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

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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, the 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 Basic concepts of electrokinetic flow

Electrohydrodynamics involves the study of electric phenomena on fluid flow. How fluids carrying electrical charges (electrolytes) react upon external electrical fields or interact with charged objects are examples of problems that arise in this field.

2.1.1 Electrical double layers

As a charged object is brought into contact with an electrolyte it is, qualitatively, easily deduced that ions with a sign of charge opposite to that of the object will be attracted to the object and ions with the same sign of charge will be repelled. These two distinct categories of ions will from hereon be referred to as counter- and co-ions respectively. In this case, for a neutral electrolyte, a surplus of counter-ions will be present in the direct vicinity of the object and a surplus of co-ions will be present at some other location further from the object.

The area with a surplus of counter-ions in an electrolyte in contact with a charged object is often referred to as an electrical double layer. Two distinct regions will be formed in this area, thus the name double layer. The two layers are often referred to as the Stern layer (adsorbed ions) and the diffusive layer (mobile ions). The Stern layer is usually several orders of magnitude thinner than the diffusive layer and is therefore seldom considered when it comes to modelling [**?**].

2.1.2 Electroosmosis

As fluid carrying a net charge, e.g. in the diffusive layer of an EDL, is under influence of an electric field, the charged particles will move due to the electric forces. As the charge particles move, they will affect the surrounding liquid, causing it move as well. This liquid motion is often referred to as electroosmotic flow. [**?**]

2.2 The potential - Poisson's equation

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, further discussed in section 2.3.2.

2.2.1 Boundary conditions

At the charged boundaries, most physical situations may be covered by either specifying the potential or the surface charge density. The former would be boundary condition of Dirichlet type:

$$\psi(\mathbf{x}) = \zeta(\mathbf{x}) \ , \ \mathbf{x} \in \Gamma \tag{2.2}$$

and the latter a boundary condition of Neumann type:

$$\nabla\psi(\mathbf{x}) \cdot \mathbf{n} = -\frac{\sigma(\mathbf{x})}{\epsilon_0\epsilon_r} \ , \ \mathbf{x} \in \Gamma \tag{2.3}$$

where Γ denotes the boundary of the domain and $\mathbf{n}$ is the normal to the boundary surface. [**?**]

2.3 The transport of charges - Nernst-Planck equation

The charge concentration in an electrolyte is indeed affected by its environment. In the model proposed here, influences from: advection of the electrolyte, diffusion due to concentration gradients and effects from the electric field originating from charged objects placed at the border or in the flow is considered. Charge conservation without any external sources of the ion density, $\mathrm{C}(\mathbf{x}, t)$ gives:

$$\frac{\partial \mathrm{C}}{\partial t} + \nabla \cdot \mathbf{J} = 0 \tag{2.4}$$

where $\mathbf{J}(\mathbf{x}, \mathrm{t})$ is the net flux induced by the effects described above. Explicit expressions for the fluxes due to advection and diffusion respectively are

$$\mathbf{J}_{adv} = \mathrm{C}\mathbf{u} \tag{2.5}$$

and

$$\mathbf{J}_{dif} = -D\nabla \mathrm{C} \tag{2.6}$$

where $\mathbf{u}$ is the advective velocity and D is the diffusion coefficient. The ionic flux due to the presence of an electric potential, $\psi(\mathbf{x}, t)$, is given by the Nernst equation [**?**]:

$$\mathbf{J}_{ele} = -\frac{zq_e D}{k_B T}\mathrm{C}\nabla\psi \tag{2.7}$$

where z is the relative charge of an ion, q_e is the fundamental charge, k_B is the Boltzmann constant and T is temperature of the fluid.

Summing up the fluxes and putting them into eq. (2.4) gives

$$\frac{\partial \mathrm{C}}{\partial t} = \nabla \cdot \left[D\nabla \mathrm{C} - \mathrm{C}\mathbf{u} + \frac{zq_e D}{k_B T}\mathrm{C}\nabla\psi \right] \tag{2.8}$$

which is a known result often referred to as the Nernst-Planck equation. The advective velocity, $\mathbf{u}$, and the potential gradient, $\nabla\psi$, are obtained from couplings to the Navier-Stokes and Poisson's equations respectively. More about the coupling between the equations will be discussed in section **??**.

2.3.1 Boundary conditions

Depending on the physical situation that is being modelled, different conditions may be imposed at the boundaries of the domain. Throughout this work, at hard boundaries (walls), the charge flux out of the boundary will be set to zero, i.e.:

$$\mathbf{J} \cdot \mathbf{n}\big|_{x\in\Gamma} = 0 \tag{2.9}$$

where $\mathbf{n}$ denotes the normal to the surface and Γ is the boundary of the domain.

2.3.2 Poisson-Boltzmann equation

Consider a system consisting of an electrolyte in contact with a (flat) charged wall. Under certain assumptions, it is possible to explicitly determine the charge density in eq. (2.8) as a function of the electric potential. E.g. if there is no advection present and if the system has reached a steady state, i.e. $\partial \mathrm{C}/\partial t = 0$ and $\mathbf{u} = \mathbf{0}$ we have:

$$D\nabla \mathrm{C} + \frac{zq_e D}{k_B T}\mathrm{C}\nabla\psi = \alpha \tag{2.10}$$

where α is some arbitrary constant. Due to the steady state assumption, what the equation above actually says is that the net flux of charge in the system is constant. Since no flux of charge is wanted to flow through the wall boundary, the flux is set to zero on the wall and since the flux is constant it will therefore be zero everywhere in the liquid, i.e. $\alpha = 0$.

Considering only a one-dimensional situation with a position variable y varying in a direction out from the wall into the liquid, eq. (2.10) reads

$$\frac{1}{\mathrm{C}}\frac{d\mathrm{C}}{dy} + \frac{zq_e}{k_B T}\frac{d\psi}{dy} = 0 \tag{2.11}$$

The charge density is determined by solving eq. (2.11) for C, 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 is assumed to have decreased to zero and where the concentrations, C^∞, of the electrolyte is known.

$$\int_y^\infty d\ln(\mathrm{C}(y')) = -\frac{zq_e}{k_B T}\int_y^\infty d\psi(y') \tag{2.12}$$

This gives an expression for $C(y)$:

$$\mathrm{C}(y) = \mathrm{C}^\infty \exp\left(-\frac{zq_e\psi(y)}{k_B T}\right). \tag{2.13}$$

In a general case, there may be several species of ions in the electrolyte, the net charge density, ρ_e, is then given by simply summing up the contributions from the different species:

$$\rho_e = q_e \sum_i z_i \mathrm{C}_i. \tag{2.14}$$

Summarising eqs. (2.1), (2.13) and (2.14) gives the Poisson-Boltzmann equation in one dimension

$$\frac{d^2\psi(y)}{dy^2} = -\frac{q_e}{\epsilon_r \epsilon_0}\sum_i z_i \mathrm{C}_i^\infty \exp\left(-\frac{z_i q_e \psi(y)}{k_B T}\right). \tag{2.15}$$

The Debye–Hückel approximation

Historically, the non-linear nature of eq. (2.15) complicates when it comes to solving it. This was a major difficulty 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. (2.15) reduces to

$$\frac{d^2\psi(x)}{dx^2} = \frac{2n^\infty q_e z}{\epsilon_r \epsilon_0} \sinh\left(\frac{z q_e \psi(x)}{k_B T}\right). \tag{2.16}$$

and the linearised equation is

$$\frac{d^2\psi(x)}{dx^2} = \frac{2n^\infty q_e^2 z^2}{\epsilon_r \epsilon_0 k_B T}\psi(x) = \kappa^2 \psi(x) \tag{2.17}$$

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

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.

2.4 The velocity field - Navier-Stokes equations

In hydrodynamics, the Navier-Stokes equations are one of the most fundamental corner stones. They describe the motion of a fluid under the influence of various internal and external forces.

For later convenience and for reference when it comes to deriving the Lattice-Boltzmann formulation of the NS equation, a brief sketch of a derivation will here be presented. A most general form of the Navier-Stokes equation follows from momentum conservation

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \mathbf{Q} = 0 \tag{2.18}$$

where, ρ is fluid density, $\mathbf{u}$ is velocity and $\mathbf{Q}$ is a momentum source term (force per volume). Expanding the time derivative and the divergence terms respectively gives

$$\mathbf{u}\left(\frac{\partial \rho}{\partial t} + \nabla \cdot \rho\right) + \rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) + \mathbf{Q} = 0. \tag{2.19}$$

By assuring mass conservation (without sources) we have that

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho = 0 \tag{2.20}$$

and eq. (2.19) reduces to

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) + \mathbf{Q} = 0. \tag{2.21}$$

which together with eq. (2.20) is a general formulation of the Navier stokes equations.

The force term $\mathbf{Q}$, is determined by the physical properties of the fluid and from its environment. In this work, only incompressible Newtonian fluids will be studied. The force contribution to $\mathbf{Q}$ involved in that case is limited to viscous forces, pressure gradients in the fluid and to external force fields. Putting that into eqs. (2.20) and (2.21) gives

$$\nabla \cdot \rho = 0 \tag{2.22}$$

and

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla \mathrm{P} + \mu \nabla^2 \mathbf{u} + \mathbf{F} \tag{2.23}$$

where P is the pressure, μ the kinematic viscosity and $\mathbf{F}$ are the contributions from external forces.

2.5 Complete physical model

2.6 Pressure-driven electrokinetic flow

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

2.7 Electroosmotic flow

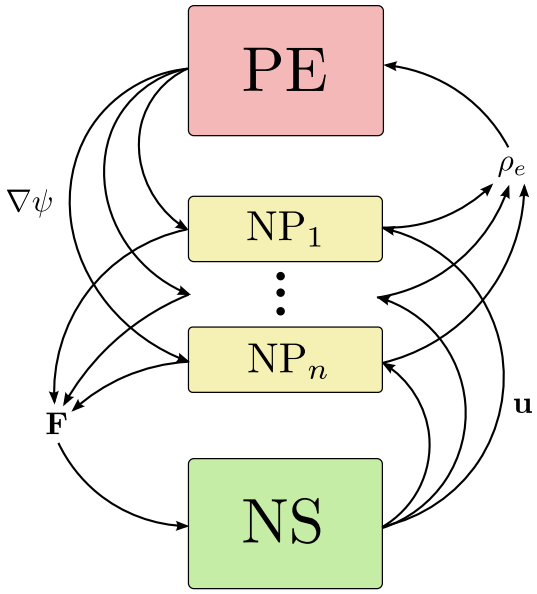

Figure 2.1: Visualisation of the coupling between the three equations present in the model. Poisson's equation (PE), The set of Nernst-Planck equations (NP_1 ... NP_n) and the Navier-Stokes equations (NS). The dependencies have also be marked with arrows indicating what quantities for a certain equation that are needed from an other.

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 flow

Navier-Stokes density + velocity profiles.

5.2 Taylor-Green vortex

5.3 Helmholtz equation

Poisson's eq.

5.4 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

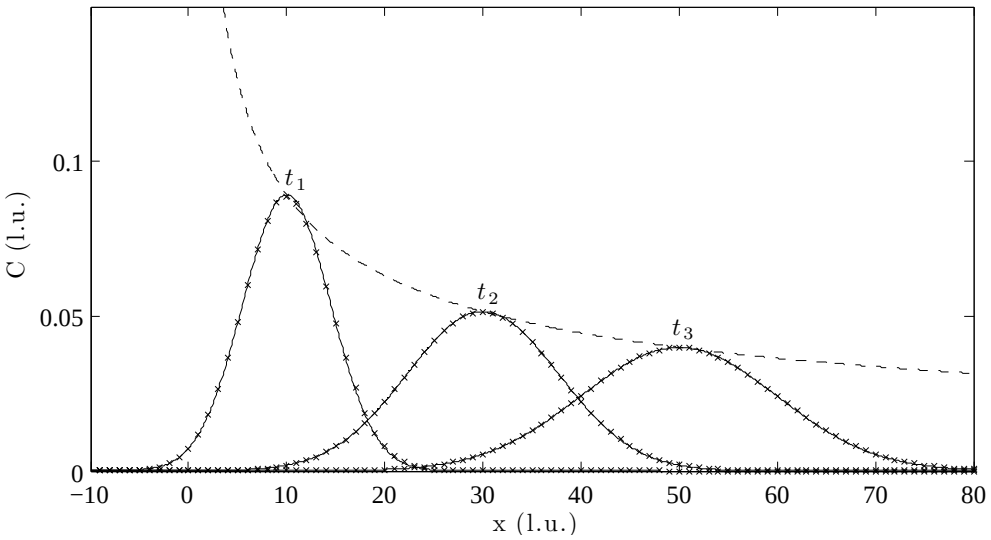

Figure 5.1: Obtained solutions (×) of the advection-diffusion equation for a point mass evolving in time and space. Three different times ($t_n = 100n$) are compared to analytical solutions (solid). The Amplitude of the solutions as function of time has also been plotted (dashed). The advecting velocity,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

the dynamics from advection and diffusion respectively. For $Pe \gg 1$ the dynamics is dominated by advection and for $Pe \ll 1$ by diffusion.

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. 5.4.

5.5 Nernst-Planck, a special case

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?