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

Contents

1

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 channels 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 and $\epsilon_r \epsilon_0$ the absolute permittivity.

Before the final model used in this project is presented, a simpler approach based on the Poisson-Boltzmann equation will be presented.

2.2 Poisson-Boltzmann model

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.

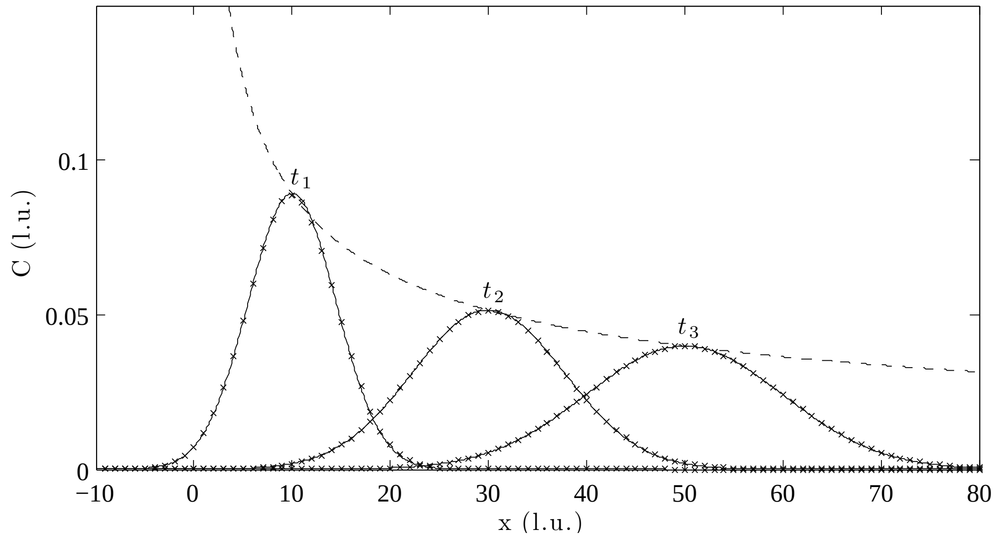

Figure 5.1: Obtained solutions ($\times$) of the advection-diffusion equation for a point mass evolving in time and space. Three different times ($t_n = 100n$) are compared to analytical solutions (solid). The Amplitude of the solutions as function of time has also been plotted (dashed). The advecting 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

6.5 3D?

7

Conclusions

And what do we conclude of this?