarising eqs. (2.1), (2.6) and (2.7) gives the Poisson-Boltzmann equation in one dimension

$$\frac{d^2\psi(x)}{dx^2} = -\frac{q_e}{\epsilon_r \epsilon_0} \sum_i z_i n_i^\infty \exp\left(-\frac{z_i q_e \psi(x)}{k_B T}\right). \tag{2.8}$$

2.2.1 The Debye–Hückel approximation

The non-linear nature of eq. (2.8) complicates when it comes to solving it. Especially in the past when the computational power at hands were rather limited. A linearisation is therefore sometimes done, this linear version of the PB equation is often referred to as the Debye–Hückel approximation. In this work, when it comes to the solving the PB equation, the full non-linear version will be considered. The solution of the linearisation gives however, something to compare with and will be used when defining a characteristic length scale of the EDL.

For a 1:1 electrolyte solution, eq. (2.8) reduces to

$$\frac{d^2\psi(x)}{dx^2} = \frac{2n^\infty q_e z}{\epsilon_r \epsilon_0} \sinh\left(\frac{z q_e \psi(x)}{k_B T}\right). \tag{2.9}$$

and the linearised equation is

$$\frac{d^2\psi(x)}{dx^2} = \frac{2n^\infty q_e^2 z^2}{\epsilon_r \epsilon_0 k_B T}\psi(x) = \kappa^2 \psi(x) \tag{2.10}$$

where κ^{-1} is the Debye length and gives a measure for the characteristic size of the EDL.

2.2.2 Limitations of the Poisson-Boltzmann model

From the derivation of the Poisson-Boltzmann equation above, two main assumptions are made. First the system is considered to be at thermal equilibrium. And second the system is assumed to infinitely large.

In this work, flows of ionic solution will be studied and the assumption with thermodynamical equilibrium does not apply. However for low-speed flows the model may still be a decent approximation, which will be investigated.

The second assumption, may also stay unfulfilled in some cases investigated here. The fluid in contact with the wall must be of substantial size in relation to the EDL thickness. There will be cases where the choice of ζ potential in combination with thin channels will make this assumption not fulfilled.

Since the PB equation is unable to model the system of interest, a different approach will be presented. However, throughout this work, references and comparisons with the PB model will be made.

2.3 Nernst-Planck

2.4 Navier-Stokes

2.5 Pressure-driven electrokinetic flow

How does the presence of el. fields affect the flow? Streaming potential etc.

2.6 Physical model

The three coupled equations described earlier...

3

The lattice-Boltzmann method

short intro of this section

3.1 Historical overview

A few words on the history of the method. Lattice automata etc.

3.2 Maybe something on asymptotic analysis

Some theory that could be useful in the chapman-enskog derivations.

3.3 Basic idea

The principle behind the method, what it does and does not.

3.4 Collision operator

discussions on different col. operators, focus on BGK since that is the one used.

3.5 Streaming

maybe not so much to say here

3.6 Boundary conditions

discussion and description of the boundary conditions

3.6.1 bounce back

accuracy, e.g. second order accurate if placed between node planes...

3.6.2 slip

3.6.3 he-zou, constant density/velocity

3.6.4 Maybe something on non-local boundary conditions

3.7 Forcing schemes

how to add a "forcing" term in the method.

3.8 LBM for Navier-Stokes

3.8.1 Chapman-Enskog

3.9 LBM for Poisson's equation

3.9.1 Chapman-Enskog

3.10 LBM for Nernst-Planck

3.10.1 Chapman-Enskog

3.11 Algorithm/Scheme for solving the coupled equations

the iterative scheme used.

4

A few notes on high performance computing

intro what is said below refer to computers of a certain architecture...

4.1 The pipeline

keep it full.

4.2 Locality

using the caches in a good way. some examples of its importance.

4.2.1 Locality and LBM

4.3 Parallelisation

shared memory, distributed memory...
data dependence, LBM good!
OpenMP/MPI

4.4 Maybe something about profiling

men kanske inte tillför något vettigt.

4.5 Choice of programming language

4.6 Some stats on the performance of the code...

Lattice updates/s

5

Model benchmarks

intro 2D

5.1 Poiseuille

Navier-Stokes density + velocity profiles.

5.2 Helmholtz equation

Poisson's eq.

5.3 Advection-Diffusion

Before the implementation of the Nernst-Planck part of the model is tested, a special case is considered, i.e. when the electrical potential in the domain is constant. This makes the source term including the electrical potential in eq. (**??**) vanish and we have to solve only for advection and diffusion.

Introducing characteristic scales for the concentration (C_0), advective velocity (u_0) and length (l_0) respectively, gives the non-dimensional advection-diffusion equation for incompressible flow:

$$\frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C = \frac{D}{u_0 l_0} \nabla^2 C. \tag{5.1}$$

All variables in (5.1) are non-dimensional. The quantity $Pe = u_0 l_0 / D$ is often referred to as the Péclet number. It determines the relation between contributions to the dynamics from advection and diffusion respectively. For $Pe \gg 1$ the dynamics is dominated by advection and for $Pe \ll 1$ by diffusion.

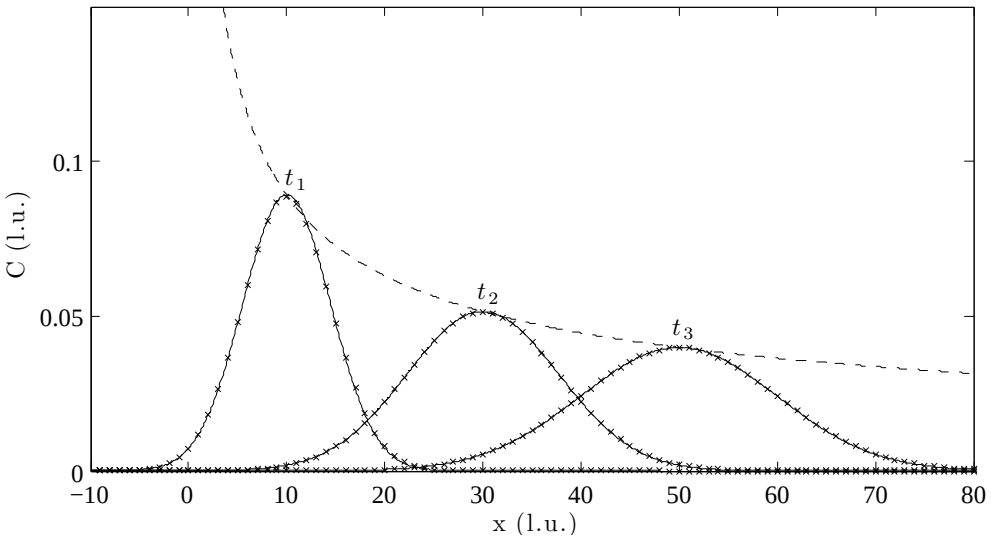

Figure 5.1: Obtained solutions (×) of the advection-diffusion equation for a point mass evolving in time and space. Three different times ($t_n = 100n$) are compared to analytical solutions (solid). The Amplitude of the solutions as function of time has also been plotted (dashed). The advecting velocity, $u_0 = 0.1$ and the Peclet number, $Pe = 10$. All units are in lattice units.

The LB model described in section **??** was tested by studying the evolution in time and space of a point mass in one dimension. The analytical solution of eq. (5.1) in one dimension with initial conditions $C(x, t = 0) = \delta(x)$ on an infinite domain is:

$$C(x,t) = \sqrt{\frac{Pe}{4\pi t}} \exp\left(-\frac{(x-ut)^2 Pe}{4t}\right). \tag{5.2}$$

In the numerical computations the parameters $Pe = 10$ and $|\mathbf{u}| = 0.1$ were used. The domain consisted of 200 lattice nodes and three snapshots in time at $t = 100, 200, 300$ were compared to the analytical solution. The result is presented in fig. 5.3.

6

Modelling of electrokinetic flow

6.1 Electric potential in 2D channel - PB

section in the channel, + debye-huckel comparision

6.1.1 It might be interesting to compare the two models Chai and Wang

6.2 Compare with Nernst-Planck

6.2.1 Potential

6.2.2 Charge distribution

6.3 Electroviscous effect

NP + PB differences?

6.4 Flow in array of charged squares

maybe other geometries as well?

6.5 3D?

only god knows...

7

Conclusions

And what do we conclude of this?