GESELLSCHAFT für
ANGEWANDTE MATHEMATIK und MECHANIK e.V.
INTERNATIONAL ASSOCIATION of APPLIED MATHEMATICS and MECHANICS

86th Annual Meeting

of the International Association
of Applied Mathematics and Mechanics

March 23-27, 2015
Lecce, Italy

Book of Abstracts - Extract

2015

UNIVERSITÀ DEL SALENTO

jahrestagung.gamm-ev.de

Scientific Program - Timetable

Sunday 22	Time	Monday 23	Tuesday 24	Wednesday 25	Thursday 26	Friday 27
	9:15		Contributed sessions (15 in parallel)	Plenary Lecture Moritz Diehl	Contributed sessions (15 in parallel)	Contributed sessions (14 in parallel)
	9:30					
	9:45					
	10:15	Registration		von Mises prize lecture		
	10:30					
	10:45					
	11:15		Coffee Break	Coffee Break	Coffee Break	Coffee Break
	11:30					
	11:45					
	12:15		Plenary Lecture Thomas Böhlke	General Assembly	Plenary Lecture Ferdinando Auricchio	Contributed sessions (11 in parallel)
	12:30					
	12:45					
	13:15	Opening	Lunch	Lunch	Lunch	
	13:30					
	13:45	Univ. Chorus Performance				Closing
	14:15	Prandtl Lecture Keith Moffatt	Plenary Lecture Enrique Zuazua	Contributed sessions (15 in parallel)	Plenary Lecture Daniel Kressner	
	14:30					
	14:45					
	15:15	Plenary Lecture Giovanni Galdi	Plenary Lecture Nikolaus Adams		Plenary Lecture Stanislaw Stupkiewicz	
	15:30					
	15:45					
Registration pre-opening	16:15	Coffee Break	Coffee Break Poster session	Coffee Break	Coffee Break Poster session	
	16:30					
	16:45	Minisymposia & Young Reseachers' Minisymposia (10 in parallel)	Contributed sessions (14 in parallel)	Contributed sessions (15 in parallel)	Contributed sessions (15 in parallel)	
	17:15					
	17:30					
	17:45					
	18:15		Public lecture Francesco D'Andria			
	18:30					
	18:45					
	19:15	Opening reception at Castle of Charles V				
	19:30					
	19:45					
	20:15			Conference dinner at Hotel Tiziano		
	20:30					
	20:45					
	21:15					
	21:30					
	21:45					

GAMM 2015

Università del Salento

Table of contents

S11: Interfacial flows

Understanding and controlling of interfacial phenomena in multiphase flows is one of the main challenges in fluid mechanics, at the crossroads of scientific disciplines like Mathematics, Physics, Chemistry and Engineering.

Examples are particle-laden flows, bubble columns, fuel atomization, casting, oil recovery, film flows, spreading and dewetting of (complex) liquids including suspensions, polymer solutions, liquid crystals, colloids and biofluids. All these systems are central for technological advances in the chemical, pharmaceutical, environmental and food industries and crucial for the development of Microfluidics and Nanostructuring. Goal of this Section is to provide a representative overview of the latest developments in this area, covering models, numerical methods and experimental techniques but also surveying new physical insights and recent technical advancements.

Simulating Free-Surface Flows with Moving Boundaries: A Combination of an Interface-Tracking and an Interface-Capturing Approach

Markus Frings, Marek Behr, and Stefanie Elgeti
Chair for Computational Analysis of Technical Systems,
CCES, RWTH Aachen University, Germany

A method is presented to simulate free-surface flows driven by a moving boundary. This kind of flow occurs for example in the numerical simulation of the high-pressure die casting process. In this simulation, a moving plunger (the moving boundary) pushes molten metal from a partially filled gating chamber (free-surface) into the die. Since the simulation is afterwards used in an automatic optimization loop, there is a need for an efficient and robust simulation model.

Both, the free-surface and the moving boundary can be treated as interfaces. In simulations with such interfaces, two main types of methods can be distinguished: (1) interface tracking (IT), and (2) interface capturing (IC). The difference lies in the description of the interface—explicitly by a boundary conforming mesh in IT and implicitly by an additional scalar field in IC.

In IT, the interface movement can be directly applied to the boundary nodes. Thereby, the computational domain is deformed based on the node movement. In order to maintain a valid mesh in the interior, the mesh node positions must be adjusted. In contrast, in the IC the computational mesh is fixed and the interface position is determained based on an additional scalar field. As the interface evolves, its movement is described by a modification of the scalar field. The IT has its strengths in the modelling of uniform and limited interface distortion. In the case of large surface deformation, a remeshing might become necessary, which is a hindrance in an automatic optimization loop. Also, the merging of two interfaces is an issue in IT. IC is suitable for the modelling of free-surface flows with large surface deformations. It allows for nearly arbitrary surface deformation and the contact of the surface with a domain wall (e.g., the top wall of the gating chamber) is not an issue.

In the approach at hand, both types of interface description are combined. The IT is applied to the moving boundary, while the IC is applied to the free surface. For the plunger movement we use a Deformable-Spatial-Domain/Stabilized-Space-Time (DSD/SST) finite element formulation in combination with a mesh update method for the interior node positions [1]. This method moves the boundary nodes according to the prescribed plunger movement. The mesh itself (containing both phases) is treated like an elastic material. As a result, the interior node positions are updated in a way that keeps the mesh valid. The free-surface flow is modelled by the level-set method [2]. The scalar field in the level-set method is the signed distance to the interface. Thus, the zero level-set describes the interface position. The sign of the function can be used to determine the density and viscosity for the flow field computations. The level-set field (and therefore also the interface) is transported with the fluid velocity.

Both methods are implemented in the in-house flow solver XNS, which employs P1P1 finite element with a Galerkin/Least-Sqares stabilization technique. Basis for the flow simulation are the incompressible and isothermal Navier-Stokes equations.

The combined approach represents an efficient and robust method appropriate for the numerical optimization of the high-pressure die casting process. Furthermore, it is possible to apply the presented approach to other applications, where a combination of a two-phase or free-surface flow with moving boundaries occurs.

References

[1] A.R. Johnson and T. Tezduyar. Mesh update strategies in parallel finite element computations of flow problems with moving boundaries and interfaces. Computer Methods in Applied Mechanics and Engineering, 119 (1994), 73–94.

[2] M. Sussman, P. Smereka and S. Osher. A level set approach for computing solutions to incompressible two-phase flow. Journal of Computational Physics, 114 (1994), 146–159.

Towards higher-order XFEM for interfacial flows

Thomas-Peter Fries
Institute of Structural Analysis, Graz University of Technology,
Lessingsstr. 25/II, 8010 Graz, Austria
fries@tugraz.at, www.ifb.tugraz.at

The simulation of two-phase flows is characterized by the presence of moving interfaces in space and time. The interfaces separate the involved fluids each having individual properties such as density and viscosity. As a consequence, the resulting physical fields such as pressure and velocity feature jumps and kinks at the interface. The accurate treatment of the discontinuous parameters and fields renders the simulation of two-phase flows a challenging task and a large number of numerical methods has evolved.

Recently, the XFEM is used increasingly for two-phase flows because it enables accurate approximations of discontinuous solutions within elements [1, 2, 4]. This is achieved by enriching the classical finite element approximation space through the partition of unity concept [5, 6]. The XFEM in combination with the level-set method enables a consistent treatment of problems with moving interfaces. Herein, the aim is to use the XFEM for higher-order accurate approximations of two-phase flows [3].

A number of issues has to be considered to achieve this aim:

- An accurate enrichment for jumps and kinks is needed in the XFEM that enables higher-order approxiomations of jumps and kinks within elements.
- A higher-order accurate time integration scheme is needed for the incompressible Navier-Stokes equations and the level-set transport equation. The discontinuous Galerkin method in time is a natural choice, i.e. higher-order space-time finite elements are realized.
- An accurate numerical integration is needed for the evaluation of the weak forms. A quadrature is proposed that captures curved interfaces within elements.
- A higher-order accurate reinitialization of the level-set function is needed.

The emphasis of this work is on the higher-order accurate integration of the weak form. The level-set function is higher-order and the resulting zero level set is curved within the elements. A consistent integration scheme is proposed that decomposes the background (space-time) elements into special sub-elements with curved faces. This integration also enables the evaluation of surface tension on the interface, which is one dimension lower than the spatial dimension of the problem.

References

[1] H. Sauerland, T.P. Fries. The extended finite element method for two-phase and free-surface flows: A systematic study. J. Comput. Phys. 230 (2011), 3369–3390.

[2] H. Sauerland, T.P. Fries. The stable XFEM for two-phase flows. Computers & Fluids 87 (2013), 41–49.

[3] K.W. Cheng, T.P. Fries. Higher-order XFEM for curved strong and weak discontinuities. J. Comput. Phys. 82 (2010), 564–590.

[4] K.W. Cheng, T.P. Fries. XFEM with hanging nodes for two-phase incompressible flow. Comp. Methods Appl. Mech. Engrg. 245 (2012), 290–312.

[5] N. Moës and J. Dolbow and T. Belytschko. A finite element method for crack growth without remeshing. Internat. J. Numer. Methods Engrg. 46 (1999), 131–150.

[6] T.P. Fries and T. Belytschko. The extended/generalized finite element method: An overview of the method and its applications. Internat. J. Numer. Methods Engrg. 84 (2010), 253–304.

Numerical Modelling of Laser-Induced Cavitation Bubbles with a Finite Volume Method

Max Koch[1], Christiane Lechner[2], Fabian Reuter[1], Karsten Köhler[1], Robert Mettin[1], Werner Lauterborn[1]

[1] CDLCME, Georg-August-University Göttingen
[2] Vienna University of Technology

We report on the numerical modelling of laser-induced cavitation bubbles with the finite volume method using the open source software package OpenFOAM [1, 2]. The goal is to correctly predict the dynamics of a laser generated bubble, including collapse and rebound, as well as the velocity and pressure field in the surrounding liquid for asymmetric situations like bubbles close to a rigid boundary or next to a second bubble.

We consider the bubble to be filled with an adiabatic van der Waals gas. Compressibility of the liquid is included via the Tait equation of state, which allows shock waves to develop upon bubble generation and collapse. At the present stage of our work evaporation and condensation is not included in the model.

The pressure-based volume of fluid solver `compressibleInterFoam` has been extended for our purpose. We show that the slow convergence of the bubble volume with grid resolution stems from a large numerical error in the mass that the bubble aquires during collapse. The violation of mass conservation for a very similar numerical scheme previously has been reported in the literature [3]. A comparativley simple correction of the bubble mass at every time step solves that problem and allows for an accurate prediction of collapse and rebound of strongly collapsing bubbles with a reasonably sized grid in axial symmetry. A further improvement of the original solver concerns the stabilization of the algorithm for the case of strong pressure waves impinging on the numerically smeared liquid/gas interface.

To validate our approach we consider spherically symmetric and axially symmetric collapse scenarios. For a spherical bubble collapsing in an unbounded liquid the bubble evolution is in very good agreement with predictions of the Gilmore model up to the second collapse as well as with the experimental data given in [4]. The pressure field in the surrounding liquid is validated by comparing form and location of the shock waves to numerical and experimental data available in the literature. Furthermore by comparing with experimental data it is shown, that the finite volume simulation can very well predict the shape of a bubble that collapses near a solid boundary.

References

[1] OpenFOAM, `http://www.openfoam.com`.

[2] The OpenFOAM-extend project, `http://www.extend-project.de/`.

[3] S.T. Miller, H. Jasak, D.A. Boger, E.G. Paterson, and A. Nedungadi. A pressure-based, compressible, two-phase flow finite volume method for underwater explosions. Computers and Fluids, 87 (2013), 132–143.

[4] S. Müller, M. Bachmann, D. Kröninger, T. Kurz, and P. Helluy. Comparison and validation of compressible flow simulations of laser-induced cavitation bubbles. Computers and Fluids, 38 (2009), 1850 – 1862.

A comparison of viscoelastic and empirical rheological models in context of squeeze flows

Stefan Descher, Olaf Wünsch
Chair of Fluid Mechanics, Institute of Mechanics, University of Kassel

For polymer melts a wide range of measurable rheological phenomena can be modelled by nonlinear differential constitutive equations. Typical phenomena are stress-relaxation, shear-thinning, normal stress differences and strain-hardening. But often empirical models which are only capable to describe the shear behaviour correctly are used. For non-newtonian squeeze flows several publications regarding slip and no-slip boundary conditions are available. A review and enumeration of publications is given by Engelmann in [1].

In this contribution an isothermal, constant velocity, no-slip squeeze flow is discussed. It is inspired by technical squeezing flows during polymer processing and validation experiments, that can be done with commercial rotational rheometers. There is a relation to investigations presented in [2], where the flow type in squeeze flows between square plates was analysed. In contrast, here the cross section of the plates is circular and the temporal progress of the averaged normal stress on the plates is evaluated. This plays a significant role in the design of presses in industrial applications. The rheological models that are used are the generalized Maxwell model with the nonlinear extension from Giesekus and the empirical Carreau-Yasuda model. The simulations are performed with the Finite-Volume-Method using *OpenFOAM*. In its framework a solver based on *pimpleFoam* (*PISO* and *SIMPLE* merged) was developed to calculate viscoelastic flows. The main difference to the standard solver *viscoelasticFluidFoam* [3] is the sequence of steps to couple pressure, velocity and stress in order to improve the convergence behaviour. The implementation of the problem domain is done by using axisymmetric boundary conditions, thus it is reduced to a wedge. Since the height of the domain is reduced due to squeezing a dynamic mesh is used.

References

[1] J. Engelmann, C. Servais, A. S. Burbige: Squeeze flow theory and applications to rheometry: A review. J. Non-Newtonian Fluid Mech, 132 (2005) 1–27.

[2] A. Al-Baldawi, O. Wünsch: Simulating of a pressing process of a viscoelastic polymer melt. Proc. Appl. Math. Mech., 12 (2012) 471–472.

[3] J. L. Favero, A. R. Secchi, N. S. M. Cordozo, H. Jasak: Viscoelastic flow analysis using the software OpenFOAM and differential constitutive equations. J. Non-Newtonian Fluid Mech, 165 (2010) 1625–1636.

On the implementation of free-slip interfaces for the immersed boundary method

Tobias Kempe, Jochen Fröhlich
TU Dresden, Institute of Fluid Mechanics, 01062 Dresden, Germany

The numerical simulation of spherical and ellipsoidal bubbles in purified fluids requires the application of the free-slip boundary condition at the bubble surface [1]. This talk presents a numerical method for the implementation of free-slip boundary conditions for immersed boundary methods as proposed and enhanced in various papers [2, 3, 4].

In contrast to other numerical approaches for multiphase flows, the realization of free-slip interfaces for immersed boundary methods is not straightforward and is not available in literature up to now. The reason is, that the method treats the liquid as well as the gas phase as a field of constant density and viscosity with a fictitious fluid inside the bubble. The motion of the disperse phase is computed explicitly by solving its momentum balance. It is coupled to the continuous phase via additional source terms in the Navier-Stokes equations. The outer fluid in the vicinity of the interface is substantially affected by the inner fluid. As a consequence, an intrinsic realization of free-slip interfaces, like for schemes with variable viscosity and density, is not possible. Several approaches to achieve such a condition were conceived and implemented. Using various tests the respective performance was assessed and compared. It turns out that an appropriate forcing is not immediate and requires to overcome certain difficulties. The new method is first described for spherical objects and then extended to general curved interfaces. The scheme is applied to spherical and ellipsoidal particles without or with prescribed constant angular velocity. It is shown that the proposed method yields the same order of convergence as the method for no-slip boundaries and does not degrade computational efficiency. The results are compared to analytical solutions for creeping flow around a sphere with free-slip surface and to numerical reference data obtained on a body-fitted grid. The numerical tests confirm the excellent performance of the new method.

References

[1] R. Clift, J. R. Grace, and M. E. Weber. Bubbles, Drops, and Particles. Dover Publications (1978).

[2] M. Uhlmann. An immersed boundary method with direct forcing for the simulation of particulate flows. Journal of Computational Physics, 209 (2005), 448-476.

[3] T. Kempe, J. Fröhlich. An improved immersed boundary method with direct forcing for the simulation of particle laden flows, Journal of Computational Physics, 231 (2012), 3663-3684.

[4] T. Kempe, J. Fröhlich. Collision modelling for the interface-resolved simulation of spherical particles in viscous fluids. Journal of Fluid Mechanics, 709 (2012), 445-489.

Linear stability of a thin non-isothermal droplet spreading on a rotating disk

K. Boettcher, T. Externbrink
Fluid Mechanics, Bio- and Biochemical Engineering, TU Dortmund

In many industrial applications solids are coated by using centrifugal forces, e.g. in spin-coating used for coating wafers. In the first step of the process a liquid droplet is placed on the disk and spreads over the solid due to gravity, centrifugal forces and wetting. During the spreading the contact line may get corrugated, giving rise to the so-called fingering instability. In a preceded work the linear stability of the contact-line was investigated for a thin isothermal droplet, using lubrication approximation and Tanners law to cover the behavior of the dynamic contact angle [1]. The results show that the stability depends on the base-state curvature of the free interface at the contact line. As the Marangoni effect can be used to alter the curvature [2], this presentation investigates the base state of the spreading including thermal gradients between the plate and the surrounding gas or in the plate itself. A linear stability analysis tries to answer the question, how those contact-line instabilities may be influenced.

References

[1] K.E.R Boettcher, P. Ehrhard. Contact-line instability of liquids spreading on top of rotating substrates. European Journal of Mechanics - B/Fluids 43 (2014), 33–44.

[2] K. Boettcher, J. Hötzel, P. Ehrhard. Temperature effects in thin droplets. Proc. Appl. Math. Meth. 12 (2012), 519–520.

A circulating gravity wave in a cylindrical tank

Herbert Steinrück,
Vienna University of Technology, Institute of Fluid Mechanics and Heat Transfer

Circulating gravity wave in a cylindrical tank A cylindrical vertical tank, partially filled with water is considered. The upper lid of the tank rotates around the cylinder axis inducing a rotational flow in the air gap between the water surface and the lid. It has been observed that above a critical angular velocity of the lid a circulating gravity wave in the water develops with an angular wave speed almost independent of the driving speed of the lid. The wave form is well known and can be described as first approximation by a potential flow. We are interested in the excitation mechanism and want to determine the critical speed of the lid by an asymptotic analysis with respect to small wave amplitudes. The key idea is to study the mechanical energy budget of the flow. Moreover, to simplify the analysis we assume that the air flow above the water given as a rotating flow with an Ekman-layer at the bottom. For small amplitudes the core flow in the water can be considered as the superposition of time periodic potential flow and a solid body rotation. The angular frequency of the gravity wave can be determined by an eigenvalue problem. By considering the boundary layers at the interface to the water and the cylinder walls the momentum an energy budget will be determined. Analytical results for the angular frequency in dependence of the driving angular speed of the lid will be given and compared to experimental results. Moreover, the minimal angular speed of the lid where the gravity wave can be observed will be given.

Experiments beyond the limits of Nusselt theory: The linear stability of gravity-driven films over undulated inclines

M. Schörner, D. Reck and N. Aksel
Dept. Applied Mechanics and Fluid Dynamics, University of Bayreuth, Germany

We present experimental results on the linear stability of gravity–driven films over strongly undulated inclines. Within our parameter study we vary the Reynolds number, the liquid's viscosity and the inclination angle of the substrate. Furthermore, we change the frequency of the linear disturbances which we impose to the basic flow. That way, we obtain stability charts which show a rich variety of phenomena induced by the undulation of the incline: We found a slight destabilization as well as a very significant stabilization of the flow compared to the corresponding Nusselt flow. Moreover, we report on transmutations from long-wave to short-wave type instabilities. Even a fragmentation of the stability chart, which leads to stable and unstable isles, is observed.

Our study extends former experimental [1, 2] and numerical [3] approaches and explores the above-mentioned complex stability behavior of gravity-driven films over strongly undulated inclines in-depth. We are now able to classify the stabilizing and the destabilizing effects. Concerning the stabilizing effects, we identified a significantly increased mean film thickness of the flow due to the undulation compared to the corresponding Nusselt flow. Consequently, this leads to a decreased free surface velocity and hence the flow is stabilized. Beyond this, we proved the destabilizing effect of hydraulic jumps and a strongly curved free surface of the liquid. This enabled us to explain the fragmentation of the stability charts and thus the existence of stable and unstable isles – phenomena which clearly exceed the limits of Nusselt's theory.

References

[1] T. Pollak, N. Aksel. Crucial flow stabilization and multiple instability branches of gravity-driven films over topography. Phys. Fluids 25 (2013), 024103.

[2] Z. Cao, M. Vlachogiannis, V. Bontozoglou. Experimental evidence for a short-wave global mode in film flow along periodic corrugations. J. Fluid Mech. 718 (2013), 304–320.

[3] Y.Y. Trifonov. Stability of a film flowing down an inclined corrugated plate: The direct Navier-Stokes computations and Floquet theory. Phys. Fluids 26 (2014), 114101.

Continuous size-dependent separation of blood components from human whole blood samples in microfluidic spirals

L. Sprenger[1,2], S. Dutz[3], T. Schneider[1], S. Odenbach[2], U. O. Häfeli[1]

[1] Faculty of Pharmaceutical Sciences, University of British Columbia, Vancouver, BC V6T 1Z3, Canada

[2] TU Dresden, Chair of Magnetofluiddynamics, Measuring and Automation Technology, 01062 Dresden, Germany

[3] Institut für Biomedizinische Technik und Informatik, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Parasites, like those causing leishmaniasis [1], appear in very small concentrations in the blood of infected humans. This makes a diagnosis challenging based solely on visual proof of the whole blood sample. In this context our work aims at developing a microfluidic point-of-care device with the focus on a simplified continuous separation process which requires no pretreatment of the blood.

The separation process is based on the so-called Dean effect [2], which denotes a double vortex structure perpendicular to the primary flow along a curved duct. The effect is characterized by the Dean number $De = \rho v D_h/\eta\,(D_h/(2R))^{0.5}$, involving the primary flow velocity v, the fluid's parameters density ρ and viscosity η, and the geometric parameters hydraulic diameter $D_h = 4A/P$ (A: cross-sectional area, P: wetted perimeter) and the duct's radius R. This flow phenomenon can be applied to focus solid components dispersed in a liquid phase. Depending on their size and presumably also their shape and concentration they migrate across the primary flow to an equilibrium position near the inner wall, where they are trapped by a balance of Dean force, inertial lift force, and wall lift force [4].

Experiments are conducted aiming at designing a microfluidic spiral capable of separating spherical particles, used as simplified model system, of the diameter of 2-18 µm by symmetrically splitting the spirals outlet. It is expected that the presence of red blood cells in the flow decreases the efficacy of the process while increasing the channel's fluidic resistance. Experiments therefore also shed light on the conflict of diluting the blood sample which decreases the particles' low inlet concentration while separation in the duct is enhanced with a positive effect on the particles' outlet concentration.

The separation efficacy is described by the ratio between the particle concentration at the inner outlet and inlet (separation ratio s_r). It must be taken into account that the symmetrical splitter can lead to a theoretical maximum of a factor of s_r=2. Inlet samples are diluted with a buffer, and experiments are carried out containing more than 20% of blood ($c_b > 0.2$), exactly 20% of blood ($c_b = 0.2$), and containing no blood at all ($c_b = 0$). If the system's parameters lead to De >1 and a ratio of particle size and hydraulic diameter of d_p/D_h >0.12 the separation efficacy results in: $c_b > 0.2 \rightarrow s_r = 1.25 \pm 0.23$; $c_b = 0.2 \rightarrow s_r = 1.6 \pm 0.28$; $c_b = 0 \rightarrow s_r = 1.95 \pm 0.23$. The use of an asymmetric splitter results in a reduction of the volumetric flow rate in the inner outlet by 25%. This leads to $c_b = 0 \rightarrow s_r = 2.25 \pm 0.16$, and therefore enhances the mean efficacy by roughly 15%. A two-step separation process with two spirals connected in a row results in $c_b = 0 \rightarrow s_r = 3.69 \pm 0.32$. Limits for two-step separation and asymmetric splitters will be stressed more in further experiments.

The experimental investigations are accompanied by a numerical evaluation of the macroscopic fluid flow of whole blood in a microfluidic channel. The blood flow is implemented by two shear-thinning models for the viscosity, namely Quemada [5] and Carreau-Yasuda [6]. The simulation reveals that by using experimentally relevant inlet velocities in a curved duct of a cross-section of 45x55 µm^2 the flow leads to such high shear gradients in the liquid that the viscosity of the blood in the duct's cross-section can be approximated by a constant viscosity of 3-4 mPa s depending on the model in use. Further simulations address the particles' trajectories in the duct considering liquid-solid interactions.

Experimental and numerical investigations show that the presented microsystem can be applied to separate rare components from highly concentrated samples such as whole blood.

Acknowledgements: Financial supports by a fellowship within the Postdoc-Program of the German Academic Exchange Service (DAAD) and by a discovery grant from the Natural Sciences and Engineering Research Council (NSERC) in Canada are gratefully acknowledged.

References

[1] World Health Organization. World Health statistics (2014).

[2] W. R. Dean. Philos. Mag. (Ser. 7) 4 (1927), 208-223.

[4] D. Di Carlo et al. Proc. Natl. Acad. Sci. USA 104 (2007), 18892-18897.

[5] A. Marcinkowska-Gapińska et al. Med. Bio. Eng. Comput. 45 (2007), 837-844.

[6] J. Boyd et al. Phys. Fluids 19 (2007), 093703.

Modeling and simulation of mobile jet agitator for a biogas plant

Aria Alimi[1], Olaf Wünsch[1]
[1] Chair of Fluid Mechanics, Institute of Mechanics, University of Kassel

Nowadays, the biogas plants are one of the major natural energy sources in the world. The mixture inside these plants, which consists of different types of slurry, has to be stirred due to the sedimentation of high-viscous component after a certain amount of time. Currently, there are submersible motor agitators in use for this purpose, which need a long time to stir the whole component and also need opening the cover of biogas plant every time. The goal of this work is to investigate a new concept to mix the content of a biogas plant having none of the above restrictions based on a mobile stirring system that works in a closed pumping process. It works on a similar principle as a jet pump of a watercraft. The content of the plant will be pumped out and then will be pumped inside with a high inlet velocity on different positions already defined on the plant body.

In order to design such a mixing process, we simulate it numerically using Finite-Volume-Method for different types of meshed cylinder geometries. The problem involves an unsteady-state flow with two unmixable phases and will be calculated using Volume of Fluid (VOF) solver. The material properties of the contents -the most important one are the density and viscosity- have to be analyzed using rheometer device. The model consists of two different phases: the high-viscous component which has a viscosity of about 40 Pas, and the low-viscous component with a viscosity of about 0.003 Pas. The mixing process will be analyzed through the study of the flow field. Furthermore, the parameter study such as different inlet velocities or inlet directions will be performed.

Regarding the validation of simulations, different experiments are carried out on a labor scale biogas plant with transparent walls. Considering the similitude theory, appropriate materials come in use for both high and low viscous components and the mixing process will be monitored closely. The mixing process in both numerical simulations and the experiments will be compared and the results would be discussed.

References

[1] M. Gerber. Ganzheitliche stoffliche und energetische Modellierung des Biogasbildungsprozeses. Dissertation, Faculty of Mechanical Engineering, Ruhr-Universität, Bochum (2009)

[2] P. Mähnert. Kinetik der Biogasproduktion aus nachwachsenden Rohstoffen und Gülle. Dissertation, Landwirtschaftlich-Gärtnerische Fakultät, Humboldt–Universität, Berlin (2007)

Interaction of a finite-size particle with a wall

Francesco Romanò, Hendrik C. Kuhlmann
Vienna University of Technology, Tower BA/E322, Getreidemarkt 9, 1060 Vienna

The motion of a particle moving near a domain boundary is investigated. If the tangential velocity along the boundary is large the streamlines are dense and the finite size of a particle can have a profound effect on its trajectory. Despite of Stokes numbers as small as 10^{-5}, this effect has been shown to be important in certain free-surface flows [1, 2, 3].

Here we consider the steady two-dimensional flow in a lid-driven cavity. We examine the particle motion using different particle motion models: perfect tracers, inertial point particles (Maxey–Riley equation) one-way coupled to the flow, and finite-size particles the flow around which is fully resolved (two-way coupling). We discuss and quantify the finite-size effect and compare the results with the particle–surface interaction model originally introduced by [1].

As a results of the simulation of the fully resolved motion of finite-size particles we directly obtain the forces and torques on the particle. This information is used to derive a particle-motion model which can be employed to simulate the transport of a large number of particles and which represents an improvement of the inelastic particle–surface interaction model originally introduced by [1].

The numerical technique used to simulate the phenomenon belongs to the hp-methods (DG-FEM, in particular) and it is coupled with the so-called "smoothed-profile method" (SPM). This approach was developed in [4] for low and moderate Reynolds numbers. More recently, it has been further extended to high-Reynolds-number flows. The strengths of this approach are (a) the absence of moving grids as are required for, e.g., the ALE technique and (b) an accurately and efficient computation of the particle motion. The latter is ensured thanks to the spectral convergence and use of high-order methods of the DG-FEM technique.

References

[1] Hofmann, E., Kuhlmann, H. C. Particle accumulation on periodic orbits by repeated free surface collisions Phys. Fluids 23 (2011), 0721106-1–0721106-14.

[2] Muldoon, F. H., Kuhlmann, H. C. Coherent particulate structures by boundary interaction of small particles in confined periodic flows Physica D 253 (2013), 40–65.

[3] Mukin, R. V., Kuhlmann, H. C. Topology of hydrothermal waves in liquid bridges and dissipative structures of transported particles Phys. Rev. E 88 (2013), 053016-1–053016-20.

[4] X. Luo, M. R. Maxey, G. E. Karniadakis, Smoothed profile method for particulate flows: Error analysis and simulations, J. Comput. Phys. 228 (2009), 1750–1769.

The magnetoviscous effect of a biocompatible ferrofluid diluted in sheep blood.

J. Nowak, S. Odenbach
Technische Universität Dresden, Institute of Fluid Mechanics,
Chair of Magnetofluiddynamics, 01062 Dresden, Germany

Ferrofluids, suspensions of magnetic nanoparticles in suitable carrier liquids, are receiving a growing importance in biomedical applications. While being used in magnetic resonance imaging with great success for several years, new approaches like e.g. magnetic drug targeting are of great interest [1]. This approach focuses on binding chemotherapeutic agents to the magnetic particles suspended in the fluid. These ferrofluids are arterially injected and concentrated in the tumor by the application of external magnetic fields in the respective region. This application being in the focus of current research has the potential to decrease side effects of conventional chemotherapy and to increase its effectiveness.

To guarantee a safe and effective application of the ferrofluids the knowledge of the flow characteristics is important. For ferrofluids used in the engineering context the magnetoviscous effect (MVE), a rise in viscosity due to the formation of particle-structures caused by the application of an external magnetic field, is well known and investigated in some detail [2]. This effect was detected for bicompatible ferrofluids as well [3]. Nevertheless up to now no extends were made to characterize the flow behavior of biocompatible ferrofluids if a dilution in blood occurs.

This experimental study focuses on the rheological investigation of a biocompatible ferrofluid mixed with sheep blood. Results measured using a specially designed shear rate-controlled rheometer [4] are compared to results measured with a novel capillary rheometer designed for the special needs of the measurement conditions existing.

The relative increase of viscosity, the MVE, if an external magnetic field is applied for pure ferrofluids is compared for both rheometers, revealing an effect above 1000 % for low shear rates. For higher shear, which have to be expected during a potential biomedical application, the MVE is still measurable using the capillary viscosimeter. If the ferrofluid is diluted with sheep blood an increasing viscosity caused by an external magnetic field can be measured as well, being significantly different if compared to water as diluting agent, Therefore particle-particle interactions of the ferrofluids nanoparticles and the cells found in the sheep blood have to be assumed.

Financial support by the Deutsche Forschungsgesellschaft under grant no. OD18/23-1 is gratefully acknowledged.

References

[1] C. Alexiou et al. Cancer therapy with drug loaded magnetic nanoparticles - magnetic drug targeting. J. Magn. Magn. Mater. 323, 1404-1407 (2011)

[2] J. Nowak et. al. The influence of hydrodynamic diameter and core composition on the magnetoviscous effect of biocompatible ferrofluids. J. Phys.: Condens. Matter 26, 176004 (2014)

[3] S. Odenbach. Magnetoviscous Effects in Ferrofluids. LNP 71, Springer, Berlin (2002)

[4] S. Odenbach, H.Störk. Shear dependence of field-induced contributions to the viscosity of magnetic Fluids at low shear rates. J. Magn. Magn. Mater. 202, 155–158 (1998)

The anisotropy of the magnetoviscous effect in a magnetite ferrofluid with weak interparticle interactions

J.M. Linke, S. Odenbach
TU Dresden, Chair of Magnetofluiddyanmics, 01062 Dresden, Germany

Ferrofluids are colloidal suspensions of magnetic nanoparticles in a carrier liquid. If the magnetic particles are large enough to interact by dipole-dipole interactions in an applied magnetic field, chain-like microstructures of associated particles are formed in the direction of the applied field. These microstructures can rupture if the ferrofluid is sheared. Both, the formation and the disintegration of the microstructures are accompanied by a change in the viscous properties of the ferrofluid. The change in viscosity, called magnetoviscous effect MVE [1], depends on the intensity of the applied field and the shear, and also on their relative orientation. While this anisotropy is known from theoretical and experimental studies, measurements of the magnetoviscous properties are generally conducted in rotational or capillary flow rheometers [2], which allow only one distinct orientation of the magnetic field with respect to the fluid flow.

In the present work, a four-coil magnet system and a specially designed slit die viscometer [3] have been used to study the anisotropy of the MVE in a magnetite ferrofluid for three different directions of the magnetic field: in the direction of the flow, in the direction of the velocity gradient, and in neutral direction parallel to the vorticity. The measurement of the three corresponding Miesowicz viscosity coefficients allows a comprehensive magnetorheological characterization of the magnetite ferrofluid. Effects like the field-induced increase of the MVE, the shear thinning and the shear stability for field directions perpendicular to the vorticity have been confirmed. A negative MVE related to the crystal anisotropy of magnetite as observed by Grants [4] for constant shear rates in neutral direction could not be confirmed.

The highest MVE has been measured in a magnetic field perpendicular to the flow and to the vorticity. Elongated microstructures oriented in this direction have the highest moment of inertia and therefore offer the highest resistance to the flow resulting in the highest change in viscosity. On the other hand, elongated structures oriented parallel to the direction of the flow offer less resistance to the flow. Hence at low shear rates the lowest MVE has been observed in a field parallel to the flow. However, if the shear rate is increased, the lowest MVE is found in a field parallel to the vorticity. This is in agreement with Shliomis' theory of non-interacting particles [5] which predicts that for individual spherical particles the viscosity increase is zero for the magnetic field parallel to the vorticity. Hence the observed anisotropy of the MVE corroborates the field-driven formation and shear-induced disintegration of elongated chain-like microstructures in the ferrofluid. Nonetheless, future experiments will have to be complemented by molecular dynamics simulations to relate microstructural changes and rheological behaviour in ferrofluids.

We gratefully acknowledge the financial support by the Deutsche Forschungsgemeinschaft (DFG grant Od18–18).

References

[1] S. Odenbach. Magnetoviscous Effects in Ferrofluids. Lecture Notes in Physics M71 (2002), Springer, Berlin.

[2] M. Gerth-Noritzsch, D.Y. Borin, S. Odenbach. Anisotropy of the magnetoviscous effect in ferrofluids containing nanoparticles exhibiting magnetic dipole interaction. J. Phys.: Condens. Matt. 23 (2011), 346002.

[3] J.M. Linke, S. Odenbach. Anisotropy of the magnetoviscous effect in a ferrofluid with weakly interacting magnetite nanoparticles. Submitted to J. Phys.–Condens. Mat.

[4] A. Grants, A. Irbitis, G. Kronkalns, M.M. Maiorov. Rheological properties of magnetite magnetic fluid. J. Magn. Magn. Mater. 85 (1990), 129.

[5] M.I. Shliomis in Ferrofluids: Magnetically Controllable Fluids and Their Applications. Lecture Notes in Physics 594, p. 85–111, S. Odenbach ed. (2002), Springer, Berlin.

An innovative phase transition modeling for reproducing cavitation through a five-equation and seven-equation models and complex equation of state

M.G. Rodio[+], P.M. Congedo [+], R. Abgrall*
([+])INRIA Bordeaux–Sud-Ouest, France
(*) Institut für Mathematik, Universität Zürich, Switzerland

This work is devoted to model the heat and mass transfer through a liquid/vapor interface in compressible two-phase models. Modeling the heat and mass transfer between the phases is of utmost importance when simulating flows in fuel injectors, turbo-pumps, nozzles, etc. Usually, in some of these applications, cavitation could appear because of a strong liquid acceleration, yielding a strong rarefaction wave and hence with vapor/gas bubbles creation. The consequences of cavitation, such as noise, performance device reduction and wall corrosion, are extremely negative. For these reasons, this phenomenon requires a good theoretical comprehension and, as consequence, an accurate predictive physical model is required.

The most important reference about the treatment of heat and mass transfer terms, for the Interface Diffusive models, is the work of Saurel et al. [1]. The authors proposed a phase transition modeling for a single velocity and single pressure model (five equations model) relying on a thermo-chemical relaxation. In fact, by obtaining the equality of temperature and chemical potential for the two phases, this relaxation assures the evolution of liquid phase from a metastable state to an equilibrium state on the saturation curve. During this evolution, the liquid phase releases mass in order to evaporate before assuming a new state on the saturation curve. Then, the authors proposed an original procedure to identify the liquid/vapor interface. In recent years, few works have been proposed for treating phase transition modeling in Interface Diffusive models [2, 1, 3, 5, 4, 6].

The first idea of the present contribution is to couple the treatment of heat and mass transfer terms proposed in [1] for a five equation model , with the procedure for solution admissibility of [5], thus preserving the positivity of the solution and reducing consistently the computational cost. The second innovative point of this work is the extension of the proposed model to six and seven-equation models, thus showing its flexibility.

For closing the compressible seven-equation two-phase model, an equation of state (EOS) is necessary to define the thermodynamic behavior of each single phase and of the liquid-vapor mixture, under the saturation curve. When complex fluids are considered, such as cryogenic, molecularly complex ones, the use of simple EOS can produce imprecise estimation of the thermodynamic properties, thus leading to the deterioration of the accuracy of the prediction. Increasing the complexity of the model and calibrating the additional parameters with respect to the available experimental data are certainly valid options for improving the model prediction. Nevertheless, this is very challenging because of the numerical difficulties for the implementation of more complex mathematical model and because of the large uncertainties that generally affect the experimental data. Actually, the most used EOS for reproducing the liquid/vapor behavior under the saturation curve is the Stiffened Gas (SG) EOS [1, 5]. The reason is that this EOS allows an explicit mathematical calculations of important flow relation. Moreover, in mass transfer problems it assures the positivity of speed of sound in the two-phase region, under the saturation curve.

So, finally, the third contribution of this work is to show how the numerical solver based on a Discrete equation Method (DEM) formulation [7] can be modified to include a more complex equations of state than the SG for the vapor region.

References

[1] R. Saurel and F. Petitpas and R. Abgrall. Modelling phase transition in metastable liquids. Application to cavitating and flashing flows. Journal of Fluids Mechanics, 607 (2008), 313–350.

[2] E. Goncalves. Modeling for non isothermal cavitation using 4-equation models. International Journal of Heat and Mass Transfer, 76 (2014), 247–262.

[3] A. Zein and M. Hantke and G. Warnecke. Modeling phase transition for compressible two-phase flows applied to metastable liquids. Journal of Computational Physics 229 (2010), 2964–2998.

[4] F. Daude and P. Galon and Z. Gao and E. Blaud. Numerical experiments using a HLLC-type scheme with {ALE} formulation for compressible two-phase flows five-equation models with phase transition. Computers & Fluids 94 (2014), 112–138.

[5] M. Pelanti and K. M. Shyue. A mixture-energy-consistent six-equation two-phase numerical model for fluids with interfaces, cavitation and evaporation waves. Journal of Computational Physics 259 (2014), 331–357.

[6] Y. Wang, L. Qiu, R. D. Reitz and R. Diwakar. Simulating cavitating liquid jets using a compressible and equilibrium two-phase flow solver. International Journal of Multiphase Flow 63 (2014), 52–67.

[7] R. Abgrall and R. Saurel. Discrete Equations for Physical and Numerical Compressible Multiphase Mixtures. Journal of Computational Physics, 186 (2003), 361–396.

Numerical investigation of a liquid displacing a gas in thin porous layers

Tim Neumann, Konrad Boettcher, Lutz Gödeke, Peter Ehrhard
Strömungsmechanik, Bio-und Chemieingenieurwesen
TU Dortmund
Emil-Figge-Str. 68, D-44227 Dortmund
Email: Tim.Neumann@bci.tu-dortmund.de

Liquid flow through a porous media is of great importance in many engineering problems, e.g. calculating the heat and mass transfer in fixed bed catalytic reactors or estimating the potential environmental risks of fracking. The cells of an lithium-ion battery may be described as thin porous layers sintered on the electrodes, with a thin and permeable layer separating these two porous domains, so that one elementary cell is composed of three porous layers with heterogeneous characteristics of the porosity. The whole battery consists of many elementary three-layer cells.
This presentation deals with a liquid displacing a gas in such an elementary three-layer cell, which occurs during the filling of the battery with the electrolyte. The investigation is based upon the volume-averaged Navier-Stokes equations, using a volume of fluid method to cover the multiphase flow. The flow is investigated with respect to the wall-effect and capillary action in porous media. The Ergun equation is used to estimate the permeability, depending on the distance to the wall. Since the layers are thin and the characteristic size of the particles is comparatively large, friction of the electrode is taken into account with respect to the mobility of the contact line. The implemented models are validated against analytical results, showing only small deviation. Thereafter, results of the displacement flow in the elementary cell are presented and discussed, showing a not negligible influence of the modeled effects onto the flow characteristics.

Mechanisms for wave generation in countercurrent air-water turbulent flows

Francesco Zonta[1], Miguel Onorato[2], Alfredo Soldati[1]
[1] Department of Elec., Manag. and Mechanical Enginerring, University of Udine, 33100 Udine, Italy.
[2] Department of Physics, University of Torino, 10125 Torino, Italy.

Mass, momentum and energy transport phenomena through a deformable air-water interface are important in many geophysical processes and industrial applications. In this study, we use Direct Numerical Simulation (DNS) of the Navier Stokes equations to analyze the dynamics of the interface between air and water when they are driven by opposite pressure gradients (countercurrent configuration). The Reynolds number (Re_τ), the Weber number (We) and the Froude number (Fr) fully describe the physical problem. We examine the problem of the transient growth of interface waves for different combinations of physical parameters. Keeping Re_τ constant and varying We and Fr, we show that, in the initial stages of the wave generation process, the amplitude of the interface elevation η grows in time as $\eta \propto t^{2/5}$. Later in time, the waves growth rate differs depending on the value of Fr,We: for small capillary waves, we do not observe substantial changes from $t^{2/5}$ law; for longer gravity waves we observe a faster growth rate. From the single wave mode analysis, we observe a similar behavior for the growth rate of the most significant modes. Simple phenomenological models have been derived to explain our results. At steady state, our data confirm previous results: wavenumber spectra, $E(k_x)$, of the surface elevation in the capillary range are in good agreement with the prediction of the Wave Turbulence Theory. Finally, we also evaluate wave-induced modifications of the average wind and current velocity profiles.

Diffuse interface models for locally inextensible vesicles

Sebastian Aland, John Lowengrub, Axel Voigt
Institut für wissenschaftliches Rechnen, TU Dresden, Germany
Department of Mathematics, UC Irvine, California, USA

The presence of lipid molecules at the membrane of lipid vesicles makes the membrane itself incompressible. This property is also termed inextensibility and implies that the surface divergence of the velocity field vanishes at the vesicle surface:

$$\nabla_\Gamma \cdot \mathbf{v} = 0 \qquad \text{on } \Gamma.$$

We present new diffuse interface models for the dynamics of such inextensible vesicles in a viscous fluid [1]. A new feature of this work is the implementation of the local inextensibility condition by using a local Lagrange multiplier harmonically extended off the interface. To make the method even more robust, we develop a local relaxation scheme that dynamically corrects local stretching/compression errors, thereby preventing their accumulation. We present numerical results that confirm the effectiveness of the proposed models in a test case scenario of vesicles in shear flow. Finally we apply the model to a problem of clathrin-mediated endocytosis. Clathrin proteins attach to the membrane and alter locally its bending stiffness and spontaneous curvature. This process can lead to budding and pinch-off of small vesicles. First numerical simulation results will be shown.

References

[1] S. Aland, S. Egerer, J. Lowengrub, A. Voigt Diffuse interface models of locally inextensible vesicles in a viscous fluid. J. Comp. Phys. 277 (2014), 32–47.

Polymer Devolatilization in a Rotating Apparatus

Stefan Hirschfeld[1], Lutz Hermann[1], Olaf Wünsch[1]
[1] Chair of Fluid Mechanics, Institute of Mechanics, University of Kassel

Devolatilization processes are of great importance in polymer processing. This unit operation is carried out several times within the production process of plastics. Devolatilization or degassing is the controlled removal of volatile compounds which are often harmful to health and environment. Furthermore, these substances downgrade the properties of the polymer products. There are two different mechanisms of devolatilization for polymer melts: film degassing and bubble degassing. Film degassing takes place on continiuous free surfaces between the liquid polymer phase and the gas phase. Mass transfer proceeds due to diffusion. Bubble degassing involves a more complex mechanism, where foaming is introduced as the solution is supersaturated. This means the ambient pressure is below the equilibrium partial pressure. Similar processes as by film degassing occur inside each bubble in the foam. Futhermore, the devolatilization equipment is classified into two main categories: rotating and nonrotating devolatilizers. Rotating devices are usually used for devolatilization of high-viscous polymers. [1, 2]

This contribution presents the experimental study of film degassing in a partial filled agitator vessel. A laminar fluid flow with a distinct free surface for the degassing process occurs. High-viscous polydimethylsiloxane with a viscosity of about 100 Pas enriched with 1,1,2-trichloro-1,2,2-trifluoroethane is used as model substance system. Degassing is introduced by purging with a nitrogen gas flow. Concentration analysis of the liquid phase is realized by thermogravimetric measurements. The exiting gas stream of the test apparatus passes through two cold-traps in series to precipitate the volatile compound. The results of the weighted condensate are compared with the concentration analysis. All experiments were performed at ambient temperature. Data for the vapor-liquid equilibrium at the phase interface are obtained by measurement of pressure, temperatur and volume flow in the gas stream. The experiments are evaluated and discussed based on the surface renewal theory or penetration theory by Higbie and Danckwerts [3]. This model assumes that the diffusion in the polymer is the rate-controlling step of devolatilization. Mass transfer is modeled as an locally unsteady process within an exposure time of liquid at the free surface. Afterwards, this degassed fluid elements are assumed to be complete mixed into the bulk of the liquid phase.

References

[1] VDI-Gesellschaft Kunststofftechnik: Aufbereitungstechnik 2006. Entgasungsprozesse in der Aufbereitungstechnik. VDI-Verlag, Düsseldorf, 2006.

[2] R.J. Albalak. Polymer Devolatilization. Hanser Publishers, München, 1996.

[3] P.V. Danckwerts. Significance of liquid-film coefficients in gas absorption. Ind. Eng. Chem. 43 (1951) 6, 1460-1467.

Gas Bubbles in Micro-Capillaries - Hydrodynamics and Mass Transfer

Peter Lakshmanan, Peter Ehrhard
TU Dortmund University - BCI - Fluid Mechanics

Process design of multi-phase unit operations on the micro-scale asks for detailed knowledge of the hydrodynamics and mass transfer behavior of discrete disperse fluid particles in confined geometries. In the present work, the focus is on single gas bubbles in vertical capillaries. Hydrodynamics and mass transfer are examined using numerical methods.

The hydrodynamic behavior of a single bubble in a capillary including its deformation is examined numerically using a modified level-set method [1]. Additionally, the influence of surface-active contaminations ('surfactants') and the resulting Marangoni effects are taken into account [2]. This enables the differentiation of bubbles with a mobile, i.e. clean, interface and those with a immobile, i.e. contaminated, interface. Based on the hydrodynamics, the mass transfer is examined, again employing numerical methods. In the present work, mass transfer is from the bubble into the bulk fluid. The system is assumed to be dilute, i.e. the concentrations are small and do not influence other fluid properties ('one-way coupling'). By using either asymptotic approximations or very high mesh resolutions, the local concentration field in and around the gas bubble can be resolved, which gives access to the local mass transfer in terms of a local Sherwood number.

Two modes of operation are examined for the cases of a mobile and immobile gas-liquid-interface: (i) A gas bubble rising in a vertical capillary filled with a stagnant liquid; (ii) A gas bubble levitated in a vertical capillary.

Results are in good agreement to experimental data and available correlations from literature. Based on the knowledge of the drag coefficients and local and also integral Sherwood numbers over a wide field of parameters (Re, Sc, $d_{\mathrm{bubble}}/d_{\mathrm{capillary}}$) and mode of operation allows for the analysis and optimization of unit operations employing multiphase micro-capillaries.

References

[1] E. Olsson, G. Kreiss. A conservative level set method for two phase flow. J. Comp. Sc. 210 (2005), 225–246.

[2] P. Lakshmanan, P. Ehrhard. Maragoni effects caused by contaminants adsorbed on bubble surfaces. J. Fluid Mech. 647 (2010), 143 –161.

Simulation of mass transfer at free liquid/liquid interfaces

Christian Heckmann, Peter Ehrhard, Peter Lakshmanan
Strömungsmechanik, Bio- und Chemieingenieurwesen
TU Dortmund
Emil–Figge–Str. 68, D–44227 Dortmund
Email: christian.heckmann@bci.tu-dortmund.de

Mass transfer in multiphase systems finds extensive application in chemical–engineering problems, like chemical reactions, extraction, or adsorption. In liquid–liquid systems, usually, the mass transfer resistance in both phases appears to be relevant – this is a conjugated problem. Hence, a detailed knowledge of the mechanisms and characteristics of the mass–transfer process in conjunction with the geometrical properties of the multiphase system appears to be crucial for the process design. Numerical simulations are certainly an ideal tool for a local examination of such mass–transfer processes, since experiments usually remain restricted to integral measurements.

We present a concept for the numerical simulation of the mass transfer at a free liquid/liquid interface, based on the open–source software package openFOAM. Starting point for the hydrodynamics of the examined two–phase system is an imported steady–state interface. On both sides of this interface (separate) computational domains for both liquids are arranged, whereas a kinematic coupling at this interface is in place. Hence, the flow can be computed within both computational domains. The mass transfer is examined, based on this steady–state hydrodynamics, by solving a transport equation of a passive (scalar) concentration at both sides of the interface. At the liquid/liquid interface, transition conditions arise from both the interfacial dissolution equilibrium and mass–flux continuity. Our numerical approach is validated against analytical limiting cases.

Three-phase contact line pinning at structured surfaces by molecular dynamics simulation

Stefan Becker, Maximilian Kohns, Martin Horsch, and Hans Hasse
Laboratory of Engineering Thermodynamics, University of Kaiserslautern, Germany

The wetting behaviour of a fluid in contact with a solid substrate is important for many applications and processes. Molecular simulation allows to investigate adsorption and wetting with atomistic resolution. In the present study, the massively-parallel molecular dynamics code *ls1 mardyn* [1] is employed to simulate adsorption and wetting in dependence on the fluid-solid interaction and the structure of the solid substrate. In this way, the influence of the surface morphology on the contact line and the contact angle is captured.

For a perfectly planar surface and a sessile droplet, both interacting by the truncated and shifted Lennard-Jones potential, the contat angle is determined from density profiles and correlated in terms of the magnitude of the fluid-wall dispersion energy [2]. The entire range between complete wetting and dewetting is covered, as well as the temperature range from the triple point up to the critical point. Contact line pinning is considered for the boundary between planar and hydrophilic rough regions in the Wenzel state, and for the epitaxial Cassie state, where a contact line of an advancing droplet is stuck at an edge.

The validity of the Gibbs inequality, which describes the range of contact angles at which pinning occurs, is confirmed down to the nanometre length scale. The precise position of the equimolar contact line, however, deviates from the edge of the substrate by a characteristic length of about 5 Å, due to the influence of the adsorbed precursor layer on the three-phase contact region.

References

[1] C. Niethammer, S. Becker, M. Bernreuther, M. Buchholz, W. Eckhardt, A. Heinecke, S. Werth, H. J. Bungartz, C. W. Glass, H. Hasse, J. Vrabec, M. Horsch, J. Chem. Theory Comput. **10**(10), 4455 (2014)

[2] S. Becker, H. M. Urbassek, M. Horsch, H. Hasse, Langmuir **30**(45), 13606 (2014)

New density based OpenFOAM solver with a stochastic fields approach for two phase flow

Michael Ranft[1], Andreas G. Class[2], Thomas Jordan[1]
[1] Institute for Nuclear and Energy Technologies, Karlsruhe Institute of Technology
[2] Areva Nuclear Professional School, Karlsruhe Institute of Technology

A new density based solver is implemented in the C++ library OpenFOAM, applying the finite volume method. For a second order accurate space discretization the provided interpolation schemes and limiters are used. The time discretization a Dual Time Stepping technique is used, whereby at each physical time step the flow is treated as a pseudo steady state problem. The equations are integrated over a so-called pseudo time τ until steady state is reached, where τ is only a relaxation factor with no physical meaning. The previous flow variables in physical time are treated as explicit source terms in the pseudo time integration. With Dual Time Stepping the physical time steps aren't limited by the Courant-Friedrichs-Lewy condition and the von Neumann criterion.

The convective fluxes through the cell faces are provided by new implemented standard flux schemes. Additional a preconditioning technique is adopted for removing the stiffness from the system of flow equations at low Mach numbers. The preconditioning scales the acoustic eigenvalues of the system until they are of the same order as the convective eigenvalues.

For time integration in pseudo time SSP Runge-Kutta time schemes are used. Whereby schemes with more stages than order extend the CFL coefficient and lead to greater pseudo time steps. Further accelerating of time integration in pseudo time without influencing the accuracy of the transient problem in the physical time is done with the following techniques. A local time step, depending on the local CFL and von Neumann criterion, allows greater time steps where local velocity is small or grid space is large. An implicit residual smoothing is done extending the stability limits of the scheme. The residuals for the Runge-Kutta stage are exchanged with a weighted average residual of neighboring cells. A bulk viscosity damping technique is added, damping error waves in the computational flow domain by adding a small value of viscosity to the momentum and optional to the energy equation. A multigrid algorithm is applied, using a series of successive coarser grids. For the interaction between the different grids a Full Approximation Storage (FAS) is used, whereby a Full Multigrid (FMG) initialize the solutions at the different meshes, beginning at the coarsest grid.

The effective turbulence viscosity and effective thermal diffusivity are provided by the k-ω SST turbulence model for the diffusion fluxes. And the stochastic field method by Valiño [1] is used for simulating the two phase flow. This approach was extended by Dumond et al. [2] for simulating a cavitating flow. Their procedure is integrated into the new density based flow solver, where the two phase flow is treated as single fluid and the stochastic fields provide the mass fractions of the two phases.

The main differences between the new solver and the published density based solver in the framework of OpenFOAM are the use of SSP Runge-Kutta schemes, instead of standard low-storage, the new integration of a FMG-FAS multigrid scheme and the extension with a stochastic field method. Solving all flow equations including stochastic field and turbulence model at each Runge-Kutta stage is another advantage.

References

[1] L. Valiño. A Field Monte Carlo Formulation for Calculating the Probability Density Function of a Single Scalar in a Turbulent Flow. Flow, Turbulence and Combustion, 60 (1998), 157–172

[2] J. Dumond, F. Magagnato, A. Class. A. Stochastic-field cavitation model. Physics of Fluids, 25 (2013).