Research strategy for

Micro and complex fluids

Introduction

Presently there is a strong trend towards miniaturizing equipment for chemical analysis and synthesis. This is made possible by development of technologies for fabricating small-scale structures that will serve as the components of a laboratory, such as pumps, valves, reactors, separators, etc, i.e. the lab-on-a-chip concept, where all of the components are built in a single device. Also, as nano-technology progresses, there is a rapidly growing need to manipulate small objects, such as carbon nano-tubes, nano-particles etc. From the view point of fluid mechanics, there is a rapidly growing research area that could be termed micro fluid dynamics or more commonly micro-fluidics, that deals with the special problems that appear when these flow systems are built in micron sizes or less. In a liquid some of the main effects that need to be addressed stem from the increased importance of surface phenomena at small dimensions. Also, whenever immiscible liquids and/or liquid/gas are handled in micro-systems, there are free surfaces and surface chemistry that must be understood and modeled. Of particular importance are bubbles and drops, evaporation and condensation, for instance used as a driving force, capillary effects, Marangoni effects, and electrostatic phenomena.

Another very active research area is that of complex fluids. Complex fluids abound in nature; with examples such as polymeric solutions, milk, foams and emulsions (mixtures of two immiscible liquid substances). Simple Newtonian liquids with immersed elastic or solid particles form suspensions that can display very complex and non-Newtonian dynamics. In general, flows of these complex fluids exhibit intriguing two-way couplings: the micro-scale dynamics of the particles affects the macro-dynamics of the flow and vice versa. One interesting and particularly challenging class of complex fluids are fiber suspensions, i.e. suspensions of elongated particles in a liquid. Examples of applications where such liquids appear are pharmaceutical, food and pulp and paper processes.

Furthermore, these two subfields are strongly connected, in that multiphase and separation problems are of prime importance in micro-fluidics, whether the particulate phase can be fibers, cells, beads, carbon nano-tubes, etc. Also, the fluid physics in both areas involve low Reynolds-number flows, strong influence of surface forces, experimental techniques where flows can be studied in small volumes, etc.

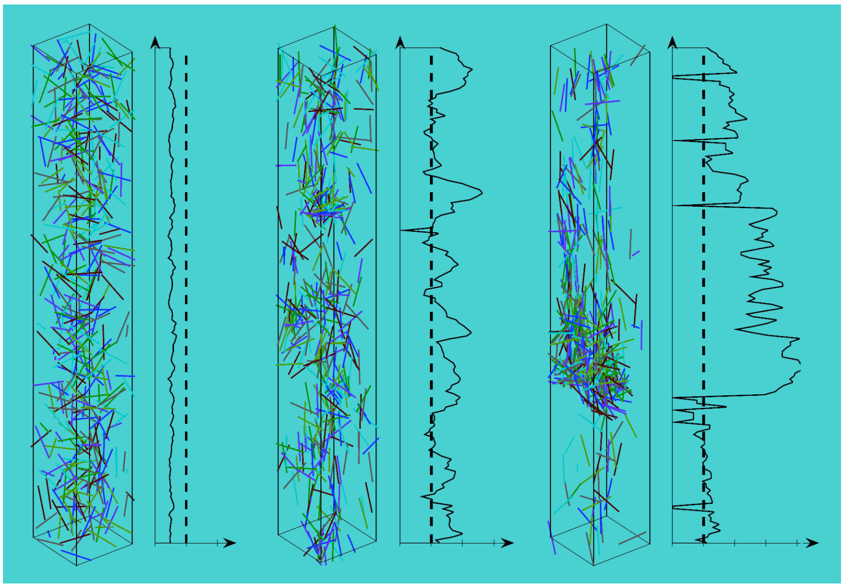

Figure 1. Simulation of sedimenting rigid fibers. The configuration is shown initially and at two later times. The clustering of fibers and their increased vertical alignment can be seen to increase their sedimentation speed, as indicated in the plot to the right of each box.

Research environment

The research environment on micro-fluidics and complex fluids within FLOW is formed by integrating several different research groups with common goals but with different expertise. The group of Prof. Gustav Amberg has an established activity concerning the numerical simulation of multiphase flow and flows driven by capillary effects. The group has mainly developed and improved upon so called phase-field methods for this purpose. In addition, it has developed a flexible software package to ease the implementation of new algorithms. The group of Prof. Gunilla Kreiss, now at Uppsala University, has worked on the development of a conservative so-called level-set method; an interface tracking method which the group has applied to immiscible multiphase flows. Dr. Anna-Karin Tornberg has formed a group which works with the design and analysis of numerical algorithms for different multiphase flows, ranging from interface tracking techniques for immiscible multiphase flow, analysis of regularization techniques often used in connection these, to boundary integral methods for solid and elastic particles in Stokes flow. Prof. Alfredsson´s group now houses research on fluid mechanics related to paper technology. Fundamental aspects of fiber suspension flows are studied, mainly experimentally. Modern image acquisition, image analysis, NMR and conductivity measurements are used to study the motion of fibres and liquids in different flow situations, ranging from very slow to turbulent. At KTH there are also excellent groups that use micro-fluidics and develop micro systems, where there is a need for knowledge of the corresponding fluid dynamics and capability to simulate such systems. The interaction with these groups will provide challenges and knowledge for such applications. The Linné Flow Centre is actively collaborating with researchers at S3 (Göran Stemme and Wouter Van Der Wijngaart) and analytical chemistry (Johan Roeraade).

Below follows a table that lists the ongoing projects within the research group involving students and/or post-docs.

Project titels	PhD stud./ Postdocs	Senior reseaerchers	Proj. Start	Sponsor
Micro-fluids				
Simuation of free boundary problems and phase change		Amberg Do-Quang	2006	VR/KTH
Microfluidic hydraulics	Amer Malik (part time)	Amberg Do-Quang	2009	VR
Contact line dynamics in two phase flow	Zahedi	Kreiss	7/2006	KTH
New surface technology -PUG	Lindbo	Tornberg	1/2007	KTH
Fluid mechanics with intelligent surfaces	Andreas Carlson	Amberg Tornberg	4/2007	FLOW
Numerical issues in micro fluidics	Engborn	Tornberg	8/2009	FLOW
Complex fluids				
Num. sim. of rigid fiber suspensions		Tornberg Gustavsson	7/2005	KTH/future faculty
Fiber dynamics in Stokes flow	Marin	Tornberg	4/2007	FLOW
Flow in consolidating networks	Bellani	Lundell Söderberg	1/2006	STEM
Estimation of flows in complex liquids	Bellani	Lundell	1/2009	STEM
Turbulence in fiber suspensions		Tanaka	1/2010	VR
Fibre suspensions in narrow conduits		Söderberg Lundell	5/2007	STEM
Differential equations on dynamic surfaces	af Klintenberg	Tornberg	1/2010	VR

Overall Research Goals

The vision for our research group is to become a leading European group in modeling and simulation of micro fluidics and complex fluids. To achieve this vision, we plan to focus on two main areas.

Within micro-fluidics, we will focus on free boundary problems, i.e. applications with interfaces separating immiscible liquids and/or liquid and gas. We aim to develop accurate and competitive simulation methods for these problems in which we will include increasingly complex surface physics. This includes phenomena such as dynamic wetting, influence of surfactants, phase change such as evaporation and condensation, electric forces and other surface chemistry phenomena. These developments will be driven by applications in micro-fluidics, and close collaborations will provide the challenges and expertise of the applications.

For complex fluids, the main focus will be enhanced understanding and modelling of macroscopic properties of particulate flows. i.e. suspensions with particles (solid or elastic of different shapes) immersed in a fluid. Initially, the focus will be on rigid fibers, but the objective is to build methodologies and knowledge that will later also be applicable to other suspensions. The long-term goal is the design, development and verification of a coupled micro-macro scale simulation algorithm which uses the direct fiber simulation algorithm on the micro-scale to calculate the evolving stress field needed for momentum balance at the macroscopic scale. A reliable, accurate and rigorously verified algorithm for macroscopic simulations would be a ground breaking tool in the study of suspensions, and would be a long awaited complement to experiments in understanding their complex dynamics.

Roadmap

Within our research group, we have a large experience of both so called sharp interface methods (e.g. front-tracking and level-set methods) and diffuse interface methods (phase field methods) for free boundary problems. To address the challenges ahead, we intend to build methods based on both diffuse and sharp interface methods and will design also combinations thereof, combining the strengths and weaknesses of these methods in an optimal manner.

For suspensions, results from physical experiments will be used in conjunction with data from numerical simulations to enhance our understanding of the dynamics of these systems. For this, the experimental techniques will be steadily improved and state-of-the art numerical techniques for simulating a large number of particles immersed in the flow will be developed.

The short-term goals are:

- To develop numerical methods for simulations of electrowetting and use these to study how the hydrophobicity of the surface can be controlled, in conjunction with experiments.
- To develop algorithms based on mathematical formulations that include dissolution of the air in an air pocket into the liquid, or evaporation and condensation of the liquid vapor. This can be naturally included in diffuse interface models. This should then allow prediction of the size and appearance or disappearance of air/vapor pockets, depending on the ambient pressure, the properties of the liquid, dissolved gases, the electric field, etc.
- To develop models and simulation methods for surfactants and Marangoni flow. Surfactants are almost always present in aqueous systems, and there is a nontrivial interaction between the surface

concentration of a surface active component, and the bulk concentration, via the flow that is driven by surface tension variations.

- To extend the sharp interface model to correctly model contact line dynamics, and develop numerical methods for the new model.
- To develop accurate and fast simulation methods for particulate flows (initially flows with rigid fibers) including the details of each particle. Use distributed computing to enable large-scale computations including large numbers of particles.
- To develop experimental techniques allowing simultaneous measurements of fiber and fluid motions in fiber suspensions. These activities include the development of scaled experiments with larger fibres in order to facilitate the measurements. The aim is to provide verification data for the simulation methods on both micro and macro scale.
- To analyze microscopic and macroscopic properties of the suspensions and of correlations in between using data from both physical and numerical experiments.