



Devices: Design & Transport

1. Efficient 3d FEM simulation of Surface Acoustic Wave fluidics via raytracing

Thomas Frommelt

This poster presents a new approach to simulate Rayleigh surface acoustic wave streaming in arbitrary 3d-geometries by FEM simulations. An efficient raytracing algorithm is applied on the acoustic subproblem to avoid the unbearable memory demands and computational time of a conventional 3d FEM acoustics simulation. The acoustic streaming interaction is modeled comprehensively by a body force term in the Stokes equation. In further comparisons between experiments and simulated flow patterns, we demonstrate the quality of the proposed technique.

2. Microfluidic mixing via Surface Acoustic Wave driven chaotic advection

Thomas Frommelt

Mixing in small amounts of fluids presents a notoriously difficult problem for the chemical and biological investigation of tiny samples of substances. Surface acoustic waves propagating on a substrate, covered partly or completely by a fluid, provide a convenient technique to generate time-dependent flow patterns. These flow patterns can be optimized in such a way that advected particles are mixed most efficiently in the fluid within a short time compared to the time pure diffusion would take. Experimental results are presented for the mixing efficiency of a thin spherical fluid layer that is periodically driven by two surface acoustic waves. The experimental results favorably agree with model calculations of the flow patterns and the resulting advective transport.

3. Multicomponent diffusional and thermodynamical cross effects in microscale fluid flow

Eugeny Kenig

In recent years, chemical micro-processes have attracted a significant interest of both chemical process industry and science. These processes occur in equipment with characteristic dimensions on a micrometer scale. As a consequence, low pressure drop, high surface areas per unit volume and small diffusion paths are achieved resulting in increased mass transfer rates.

Due to small dimensions and prevailing laminar flow conditions, diffusion becomes the mass transfer limiting phenomenon pre-determining its overall rate.

Besides, most chemical systems comprise several components, and thus, multicomponent diffusional interactions appear. This brings about phenomena which are qualitatively more complex than those in binary systems. During multicomponent diffusion, the direct proportionality between the component mass flux diffusion and its driving force may break up resulting in unusual phenomena, e.g. diffusion barrier (no mass transport despite the existing component concentration gradient), osmotic diffusion (component transport without its own driving force) and reverse diffusion (component transport against its own driving force). These phenomena are often called cross effects. Another interesting cross effect encountered in multicomponent mixtures is related to the thermal diffusion (or Soret effect). When a temperature gradient exists in a mixture, not only does it cause a heat flux, but it also enhances diffusion. In large-scale equipment, the cross effects are usually neglected, due to the dominant role of convection. However, on microscale, they should play an important part and worth a special analysis. Besides, a significant interaction could be expected between multicomponent mass transport and microscale hydrodynamics.

The basis of a physically consistent description of multicomponent cross effects is given by the Maxwell-Stefan equations which can be derived from the kinetic theory of gases. These equations will be used in the anticipated project.

As a test system for the study, the water shift reaction inside a rectangular microchannel is selected. One side of the channel is covered by a catalyst, whereas the opposite site represents a porous wall (a membrane) to ensure mass transport in the channel. The heterogeneous reaction takes place on the catalytic surface. Different temperature gradients will be applied to study the effect of the thermal diffusion. A commercially available computational fluid dynamics tool (probably CFX-11.0 by ANSYS Inc) will be used. This tool will be supplemented by our own subroutines (in Fortran) in order to take account of the cross effects.

From this study, valuable conclusions will be drawn concerning the significance of the cross effects on microscale. For instance, regions of importance will be identified for various operating and physicochemical parameters. In case of success, we plan to study another multicomponent system with more components in order to extend the added value and reliability of the research results.

4. FET Flow Sensor: Direct Probing of the Solid-Liquid-Interface

Pagra Truman
(without abstract)

5. Separation of Binary Liquid Mixtures on Gradient Surfaces

F. Varnik, B. Wu, D. Raabe, P. Truman, P. Uhlmann, M. Stamm, J.-F. Moulin, P. Mueller-Buschbaum
Via flow experiments as well as mesoscopic computer simulations, we show that a spatial change of substrate wettability may give rise to driving forces strong enough for a significant change of the dynamics of a fluid droplet. Since these forces scale with the area of the liquid-solid contact, they become increasingly more important as the surface to volume ratio increases. As a consequence, in micro-fluidic devices, full control of flow may be achieved via a spatially variable substrate wettability. In this poster, we present, how various aspects of this interesting phenomena may be investigated by mutual collaboration of experts on surface characterization, microfluidic chip design and mesoscopic computer simulation.

Probing the Boundary Conditions: Slippage and Beyond

6. On particle based velocimetry: Brownian particle near walls

Laura Almenar, Markus Rauscher
Motivated by particle based velocimetry techniques, in particular by double focus correlation spectroscopy experiments, we study the dynamics of Brownian particles in shear flow in the vicinity of planar walls. The experiments are designed to measure hydrodynamic slip in polar liquids. However, wall effects such as the fact that the particles cannot penetrate into the wall, the electrostatic double layer force, and the reduced particle mobility in the vicinity of the wall have to be taken into account in the data analysis in order to avoid spurious slip. We model the dynamics of the Brownian particles by a drift-diffusion equation taking into account the impermeability of the wall, the electrostatic double layer force, and the reduced mobility of the particles in the vicinity of the wall. The latter turns out to be irrelevant for the experimental system. We use analytical as well as numerical tools to simulate the experiments and to quantify the spurious slip that one would measure if the data was analyzed in a naive way. Here, we find qualitative agreement with the experiment. It turns out that for a more careful analysis of experimental data one needs more detailed information on the electrostatic particle-wall interaction.

7. Stochastic Hydrodynamics for Capillary Waves

Kerstin Falk, Thorsten Hiester, Klaus Mecke
The hydrodynamical predictions for fluid dynamics neglect the molecular motion of particles on short length and time scales. In particular, the dynamical behavior of liquid-vapor interfaces is expected to be different on microscopic scales due to the underlying bulk fluctuations.

Stochastic hydrodynamics provide an appropriate procedure to study fluctuation effects on the hydrodynamics of liquid-vapor interfaces. By extending the Navier-Stokes equations with thermal noise terms, we have calculated the dynamical capillary wave spectrum for both, incompressible and compressible fluids. In particular, the resulting dispersion relations for finite depth are discussed.

8. Rheology and the Structure Factor -- do they tell the same story?

Nicole Voss, Marco Walz, Max Wolff, Andreas Magerl, Hartmut Zabel
Shear anomalies may manifest themselves by unusual solid-liquid interface properties. These can be studied by GISANS and reflectometry which can be tuned to be particularly surface sensitive. However, the scattering contrast for x-rays usually is low, and laboratory diffraction is inappropriate. This shortcoming can be overcome if electron-rich salts are added. We show by rheology that the topology of the phase diagram of aqueous solutions of tri-block copolymers remains unchanged. A comparison with neutron structure factor measurements provides new insights into the origin of the phase transitions.

9. Crystallisation of micelles: a grazing incident neutron scattering study

Maximilian Wolff
Block copolymers can self-assemble into ordered mesoscopic superstructures, (length scale: 1-1000 nm). Such structured materials are not only fascinating but also of great importance in e. g. high-performance materials while miniaturising technology. Small angle neutron scattering is known since long to provide information on the structural arrangements of polymer systems. For crystalline systems often shear was used to bring the samples into a single domain state and allow long range correlations. Another possibility of introducing anisotropy is to confine the polymer close to a solid substrate. The adequate scattering technique to extract the structural information is then grazing incident or near surface small angle neutron scattering (GISANS or NS-SANS). In this presentation we will sum up the similarities and differences of normal and NS-SANS. The crystallisation of one particular block polymer will be discussed in great detail. The sample is the three block copolymer called Pluronic F127 that tends to agglomerate into micelles when solved in water. For higher concentrations or temperatures the micelles will crystallise into a cubic structure. Solid surfaces

with different degrees of hydrophobicity were employed as solid substrates. We find a preferred crystallisation of the micelles close to an attractive, with respect to the micelle shell, interface whereas crystallization is suppressed close to a repulsive one. In addition the epitaxial growth of crystallites starts at well separated germs at the solid interface resulting first in crystallite sizes of several μm . Deeper in the crystalline phase different crystallites start to interpenetrate resulting in a reorientation (texture) of the crystallites but on the other hand in a reduction of the correlation length parallel to the interface. Entering the crystalline phase from different liquid phases (high and low temperatures) results in distinct crystalline structures or intermediate phases.

10. Looking closer to the interface: Investigation of polymer dynamics under grazing incidence neutron scattering

Marco Walz, Max Wolff, Nicole Voss, Andreas Magerl, Hartmut Zabel

In more complex fluids the conventional non-slip boundary condition becomes microscopically void, and the slip length b may become macroscopic. For a deep understanding of boundary slip the structural and dynamical properties of interfaces on short length scales are essential. Experimental methods with pronounced interfacial feedback are needed. To highlight the properties of the boundary layer we carried out for the first time a neutron spin echo experiment under condition of grazing incidence (GINSE). With an aqueous solution of a tri-block copolymer with micellar orderings we could verify that the investigation of the dynamics of the sample with GINSE is well feasible and we will present a first data set taken near the critical angle of total reflection.

Soft Objects in Fluid Flow

11. Microchannel devices enable dynamic studies of the extracellular proteins fibrin and collagen

Heather M. Evans, Sarah Köster, Thomas Pfohl
Microfluidic structures are particularly amenable to controlled investigations of protein bundle and network formation. Hydrodynamic focusing is utilized to create a diffusion-controlled gradient of reactants, enabling non-equilibrium investigations. We present studies of the blood clotting protein fibrin, a three-dimensional network formed from the enzymatic cleavage of fibrinogen monomers by the protein thrombin. Fibrin is a vital component of blood clots, and has been implicated in a variety of diseases. Real-time fluorescence microscopy and x-ray micro-diffraction are used to quantify supramolecular assembly and provide snapshots of the evolution of fibrin network formation. We also show that collagen, a ubiquitous extracellular protein, can be bundled in situ through the use of a pH gradient. An outlook toward artificial blood vessels arises from the insight that both fibrin and collagen can easily be used to coat microchannel structures. The resulting mesh

forms an ideal environment for red blood cells and other cell types.

12. A Brownian Dynamics Study of Electrophoresis

Sebastian Fischer, Ali Najj, Roland R. Netz
We investigate the electrophoretic mobility of a long polyelectrolyte segment oriented parallel or perpendicular with respect to an external electric field by means of the Brownian Dynamics technique. Within our modeling approach counterions are accounted for explicitly. For large Manning parameters the well-known phenomenon of counterion condensation at long charged polymers tends to decrease the electrophoretic mobility of the polymer chain. In this case we observe considerable sensitivity of the electrophoretic mobility to the local chain architecture which we vary through either the charge spacing along the polymer backbone or the monomer-to-counterion size ratio. As opposed to the common assumption made in some theoretical publications we find that there is substantial slip between the condensed counterions and the polyelectrolyte. Depending on salt concentration the mobility of condensed counterions exhibits a change of sign which is due to partial screening of long-range hydrodynamic interactions.

13. Interaction of turbulent near-wall flow and flexible polymers

Sebastian Große, Wolfgang Schröder, Christoph Brückner

Micro-fabricated elastomeric pillars are used to position the macromolecules/flexible filaments in a defined wall distance in a shear field and to measure the deformation and drag forces of the polymers via pillar bending. The interaction of the pillars and the anchored filaments with the flow is studied using Particle-Image Velocimetry at micro-scale (μPIV). The experimental study allows a detailed analysis of the flow field modification by the presence of the polymers.

14. Hydrodynamic manipulation of active transport along actin cortex models II: microfluidic channels in extreme conditions

Tamas Haraszti, Simon Schulz, Kai Uhrig, Felix Bonowski, Joachim P. Spatz
(without abstract)

15. Dynamics of micro-capsules in shear flow using spectral methods

Steffen Kessler, Reimar Finken, Udo Seifert
The deformation of an elastic micro-capsule in an infinite shear flow is studied numerically using a spectral method. The shape of the capsule and the hydrodynamic flow field are expanded into smooth basis functions. Analytic expressions for the derivative of the basis functions permit the evaluation of elastic

and hydrodynamic stresses and bending forces at specified grid points in the membrane. Compared to methods employing a triangulation scheme, this method has the advantage that the resulting capsule shapes are automatically smooth, and few modes are needed to describe the deformation accurately. Better stability properties compared to simple boundary integral methods follow from this strategy. Computations are performed for capsules both with spherical and ellipsoidal unstressed reference shape. Results for small deformations of initially spherical capsules coincide with analytic predictions. For initially ellipsoidal capsules, recent approximative theories predict stable oscillations of the tank-treading inclination angle, and a transition to tumbling at low shear rate. Both phenomena have also been observed experimentally. Using our numerical approach we could reproduce both the oscillations and the transition to tumbling. The full phase diagram for varying shear rate and viscosity ratio is explored. While the numerically obtained phase diagram qualitatively agrees with the theory, intermittent behaviour could not be observed within our simulation time. An analysis using Poincaré mappings suggests that initial tumbling motion is only transient in this region of the phase diagram

16. Hydrodynamic manipulation of active transport along actin cortex models I: pillar fields or particles in optical trap arrays

Simon Schulz, Tamas Haraszti, Kai Uhrig, Reiner Kurre, Joachim P. Spatz
(without abstract)

17. Simulations of polymers in external fields

Christian Sendner, Roland R. Netz
Using Brownian Dynamics Simulations, we investigate the dynamics of polymers in external fields. We explicitly take hydrodynamic interactions in the limit of zero Reynolds number into account. The response of grafted DNA chains to alternating electric fields is examined, addressing important parameters like the bending rigidity. Terminally attached ligands change the dynamics of that system leading to possible biosensing applications. In another project we analyse the influence of a solid-liquid interface on stiff polymers, driven parallel to the surface. This leads to a preferred orientation of the rod with respect to the wall, and gives rise to an effective repulsion away from the surface. We give scaling results for this very long ranged repulsion in the high temperature limit. This purely hydrodynamic effect could lead to desorption transitions for short polymer chains which could be important for applications in the field of DNA chips.

18. Statics and dynamics of a cylindrical droplet on a substrate

Cem Servantie and Marcus Mueller

We report a study of the rolling and sliding motion of droplets on a substrate. We show that the contact angle is independent of the droplet size in the cylindrical geometry. A scaling law predicting the dependence on size of the center of mass velocity is derived. Moreover, we show that the relative importance between surface and volume dissipation is larger in droplets with large contact angles.

Wetting and Flow in Confined Geometries

19. Capillary Rise and Flow of Complex Liquids in Nanopores

Simon Grüner, Patrick Huber

We have designed and built a membrane flow apparatus to measure the volume flow rate (liquid permeability) of porous monoliths, e.g. nanoporous silica, as a function of applied pressure difference and temperature. The pore structure of the matrix (mean pore diameter, λ) is characterized by nitrogen sorption isotherms. First porosity measurements of the flow properties of n-hexane through mesoporous Vycor are presented.

20. Wetting morphologies in rectangular and triangular grooves

Krishnacharya Khare, M. Brinkmann, J.-C. Baret, B. M. Law, S. Herminghaus and R. Seemann
(without abstract)

21. Liquids on Structured Substrates - Open Microfluidic Systems

Markus Rauscher

We present an idea how to drive tiny amounts of liquid on structured substrates, e.g., in open micro- and nanofluidic systems and some recent findings on the behaviour of nano-droplets in the vicinity of topographic surface features (e.g., steps or wedges), which we recently extended to chemical steps. Driving fluids in open micro- and nanofluidic systems is less straight forward than in closed pipes since one cannot apply pressure differences and it is unclear whether electroosmosis would work. We suggest to drive the fluid by shear in a covering liquid, which could also prevent evaporation. Estimates of power input and throughput suggest that devices of the size of a miniature computer hard disk could be possible [PRL **98**, 224504 (2007)]. Studying the dynamics of nano-droplets in a 2D mesoscopic hydrodynamic model we found, that the direction of motion of the droplets is determined by van der Waals forces, but not the equilibrium contact angle [PRL **97**, 236101 (2006)]. Recently we generalized this method to chemically heterogeneous substrate. Again, the direction of motion is dominated by van der Waals forces, which can lead to droplets moving towards a less wettable region [arXiv:0706.0337].