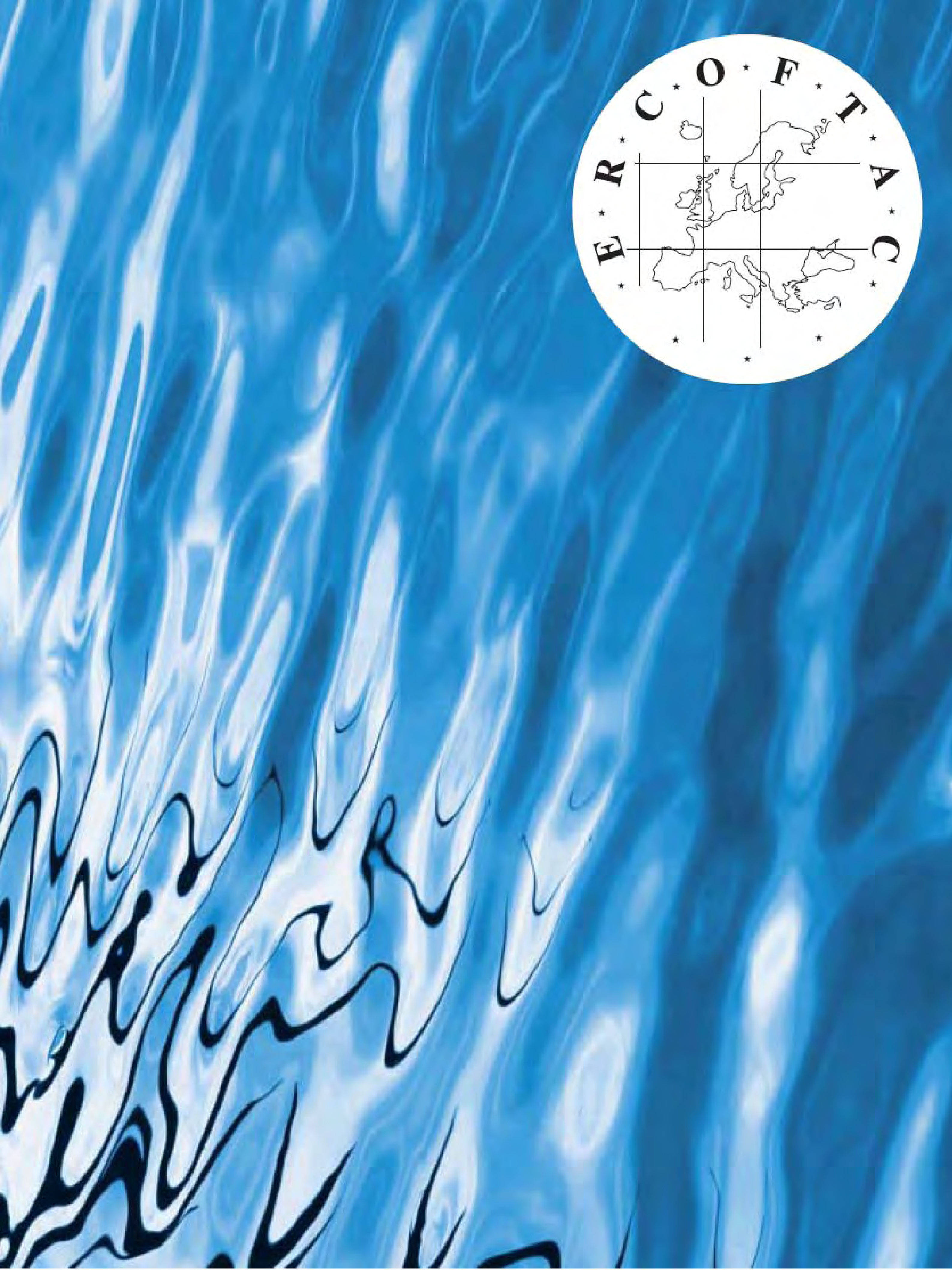

ERCOFTAC Bulletin *December 2009* **81**

European Research Community On Flow, Turbulence and Combustion

ERCOFTAC is a leading European association of research, education and industry groups in the technology of flow, turbulence and combustion. The main objectives of *ERCOFTAC* are: To promote joint efforts of European research institutes and industries with the aim of **exchanging technical and scientific information**; to promote **Pilot Centres** for collaboration, stimulation and application of research across Europe; to stimulate, through the creation of **Special Interest Groups**, well-coordinated European-wide research efforts on specific topics; to stimulate the creation of advanced training activities; and to be influential on funding agencies, governments, the European Commission and the European Parliament.

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ERCOFTAC Bulletin 81, December 2009

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Next *ERCOFTAC* Events

ERCOFTAC Spring Festival
17th May 2010
TU Delft, The Netherlands.

ERCOFTAC SPC, IPC & EC Meetings
18th May 2010
TU Delft, The Netherlands.

The ERCOFTAC Best Practice Guidelines for Industrial Computational Fluid Dynamics

The Best Practice Guidelines (BPG) were commissioned by ERCOFTAC following an extensive consultation with European industry which revealed an urgent demand for such a document. The first edition was completed in January 2000 and constitutes generic advice on how to carry out quality CFD calculations. The BPG therefore address mesh design; construction of numerical boundary conditions where problem data is uncertain; mesh and model sensitivity checks; distinction between numerical and turbulence model inadequacy; preliminary information regarding the limitations of turbulence models etc. The aim is to encourage a common best practice by virtue of which separate analyses of the same problem, using the same model physics, should produce consistent results. Input and advice was sought from a wide cross-section of CFD specialists, eminent academics, end-users and, (particularly important) the leading commercial code vendors established in Europe. Thus, the final document can be considered to represent the consensus view of the European CFD community.

Inevitably, the Guidelines cannot cover every aspect of CFD in detail. They are intended to offer roughly those 20% of the most important general rules of advice that cover roughly 80% of the problems likely to be encountered. As such, they constitute essential information for the novice user and provide a basis for quality management and regulation of safety submissions which rely on CFD. Experience has also shown that they can often provide useful advice for the more experienced user. The technical content is limited to single-phase, compressible and incompressible, steady and unsteady, turbulent and laminar flow with and without heat transfer. Versions which are customised to other aspects of CFD (the remaining 20% of problems) are planned for the future.

The seven principle chapters of the document address numerical, convergence and round-off errors; turbulence modelling; application uncertainties; user errors; code errors; validation and sensitivity tests for CFD models and finally examples of the BPG applied in practice. In the first six of these, each of the different sources of error and uncertainty are examined and discussed, including references to important books, articles and reviews. Following the discussion sections, short simple bullet-point statements of advice are listed which provide clear guidance and are easily understandable without elaborate mathematics. As an illustrative example, an extract dealing with the use of turbulent wall functions is given below:

- Check that the correct form of the wall function is being used to take into account the wall roughness. An equivalent roughness height and a modified multiplier in the law of the wall must be used.
- Check the upper limit on $y+$. In the case of moderate Reynolds number, where the boundary layer only extends to $y+$ of 300 to 500, there is no chance of accurately resolving the boundary layer if the first integration point is placed at a location with the value of $y+$ of 100.
- Check the lower limit of $y+$. In the commonly used applications of wall functions, the meshing should be arranged so that the values of $y+$ at all the wall-adjacent integration points is only slightly above the recommended lower limit given by the code developers, typically between 20 and 30 (the form usually assumed for the wall functions is not valid much below these values). This procedure offers the best chances to resolve the turbulent portion of the boundary layer. It should be noted that this criterion is impossible to satisfy close to separation or reattachment zones unless $y+$ is based upon $y*$.
- Exercise care when calculating the flow using different schemes or different codes with wall functions on the same mesh. Cell centred schemes have their integration points at different locations in a mesh cell than cell vertex schemes. Thus the $y+$ value associated with a wall-adjacent cell differs according to which scheme is being used on the mesh.
- Check the resolution of the boundary layer. If boundary layer effects are important, it is recommended that the resolution of the boundary layer is checked after the computation. This can be achieved by a plot of the ratio between the turbulent to the molecular viscosity, which is high inside the boundary layer. Adequate boundary layer resolution requires at least 8-10 points in the layer.

All such statements of advice are gathered together at the end of the document to provide a 'Best Practice Checklist'. The examples chapter provides detailed expositions of eight test cases each one calculated by a code vendor (viz FLUENT, AEA Technology, Computational Dynamics, NUMECA) or code developer (viz Electricité de France, CEA, British Energy) and each of which highlights one or more specific points of advice arising in the BPG. These test cases range from natural convection in a cavity through to flow in a low speed centrifugal compressor and in an internal combustion engine valve.

Copies of the Best Practice Guidelines can be acquired from:

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The price per copy (not including postage) is:

Non-ERCOFTAC members:	150 Euros
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ERCOFTAC members:	100 Euros
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2009 Report from the Industry Engagement Officer

Richard Seoud
richard.seoud-ieo@ercoftac.org

Dear Members,

As you have seen from the ERCOFTAC News, on our website, I have been introducing activities based on best practice guidance courses/seminars, and technology awareness seminars.

ERCOFTAC is rather unique in the field of best practice guidance, as we have published two books so far, more in the pipeline, and I will be offering more courses/seminars around these and future books. Such a strategy would clearly indicate to the world our intentions of being leaders in this very important field.

On the topic of Technology Awareness, again, the diverse knowledge available in ERCOFTAC makes it rather unique, one only has to look at the topics covered in the Special Interest Groups (SIG). My aim is to extract cutting edge technologies and present them to the world. These technologies would be residing either in academia, or national research institutions, which in five years from now could become strong candidates, for entry into an industrial R&D cycle.

Now, in 2009, I would have delivered some 5 activities, all held within the EU. Countries like the UK, Germany, Italy, The Netherlands and Sweden. I would have held more activities, but not for the global economic downturn, that has gripped the world. The impact of which has been rapid declines in industrial output, personal income, and lest we not forget the steep rise in unemployment. I believe 2010 may offer a better picture than 2009, based on recent economic indicators, such as the Gross Domestic Product (GDP), and the Purchasing Manager Index (PMI), of France, Germany, China, and the USA, who are all technically out of recession. The UK is on the verge of exiting the recession. The economic health of such powerhouses is vital to the world of applied fluid mechanics, and to a certain extent, the level of activities undertaken by myself.

In respect of the delegate feedback forms, on the activities undertaken so far in 2009, all are overwhelmingly positive. Delegates tell us that they love what has been done, and encourage me to do more. From the quality of speakers, to venues and services on the day, all seems to be very much appreciated.

So, I would like to say thank you, to all those who are involved in helping me realise these activities, to the strong support from the executive committee, and to our delegates for their attendance.

Below I offer a brief on some of the activities that have taken place in 2009.

Finally, the aim in the future is to deliver a reasonably large set of activities that covers a wide spectrum of topics, and hopefully touches on most of our members' scientific and engineering interests, under the FTAC umbrella. However, as you all know , this takes time, and this is a start.

Best Regards,

Dr. Richard E. Seoud,
ERCOFTAC Industry Engagement Officer.

Technology Awareness Seminar - Advances in Mixing and Combustion
April 2009.
GE, Garching, Germany.

The aim of the technology awareness seminar is to inform our delegates about cutting edge ideas that are amenable, in say 5 years time, to an industrial R&D cycle. This seminar was well received, the feedback forms where pretty positive. We had a set of presentations that showed some impressive ideas, from Large Eddy Simulations (LES) applied to vertical short take-off and landing fighter aircrafts, beautiful ignition sequences using Direct Numerical Simulations (DNS), and how one can use fractal geometries to deliver on one side, designer turbulence, and the other, precise flow metering.

Location wise the GE Centre is not far from the airport. The GE auditorium is superb - thank you GE and Dr. E. Gharaibah.

Best Practice Guidance Course - Hybrid RANS-LES Methods for Industrial CFD.
June 2009.
GE, Garching, Germany.

The aim of this course is to introduce CFD practitioners in the field of turbulence modelling, to the topic of Hybrid RANS-LES. The Hybrid RANS-LES represents a large family of turbulence models. The course offers an overview, guidance and examples, with an emphasis on one class of models, the Detached Eddy Simulation (DES). Again, the course was very well received, overwhelmingly positive feedback forms. Once again, the GE auditorium delivered a sterling service.

The delegates received very nice booklets of the course presentations, and I am still in discussions with the exec committee on whether we offer CDs in the future, as some delegates wanted that. A case of watch this space.

Best Practice Guidance Seminar - CFD for Dispersed Multi-Phase Flows
October 2009.
La Sala Strozzi, Florence, Italy.

The seminar was delivered by the editors of the book. The seminar and the book were both welcomed for the fact that there is nothing similar on the market. Multiphase flow is a huge topic, and the book addresses the CFD of incompressible turbulent dispersed multi-phase flow. The feedback forms were very positive, and each delegate received a personal copy of the book. Also, I will be discussing with the executive committee the delivery of a two day course, as most of the delegates wanted to see something along those lines.

As a venue, well, it was held at the natural history museum in Florence, Italy, not much to argue about. The service and support were superb.

Thank you Univ. of Florence and Prof. F. Martelli.

Technology Awareness Seminar - Microfluidics and Microheat
November 2009.
Philips Applied Technologies, Eindhoven.

The day started with a welcome statement by the centre Vice President, and closed with a tour of Philips' world class facilities.

Best Practice Guidance Course in Industrial CFD - Hybrid RANS-LES Methods in Industrial CFD
November 2009.
FOI, Swedish Defence Agency, Sweden.

The course is running again, this time at FOI, Stockholm, in Sweden, and hopefully we can serve you all, and as many of our Nordic members as possible, who are engaged in the modelling of turbulent flows.

'DLES8' Workshop on Direct and Large-Eddy Simulation

EINDHOVEN, THE NETHERLANDS, 7-9 JULY 2010

Following the spirit of the series, the goal of this latest workshop is to establish a state-of-the-art of DNS and LES techniques for the computation and modeling of transitional/turbulent flows covering a broad scope of topics such as aerodynamics, acoustics, combustion, multiphase flows, environment, geophysics and bio-medical applications and fundamental aspects of LES. This gathering of specialists in the field should once again be a unique opportunity for discussions about the more recent advances in the prediction, understanding and control of turbulent flows in academic and industrial situations.

Authors wishing to contribute to the colloquium are invited to submit an abstract before January 15, 2010. Notification of acceptance will be given by March 15, 2010. Details about abstract submission will be announced on the website. Full length papers will be published as an ERCOFTAC Book Series.

www.dles8.tue.nl

Invited speakers

- Josette Bellan (Jet Propulsion Laboratory, California Institute of Technology, USA)
- Hester Bijl (Delft University of Technology, The Netherlands)
- Javier Jimenez (Universidad Politécnica de Madrid, Spain)
- Marc Parlange (EPFL, Switzerland):
- Heinz Pitsch (Stanford University, USA)
- Neil Sandham (University of Southampton, UK)
- Eric Serre (CNRS/Aix-Marseille Université, France)
- Claus Wagner (DLR, Germany)
- Grégoire Winckelmans (Université Catholique de Louvain, Belgium)

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ERCOFTAC 'Da Vinci Competition' 2009

Michael Leschziner

Chairman of the ERCOFTAC Scientific Programme Committee

The annual *da Vinci Competition* is one of the most important events in ERCOFTAC's calendar. Its importance arises from the fact that it is the principal ERCOFTAC forum for the youngest, most gifted researchers in our field in Europe to present the products of their endeavours. The hope, indeed expectation, is that these young researchers will progress to become Europe's leaders in Flow, Turbulence and Combustion, and will act as ERCOFTAC's most eminent ambassadors.

Every year, an invitation goes out to all Pilot Centres with the request to each nominate three outstanding research studies of PhD students or recent PhD graduates. Extended summaries submitted by the nominees to the SPC are then reviewed by a panel of eight judges, leading to the selection of five top candidates for the *da Vinci Prize*. These candidates are then invited to present their research at the *da Vinci Day* . The *da Vinci Prize* - 1000 Euros a Certificate and a medal - is awarded to the competitor judged by the jury to have demonstrated the best combination of scientific merit and presentational quality.

This year, the *da Vinci Competition* attracted 23 entries from 10 countries. The *da Vinci Day* was held at EPFL, Lausanne, on 1st October 2009. The summaries of the five selected presenters are published below, and bear witness to the outstandingly high technical quality of the large majority of the submissions made to the *da Vinci Competition*.

As usual, the winner emerged only after much discussion and argument. In the end, the Jury agreed unanimously to award the 2009 da Vinci Prize to **Dr.-Ing. Florian Schwertfirm**, from the Technical University of Münich, for his paper '**Direct Simulation and Modelling of Micromixing in high Schmidt Number Flows**'. The jury's collective view was that this research was of outstanding international standard, as well as being thematically very well aligned with ERCOFTAC's field of activity.

The jury and the SPC are grateful to all members of the ERCOFTAC Coordination Centre at EPFL, especially to Dr. Navid Borhani and Prof. John Thome, for their efficient and generous hosting of the meeting. Thanks are also due to Prof. Charles Hirsch for arranging the production of the medals awarded to the finalists and the certificate awarded to the winner.

Direct Simulation and Modelling of Micro-Mixing in High Schmidt Number Flows

F. Schwertfirm

Fachgebiet Strömungsmechanik Technische Univeristät München, Germany.

Introduction

The prediction of chemical and biological reaction processes in liquids has undergone enormous advances during the past years. One of the main reasons for this advancement lies in the development of numerical tools for the description of turbulent flows and mixing taking place herein. Several strategies are available for this task of which Direct Numerical Simulation (DNS) is the most reliable one as all turbulent length and time scale are resolved by the numerical method. If scales down to the Kolmogorov scale η_K are resolved by the computational grid, then no further turbulence model is required for the flow field. The smallest length scales of the scalar concentration field is, however, given by the Batchelor scale η_B, that scales in comparison to the Kolmogorov scale with the inverse of the square root of the Schmidt number $\eta_B = \eta_K/\sqrt{Sc}$ (Batchelor, 1959). The Schmidt number, defined as the ratio of diffusion vs. viscous time scale, can easily reach values of more than $Sc = 1000$ in liquids which renders the direct computation of turbulent scalar fields in a liquid unfeasible. Modeling of micro-mixing, i.e. mixing on scales smaller than Kolmogorov scale, is therefore necessary in such flows. As a severe consequence, chemical and biological reaction rates can not be described by quantities filtered at Kolmogorov scale as the sub-Kolmogorov scales dominate the concentration fluctuations of the species involved. Predicting reaction rates in liquid systems requires either modeling of the reaction rate itself or a correct representation of the sub-Kolmogorov fluctuations which can be done in a method based on probability density function (PDF) in which the reaction term in the convection-diffusion equation can be obtained in closed form (Pope, 1985). In these methods, the problem of modeling the reaction rate reduces to the problem of finding the correct mixing model with its corresponding time scale.

In this work a novel method is developed that couples a DNS of the flow field with a filtered density function (FDF) method for the sub-Kolmogorov fluctuations of the scalar field. The resulting equations are solved by a stochastic Lagrange-method in which the reaction term is available in closed form. The micro-mixing is modeled by the linear mean square estimation (LMSE) model that is shown to be sufficient to represent sub-Kolmogorov mixing. A novel spectral relaxation model is developed for the micro-mixing frequency. In order to validate this model a DNS of passive scalar transport in turbulent channel flow at Schmidt numbers up to $Sc = 49$ is performed and analyzed. These simulations delivered not only data for the validation of the micro-mixing model but also new insights into passive scalar transport in turbulent channel flows at high Schmidt numbers including a new formulation for the turbulent mass transfer coefficient as a function of Schmidt number.

DNS of passive scalar transport in turbulent channel flow at high Schmidt numbers

The development of mixing models and the validation of the method requires detailed DNS data of passive scalar transport. To this end DNS of passive scalar transport in turbulent channel flow were performed at high Schmidt numbers. To reduce the numerical effort and make the simulation possible, two numerical techniques were developed in the framework of this thesis, an approximate deconvolution preprocessing scheme to improve the spatial resolution characteristics of the used finite volume scheme (Schwertfirm, 2008) and a hierarchical grid method to transport the scalar field on a grid that is finer than the fluid grid. The latter uses a conservative prolongation of the coarse grid velocity field to the fine grid used to solve the passive scalar transport equation with a subsequent solution of a pressure-Poisson problem to obtain the conservative velocity fluctuations within each cube defined by a coarse grid cell.

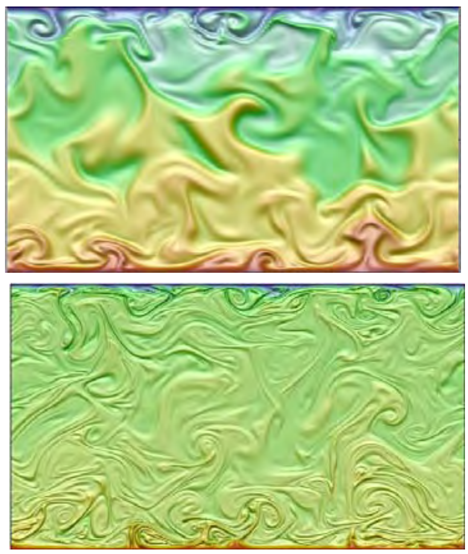

Figure 1: *Instantaneous scalar field in y-z plane: (top) $Sc = 3$, (bottom) $Sc = 49$.*

These methods were employed to perform DNS of passive scalar mixing in turbulent channel flow at $Re_\tau = 180$ and up to $Sc = 49$ (Schwertfirm, 2007). These simulations establish results for the highest Schmidt number so far in turbulent channel flow. Fig. 1 demonstrates the structural change of the scalar field with increasing Sc. A careful grid resolution study renders the results as reliable so that they can be used as reference data. Besides using the data for the development of the micro-mixing model for the DNS-FDF method, these data gave a number of new insights into and results for passive scalar transport in turbulent channel flow of which a new formulation for the scaling of the heat transfer coefficient with Schmidt number can be considered as the most important. This coefficient is expressed in terms of the thickness of the conductive sub layer which is shown to scale with $Sc^{-0.29}$. A formulation (1) can be obtained which describes and explains the asymptotic behavior of the mass transfer coefficient reported in literature for small as well as for high Schmidt numbers together with its dependence on Reynolds number.

$$K^{+} = \frac{1}{\frac{1}{0.27}\ln Re_{\tau} + 11.5Sc^{0.71} + \frac{0.29}{0.27}\ln Sc - \frac{1}{0.27}\ln 11.5} \quad (1)$$

Filtered Density Function simulation of micro-mixing

In this work the filtered density function (FDF) is used to describe the sub-Kolmogorov scalar fluctuations in the context of DNS/Lagrangian stochastic framework. The unique feature of the approach is to use the FDF method together with a DNS of the flow field. In this approach the mixing model has to represent only the viscous-inertial range between Kolmogorov and Batchelor scales thus being able to deliver conceptually the highest affordable accuracy to date. The FDF governing equations can be derived by applying a filter operation to the field variables with a filter width in the same order of magnitude as the Kolmogorov scale $\Delta \approx \eta_K$. Therefore the velocity fields are unchanged by the filter operation and for high Sc flows only the small scale fluctuations of the scalar field are removed $\Phi = \overline{\Phi} + \Phi'$. With this filter the FDF is defined:

$$P_L(\Psi; x_i, t) = \int_{-\infty}^{+\infty} \varrho\left[\Psi, \Phi(x_i', t)\right] G(x_i' - x_i) dx_i'. \quad (2)$$

Under the assumption that the velocity distribution is linear within the filter width the FDF transport equation for a passive scalar results in

$$\frac{\partial P_L}{\partial t} + u_i \frac{\partial P_L}{\partial x_i} = -\frac{\partial}{\partial \Psi}\left\{\left(\Gamma\frac{\partial^2 \overline{\Phi}}{\partial x_i^2} + \Gamma\overline{\frac{\partial^2 \Phi'}{\partial x_i^2}|\Psi} + \omega(\Psi)\right) P_L\right\}, \quad (3)$$

where the only unclosed term is the second term on the rhs that describes micro-mixing. To close this term the linear mean square estimation model is proposed which has some known deficiencies in a RANS context:

$$\Gamma\overline{\frac{\partial^2 \Phi'}{\partial x_i^2}|\Psi} = -\Omega_M\left(\Psi - \overline{\Phi}\right). \quad (4)$$

However, an a-priori analysis of DNS data of mixing in turbulent channel flow up to $Sc = 49$ shows that LMSE model gives a good representation of the dynamics of the micro-mixing term along Lagrangian paths, as shown in figure 2. The mixing frequency is defined as

$$\Omega_M = -\frac{1}{2\overline{\Phi'^2}}\left(\Gamma\frac{\partial^2 \overline{\Phi'^2}}{\partial x_i^2} - 2\Gamma\overline{\frac{\partial \Phi'}{\partial x_i}\frac{\partial \Phi'}{\partial x_i}}\right). \quad (5)$$

It can be shown that the molecular transport of scalar variance in the definition of the mixing frequency (5) can be neglected and that in the limit of high Sc the total dissipation of the scalar variance stems from the sub-grid scalar dissipation rate. The direct consequence of this is that the sub-grid scalar dissipation rate ϵ_Φ is the key parameter in micro-mixing modeling and, as it can not be computed from the FDF, has to be modeled also.

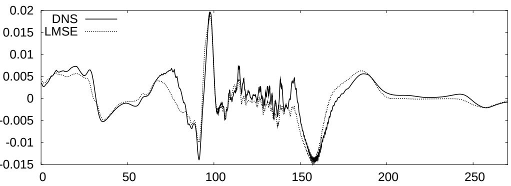

Figure 2: *Sub-filter scalar diffusion along a Lagrangian trajectory in turbulent channel flow. Comparison of DNS data with LMSE model at $Sc = 25$.*

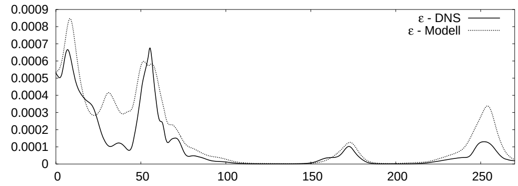

Figure 3: *Sub-filter scalar dissipation rate along a Lagrangian trajectory in turbulent channel flow. Comparison of DNS data with model equation (6) at $Sc = 25$.*

The scalar dissipation rate can be analyzed in the DNS data of high Schmidt number passive scalar transport in turbulent channel flow. A new transport equation, based on the spectral relaxation model of Fox (1995), for the sub-filter scalar dissipation rate is developed:

$$\frac{\mathrm{D}\epsilon_\Phi}{\mathrm{D}t} = \frac{C_D}{\ln(Sc)}\left(\frac{\epsilon}{\nu}\right)\Phi^{*2} + C_s\left(\frac{\epsilon}{\nu}\right)^{1/2}\epsilon_\Phi - C_d\frac{\epsilon_\Phi}{\overline{\Phi'^2}}\epsilon_\Phi. \quad (6)$$

With a priori analysis it is possible to determine the model coefficients in such a way that the dynamics of the sub-filter scalar dissipation can be predicted sufficiently accurate on Lagrangian trajectories both in an ensemble averaged and an instantaneous way. Figure 3 shows the scalar dissipation rate as predicted by the model compared to DNS data of the turbulent channel flow along a Lagrangian trajectory. The model shows a very good performance for the scalar transport in turbulent channel flow and works in homogeneous as well as in inhomogeneous flows that are not in spectral equilibrium.

Conclusions

The presented DNS/FDF model is a novel development that considerably enlarges the predictive capability of mixing and reaction processes in turbulent high Schmidt number flows. A number of novel results concerning high Schmidt number mass transport render the value of this investigation. The developments made in this thesis enabled the successful prediction of the precipitation process of nano-particles in a static mixer at a completely new level of accuracy.

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Experiments for the Validation of Large Eddy Simulations: Turbulence-Flame Interactions in Extinguishing Turbulent Opposed Jet Flames

Benjamin Böhm

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Abstract

A comprehensive experimental dataset on stable and extinguishing, turbulent, partially premixed, methane/air, opposed jet flames is provided for the validation of turbulence-chemistry interaction models in the context of large eddy simulations (LES). Data on the spatial structure and dynamics of the turbulent flow field are provided including inlet boundary conditions. A combination of particle image velocimetry (PIV) and planar laser induced fluorescence (PLIF) of OH was applied simultaneously to measure flow field statistics conditioned on the flame. Conventional statistically independent 10 Hz measurements were performed, providing accurate data with high spatial resolution. Additional high-speed measurements at 5 kHz sampling rate were recorded to characterize the temporal behavior of the flow. A newly introduced multidimensional conditioning technique to avoid spatial and temporal smearing of important flow field information was developed in order to compare individual extinction events in a meaningful, statistical manner. The conditional statistics show that vortices tend to align around the flame and generate high strain in the region where the flame is about to extinguish.

Introduction

The design of future combustors relies increasingly on computational fluid dynamics (CFD). CFD tools are required, which are able to predict extinction accurately, in order to design efficient, low emission combustors. LES emerged as a method to predict complex flows and to capture transient phenomena. Because extinction processes are caused by the interplay of chemical reactions and the underlying turbulent flow field, improved models are being developed, to predict these interactions correctly. A detailed validation is required to prove the predictability of these models. For this reason complete sets of validation data for idealized lab flames are needed which can be simulated with LES based combustion models.

The transient process of extinction in turbulent flames was investigated and characterized in this work. Because LES validation requires data far beyond statistical moments of quantities [1, 2], as they are provided traditionally by experiments for the validation of Reynolds averaged Navier stokes (RANS) simulations, the current work provides additional data on the spatial structure and dynamics of the turbulent flow field of stable and extinguishing opposed jet flames. These are well accepted reference flames in the combustion community especially to study extinction. The opposed jet burner allows the use of a relatively small computational domain and has the advantage that extinction can be brought on easily by increasing the flow's momentum. Extinction was observed frequently in the region of the stagnation point although it appeared randomly in time and space. Thus, measurements could be constrained to a small region of the flow, enabling high spatial resolutions.

Until recently, only spatial or temporal correlations were generally available. In the meantime, by improvements in all-solid-state diode-pumped laser and CMOS (complementary metal oxide semiconductor) camera technology, planar imaging techniques are extended to rates in the kHz regime. These high repetition rates enable the tracking of transient events in turbulent combustion such as flame extinction, giving new perspectives on turbulent combustion. These techniques are very useful for studying the evolution of combustion in a time resolved manner. Because of limitations in laser power, and the number of active pixels in CMOS cameras operating at high repetition rates, conventional 10 Hz measurement systems are still preferable for achieving high spatial resolutions.

To capture the interplay between the flow field and the reaction zone both have to be measured simultaneously. In this work PIV was used to capture the flow field and OH-PLIF to mark the reaction zone. Thus measuring the flow field with respect to the flame allowing to build up flow field statistics conditioned on the flame. The focus of the present work is on acquiring meaningful statistics on the random and individual transient event of extinction, in order to validate numerical simulations, especially LES.

Experimental Setup

The experiments were performed in turbulent, partially-premixed, methane/air flames in an opposed jet configuration as presented by [3]. The opposed jet burner consists of two vertically aligned, opposed, contoured nozzles (Figure 1). Fuel from the lower nozzle and oxidizer from the upper nozzle impinge on each other with equal momentum in the horizontally aligned stagnation plane. The nozzles, each 30 mm in diameter, were separated by 30 mm. Turbulence generating plates (TGP) with hole diameter of 4 mm and a blockage of 45%, were located 50 mm upstream of the nozzle exits to enhance turbulence levels. Both opposed jets were surrounded by 60 mm wide concentric co-flows of nitrogen to avoid secondary air entrainment and the formation of a recirculation zone.

The Reynolds number was varied for different equivalence ratios to access stable and extinguishing flames. Two selected flames with an equivalence ratio of 2 are presented here. Flame TOJ2C with a Reynolds number of 5000 is a stable flame, whereas TOJ2D with Reynolds number 6650 is 10% below the bulk velocity extinction limit. Under these conditions the near-extinction flame was seen to persist for 30 sec (on average) before extinction occurs.

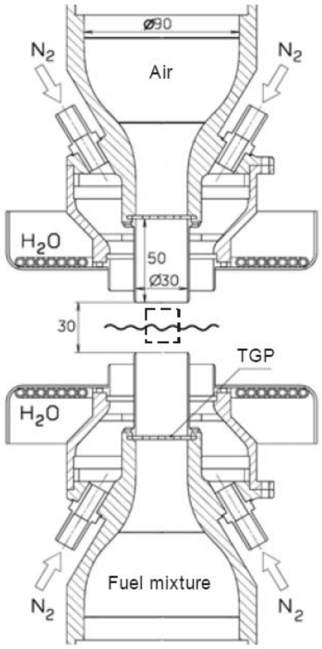

Figure 1: *Sketch of the turbulent opposed jet burner. All quantities are given in mm.*

Results

A first impression of the flame and the development of extinction was obtained by high-speed imaging of chemiluminesence at 10 kHz using a high-speed camera with a lens-coupled intensifier. Figure 2 shows a sequence of flame TOJ2D recorded under an angle from below. The flame is distorted by eddies forming bulges and inclining the flame locally. Local extinction is found frequently. Extinction was not only found to be limited to the region at the centreline but only extinction occurring in this region leads to global extinction.

PIV was used to capture the flow field. First isothermal flow field measurements were performed starting from the TGPs, in order to provide detailed inflow boundary conditions, up to the stagnation plane where the turbulent flame is stabilized. Then the reactive flow was measured and averaged in a laboratory fixed coordinate system. This revealed already a significant change in the flow. Maxima of vorticity and strain were found in the vicinity of the stagnation plane. In the next step combined simultaneous PIV/OH-PLIF measurements were performed at 1 Hz enabling the evaluation of conditional flow field statistics as demonstrated in Figure 3. PIV was thus used to measure the flow field and OH-PLIF to mark the reaction zone. While the turbulent flame moves up and down in a laboratory-fixed coordinate system, the flame was used as the point of reference. The origin of the axial coordinate z is now fixed for every single instantaneous snapshot at the lower OH contour which coincides approximately with the reaction zone. With this conditional coordinate system the intermittent character of turbulence is masked out and the statistics give now more detailed insight into the structure of flow properties in respect to the flame (detailed results are published in [4]). The results show that peak values of vorticity are found particularly close to the reaction zone where radial strain acting extensively exhibits a maximum as well. In contrast, for the compressively acting axial strain a local maximum is found directly at the reaction zone. Measurements for different equivalence ratios and Reynolds numbers showed that approaching the extinguishing flame conditions only gradually changed the conditional flow field statistics. Figure 3 shows PDFs of strain revealing a more complex distribution for the extinguishing flame (TOJ2D), where samples of high strain rate contribute more frequently to the wing of the PDF. Because the flame burns for 30 sec on average before it extinguishes, most of the acquired data are associated with a stable burning flame, while only very few measurements are related to extinction which is expected at high strain rates.

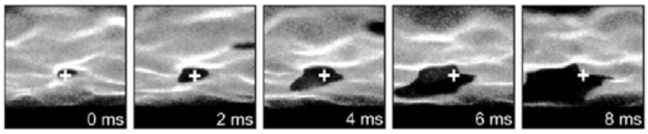

Figure 2: *Temporal sequence of chemiluminesence images showing events of extinction (visible as dark holes) for flame TOJ2D. Every 20th image is shown from data taken at 10 kHz. The white cross marks the stagnation point.*

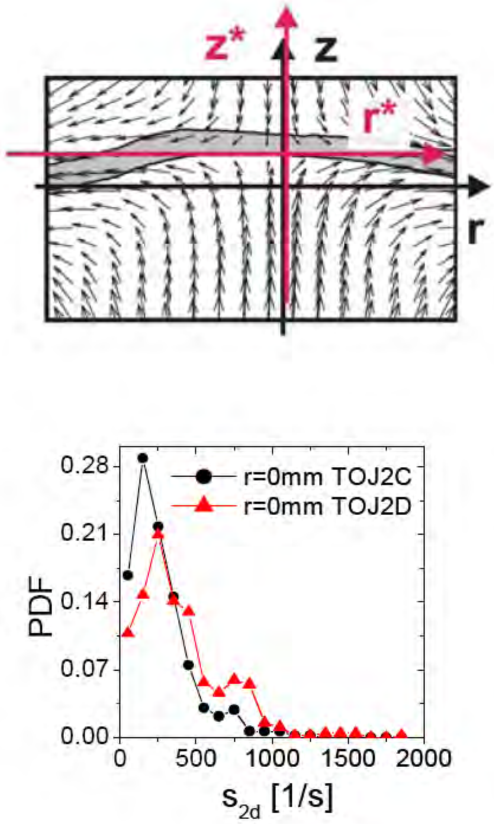

Figure 3: *Sketch demonstrating data post processing for the flame-fixed coordinate system obtained from the simultaneous PIV/OH-PLIF. The lab-fixed coordinates z and r have their origin at the stagnation point while the origin of $z*$ is now fixed to the lower OH contour (top). PDF of conditional instantaneous 2d-strain for the stable (TOJ2C) and extinguishing (TOJ2D) flame (bottom).*

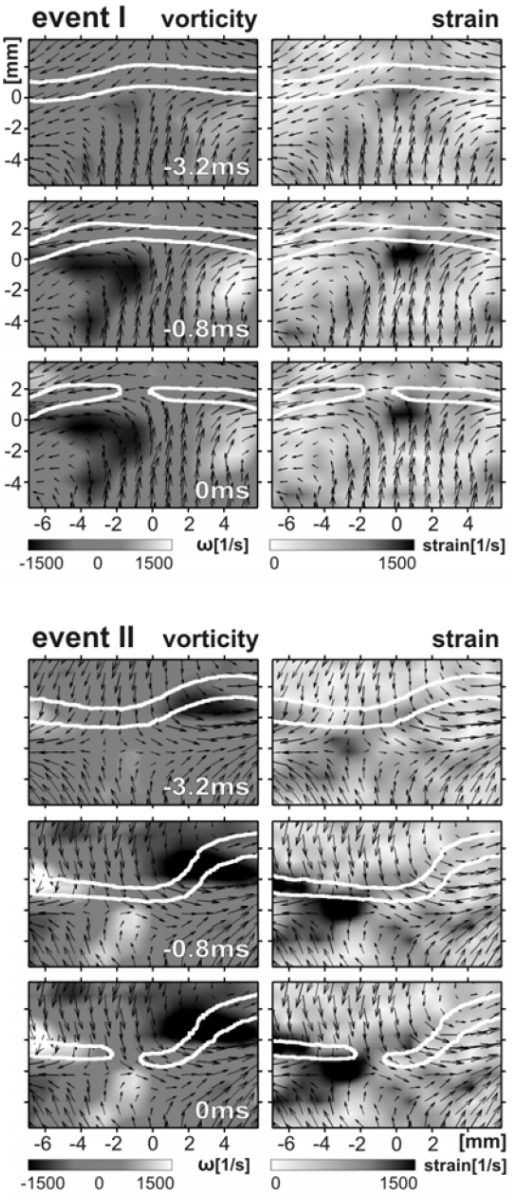

Figure 4: *Two individual sequences of extinction. Vorticity and strain are superimposed by the gray scale on top of the in-plane velocity vectors. Instantaneous locations of the OH contours are represented by white lines.*

Time averaged flow statistics are therefore not sufficient to describe extinction because this transient phenomenon relies on the actual instantaneous flow field. Therefore, simultaneous PIV/OH-PLIF measurements were extended from 1 Hz to 5 kHz. This enabled the acquisition of statistically dependent datasets and allowed tracking of the evolution of vortex-flame interactions in real time (Figure 4). The technique employed in this work allows one to focus specifically on the small fraction of measurement time directly relevant to extinction, thus increasing the physical insight of experiments into this important phenomenon (results published in [5]). The newly introduced technique of multidimensional conditioning used new criteria to compare individual extinction events in a meaningful, statistical manner without smearing important spatiotemporal information (Figure 5). It was found that turbulent vortices generated strain close to the flame and that extinction occurred when the resulting increase in strain exceeded critical values for sufficient time.

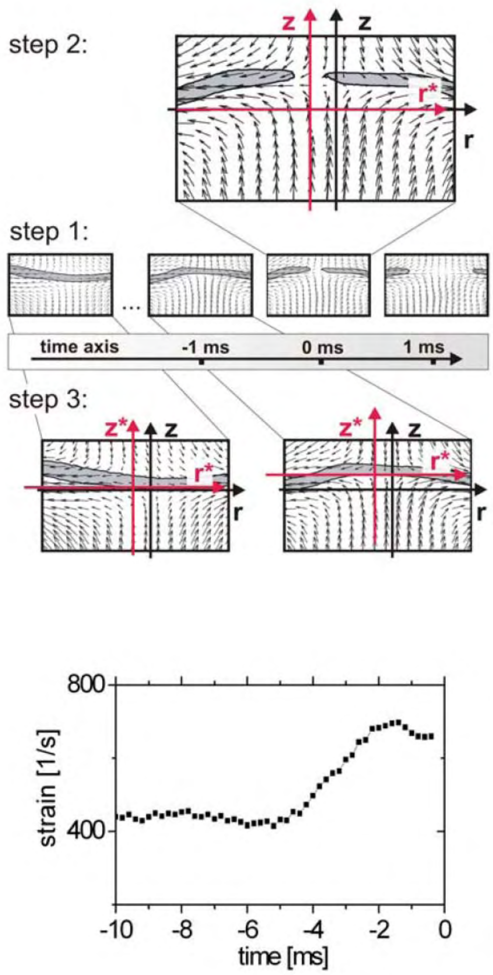

Figure 5: *Exposure of data for multidimensional conditioning post processing. Flame contour/velocity maps are recorded over thousands of frames including the time history prior to the first breach leading to global extinction (top). Temporal trace of conditional averaged strain at the origin of the new coordinate system (bottom).*

Conclusions

The combination of high-speed PIV and OH-PLIF to visualize the time resolved motion of the flame front in the resolved turbulent flow field is a new and unique method applied in the field of combustion. Additional information on the time history allowed viewing the transient process of extinction from completely new perspectives. Valuable physical insights have been gained by the introduction of a new coordinate system based on the temporal information and the flame location. This work demonstrated the high potential of high-speed measurement techniques and provided a challenging validation dataset for LES simulations.

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Lagrangian Simulations of Large Scale Non-Hydrostatic Surface Flows with SPH

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Abstract

In this paper we focus on the Smoothed Particle Hydrodynamics (SPH) method to solve the weakly compressible Navier-Stokes equations for applications to environmental problems. The new robust and parameter free formulation proposed by the author and published in [1] has been used. It is able to compute an accurate and little oscillatory pressure field accurately and also to track correctly complex three-dimensional non-hydrostatic free surface flows.

Thanks to the parallelization of the SPH code using the Message Passing Interface (MPI) paradigm with a dynamic load-balancing strategy, a considerably improvement of the computational efficiency of the code has been achieved. Thus, simulations involving millions of particles can be run on modern massively parallel supercomputers of HLRS in Stuttgart and HLRB2 in München, in Germany. A very good performance has been obtained, as confirmed by a speed-up analysis. Three-dimensional applications have been computed and the solutions obtained with our SPH code have been compared with either experimental data or with other numerical reference solutions. A large scale mudflow has been simulated involving very complex geometry and a non-Newtonian rheology. In all tests a very satisfactory agreement and results have been obtained.

1 Introduction

The SPH method is a meshless scheme based on the Lagrangian approach and it can handle moving material interfaces and large deformations of the computational domain avoiding critical mesh distorsions. The fluid is discretized by a finite set of moving points, the so-called particles, that interact with each other through an interpolation procedure based on the reciprocal positions of the interpolation points. The purpose of this work is to solve the weakly compressible Navier-Stokes equations, thus modelling accurately fully three-dimensional non-hydrostatic free surface flows as well as impact problems of inviscid and viscous fluids applying a new SPH scheme.

Starting from a thorough literature review of the classical SPH method, the lack of zeroth order consistency and even the lack of linear stability and the non-monotonicity in the pressure field are the weak points of the standard SPH scheme. For details see [1-5].

The research work has led to a new SPH formulation that can be actually considered as a breakthrough in the SPH community because it resolves all of the abovementioned issues without artificial diffusion and without any numerical parameters to calibrate, typical of other SPH approaches published so far in literature, such as in [6] by Monaghan. In particular, a monotone pressure field is computed without the need of density reinitialization [7] and without producing spurious oscillations, even at the solid wall boundaries.

This is achieved without smearing the free surface profile, unlike the Ben Moussa and Vila approach [8-9], that cannot simulate violent free surface flows due to the extremely high diffusion in the particle position, that has been introduced to stabilize the SPH scheme.

Then, the high accuracy in computing the pressure field and in tracking the free surface profile have not been achieved together before by any other published SPH scheme. The goodness and robustness of the new approach have been assessed in detail by comparing the SPH results with experimental and numerical reference solutions, as shown in the following.

2 The new SPH method

The new robust and accurate SPH scheme in Eulerian coordinates is based on a new SPH approach for inviscid and viscous weakly compressible non-hydrostatic three-dimensional free-surface flows.

The new scheme is written as follows:

$$\frac{d\rho_i}{dt} = -\sum_{j=1}^{N} m_j \left((\vec{v}_j - \vec{v}_i) \cdot \vec{\nabla}_i W_{ij} - \vec{n}_{ij} \cdot \vec{\nabla}_i W_{ij} \left(\frac{c_{ij}}{\rho_j} (\rho_j - \rho_i) \right) \right)$$

$$\frac{d\vec{v}_i}{dt} = -\sum_{j=1}^{N} m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) \cdot \vec{\nabla}_i W_{ij} - \sum_{j=1}^{N} \vec{F}_{ij}^{V} + \vec{S}_i,$$

$$\frac{d\vec{x}_i}{dt} = \vec{v}_i,$$

where the term d/dt denotes the total derivative that follows the motion of the fluid and the variables are the density ρ, the velocity v, the pressure p, and the position x. The vector S represents the body forces per unit mass, typically it is the gravity acceleration g. Moreover, c denotes the celerity, n is the unitary vector of the distance between the i^{th} and j^{th} points and W is interpolating kernel, i.e. the cubic B-spline in all our applications:

$$W_{ij} = \frac{c}{h_{ij}^{\nu}} \begin{cases} 2/3 - q_{ij}^2 + q_{ij}^3/2, & \text{if } 0 \leqslant q_{ij} < 1, \\ (2 - q_{ij})^3/6, & \text{if } 1 \leqslant q_{ij} \leqslant 2, \\ 0, & \text{if } q_{ij} > 2, \end{cases} \qquad q_{ij} = \frac{|\vec{x}_j - \vec{x}_i|}{h_{ij}}$$

where ν is the space dimension. Finally, the vector FV denotes the viscous components:

$$\vec{F}^V_{ij} = \left(\frac{7}{3}\frac{\mu}{\rho_i} m_j \frac{\vec{v}_j - \vec{v}_i}{\rho_j} + \frac{5}{3}\frac{\mu}{\rho_i} m_j \frac{\vec{n}_{ij}}{\rho_j} \vec{n}_{ij} \cdot (\vec{v}_j - \vec{v}_i) \right) \Theta_{ij},$$

$$\Theta_{ij} = -\frac{\vec{n}_{ij}}{|\vec{x}_j - \vec{x}_i|} \cdot \vec{\nabla}_i W_{ij}.$$

The key idea of the new SPH method is the use of a monotone upwind flux in the semi-discrete form of the density equation. In our particular implementation, the author has used the simple and robust Rusanov flux. The monotone upwind flux, which does not contain any parameter that has to be tuned, corresponds to the introduction of an explicit penalty term for density jumps. This penalization of density fluctuations is consistent with the physics of nearly incompressible flow, where the density variations should tend to zero anyway for $M \rightarrow 0$, and automatically stabilizes the density field. As a consequence it also stabilizes the pressure field, computed by the standard Tait equation of state used to model weakly compressible water:

$$p = k_0 \left(\left(\frac{\rho}{\rho_0} \right)^{\gamma} - 1 \right)$$

In contrast to the traditional SPH approach of Monaghan [6], which contains an artificial viscosity term, the author applies a simple centered discretization of the pressure terms in the velocity equation. This is also physically justified, since pressure waves do not have any preferred direction to propagate. After these modifications with respect to the classical SPH method, the new SPH scheme proposed therefore recalls the advection-upstream-splitting-method (AUSM) of Liou and Steffen [10], developed in the Eulerian finite volume framework, which also uses a centered discretization of the pressure terms together with an upwind method for the convection. Now, since the SPH method is a Lagrangian scheme, the convection terms do not appear explicitly because they are already included in the material derivatives of the flow quantities.

For the fully discrete scheme, i.e. including the time discretization, further stabilization is obtained using a third order accurate TVD Runge-Kutta time stepping scheme, as successfully proposed by Shu and Osher [11] in the context of high order essentially non-oscillatory finite volume and finite difference schemes for hyperbolic conservation laws.

This new SPH formulation has been published in [1].

3 Boundary conditions

An improvement of the non-penetration boundary condition at the solid interfaces for the SPH particles has also been carried out. A new flexible approach to impose the boundary conditions at solid walls is proposed in this work using boundary particles, whose flux contribution is calculated via virtual (non-existing) ghost particles using local point-symmetry, as shown in figure 1. For details, see [1]. This new treatment of the boundaries is flexible, accurate and able to handle any moving rigid body with arbitrarily irregular geometry. It preserves well hydrostatic pressure distributions without introducing spurious pressure oscillations at the wall and it does not have a restrictive impact on the stability condition of the explicit time stepping method, unlike the usual repellent boundary forces of Monaghan, which may lead to stiff ODE systems if the fluid particles are very close to the boundary particles and thus deteriorating significantly the computational efficiency of the whole scheme. As a further important benefit, it does not contain any parameter that has to be calibrated.

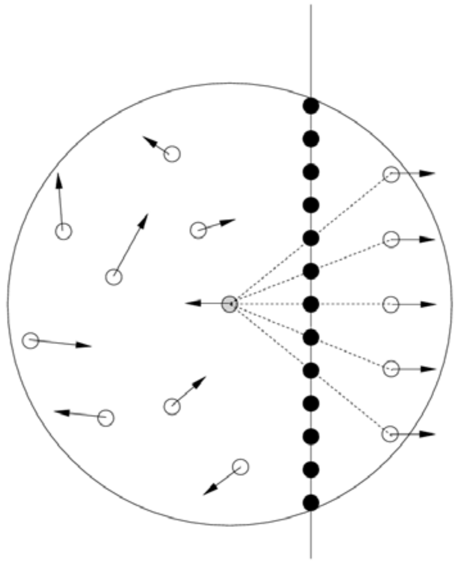

Figure 1: *The sketch of the new approach of implementing the boundary conditions in SPH scheme.*

4 MPI parallelization

The new 3D SPH method has been implemented by the author fully in parallel using the standard Message Passing Interface (MPI) paradigm together with a dynamic load-balancing strategy to improve the computational efficiency of the scheme.

The moving SPH particles need to be implemented in a very flexible data structure in order to avoid too much memory requirements and to achieve high performance to compute realistic simulations. For this reason, the particles in our 3D SPH code are organized in a tree of doubly-linked lists implemented in Fortran 95 language.

A doubly-linked list consists of a sequence of nodes, each containing arbitrary data fields and two references (links) pointing to the next and previous nodes of the same type. This data structure permits the insertion and the removal of nodes at any point in the list, but only requires to update carefully the references of the pointers of adjacent nodes. Then, the advantages of the linked lists over the array data structure are especially evident when the number of the stored items is very high and new SPH particles go in by the boundaries. An array will eventually either fill up or needs to be resized, a very expensive operation from the computational point of view that may not even be possible if memory is fragmented. The implementation of the linked lists has proven to be extremely powerful especially when it is coupled with the parallel programming. In our opinion, only this type of data structure allows to achieve high performance computing on several hundred of CPUs in three dimensional SPH simulations.

Due to the Lagrangian approach of the SPH method, the dynamic redistribution of particles amongst the CPUs during the simulation is a very crucial point in order to obtain an efficient scheme. This is done calling the standard library METIS [12] for graph and domain decomposition. Thus, simulations involving millions of fluid and solid particles can be run on modern massively parallel supercomputers in order to simulate large-scale environmental problems.

All 3D simulations have been carried out on two of the most powerful High Performance Computing (HPC) facilities in Europe, namely they are the Bundeshöchstleistungsrechenzentrum at the University of Stuttgart (HLRS) and the HLRB-II supercomputer at the Leibniz-Rechenzentrum of the Bavarian Academy of Sciences in München, Germany. A very good parallel performance has been achieved on up to 256 CPUs, as also confirmed by a thorough speed-up analysis. The results are plotted in figure 2. It represents the computational efficiency of the code using an increasing number of CPUs (2, 4, 8, 16, 32, 64, and 128). The computational time corresponds to the time required by the CPUs to complete the same computational job, that is a non-trivial 3D free surface dam break flow with the impact against a wall, computed using 500'000 particles. In the graph in logarithmic scale, the optimal theoretical performance (supposing 100% MPI efficiency) is represented by the green line. The measured performance of the code produces satisfactory results, especially considering the fact that the scheme is a meshless Lagrangian method with high order Runge-Kutta time integration, which requires quite a lot of MPI communication.

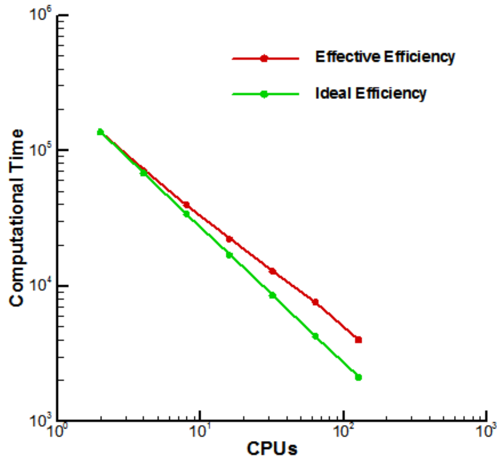

Figure 2: *Speed-up graph, comparing the measured (red) and the ideal (green) computational time from 2 to 128 CPUs.*

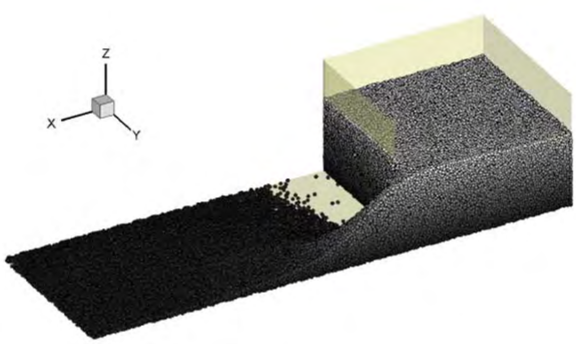

Figure 3: *Visualization of the SPH solution at time t=1s.*

5 Applications

The numerical applications consist of environmental flow problems, namely the overflow after a dam break and a realistic large scale debris flow.

First, we analyze the wave propagation on a plane bottom in order to reproduce a hypothetical scenario associated with overflow phenomena that can happen after a dam rupture. Experimental and numerical research about this dam break-type problem has been published by Fraccarollo and Toro [13]. Their laboratory setup consists of a tank (wide 2m, long 1m) connected to a rectangular plate. Initially, still water with a depth of 0.6m is in the tank. Dry bed conditions downstream the exit have been imposed. The opening time lapse is very short, less than 0.1s. After that the front propagates downstream on the horizontal plane bottom and the water overflows at the open boundaries on all three sides. The experimental data in [13] refer to the free surface depth, the pressure value and the velocity field during a period of 10s. After that time the water flow reaches the uniform motion conditions with hydrostatic pressure distribution.

The solution provided by our SPH scheme has been computed using 600,000 fluid particles on 130 CPUs.

Figure 3 shows a snapshots of the three-dimensional SPH free surface flow at time t=1s after the removal of the gate. It is cut along the symmetry $x - z$ plane.

Position	0	-5A
x [m]	0.	-0.82
y [m]	0.	0.

Table 1: *The coordinates of the gauges located on the plane bottom. The origin of the coordinates is located at the middle point of the exit.*

Figures 4 and 5 refer to the water depth and pressure at the gauges 0 and -5A, see table 1. The SPH profiles have been compared with the experimental data and also with the reference solution presented in [13] computed by the finite volume (FV) scheme on a regular mesh of 150x50 grid points using the shallow water equations (SWE). Since the SWE model assumes a negligible velocity along the gravity direction and a hydrostatic pressure, substantial deviations from the experimental data are apparent in the SWE-FV depth-average and pressure profiles soon after the gate removal at gauge 0 until 2s. A time delay after the gate removal is also present in the SWE profile to receive a depth-variation signal in the tank at gauge -5A. That is the time required by the gravity waves to propagate to gauge -5A. Instead, the 3D SPH model contains a much larger signal speed, so that the pressure signal produced by the opening of the gate reaches all the gauges after a very short time, which is consistent with experiments. The three-dimensional effects of the flow are also evaluated very well reproducing the time-dependent evolution of the free surface depth and the pressure at the exit (at the gauge 0) and in the tank (at the gauge -5A).

Then, the application of the fully three-dimensional Navier-Stokes equations significantly improves the solution in comparison with the simplified SWE model. Only at large time scale, the SWE assumptions are satisfied because the water flow reaches the uniform steady conditions. This is proved by the results plotted in figures 4 and 5. Asymptotically the SWE-FV profiles agree very well with the experimental measurements, as well as the SPH solutions.

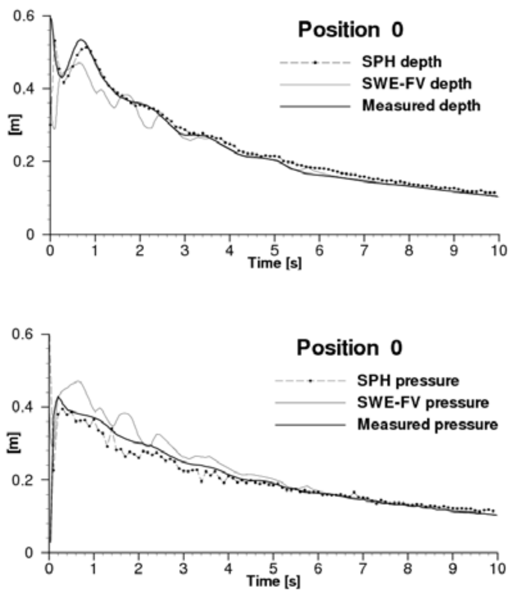

Figure 4: *Plot of the free surface depth (on the top) and pressure (on the bottom) profiles at gauge 0 until 10s.*

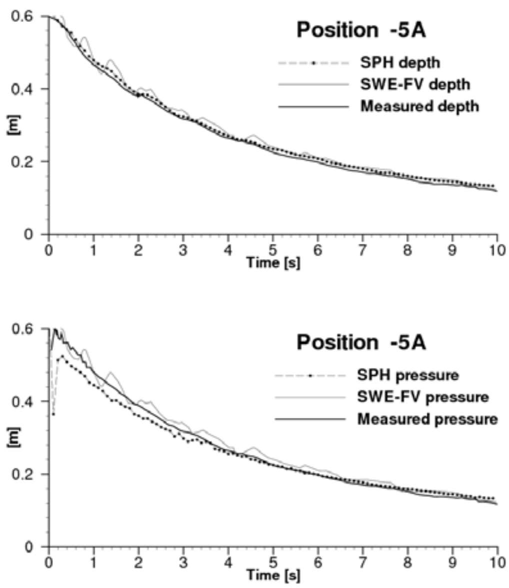

Figure 5: *Plot of the free surface depth (on the top) and pressure (on the bottom) profiles at gauge 0 until 10s.*

Another application presented in this paper consists of a catastrophic mudflow, happened in 1985 in Stava, Italy. This simulation is a big challenge even for sophisticated numerical methods due to the very large CPU times that is needed and also due to the very complex geometry (accuracy of 10m) that requires a tremendous effort in terms of computer memory. From the physical point of view, the mudflow computation involves difficulties regarding the complexity of the failure evolution of the tailing dams and the non-trivial non-Newtonian rheology of the fluid, as well as the development of turbulence, for details see [2]. The aim is to reproduce the wave propagation, especially at the beginning where the mudflow follows a natural bend of the valley and the SWE assumptions fail due to the three-dimensional effects. Millions of fluid and solid particles have been used to discretize the natural geomorphology and the non-Newtonian fluid.

The three dimensional SPH solution of the front propagation of the mudflow is plotted in figure 6. The plots refer to times t=30s and 60s. The colours denote the numerical velocity field. After the dam collapse at time t=30s, the slurry wave flows downstream on the complex topography of the valley expanding its front width on the open terrain. The mudflow strongly accelerates on the high slope (more than 10ř) and impacts against the opposite mountainside. The velocity field is fully three-dimensional and the mudflow produces adherence phenomena due to the no-slip condition of the slime at the natural bottom. The free surface is strongly deformed with a super elevation on the curved path of the flow. The slurry front flows on downstream into the narrow valley following the River Avisio in the direction of the village Tesero increasing the velocity field. From here the wave is forced to flow into the narrow valley of the River Stava as in a quasi one dimensional channel.

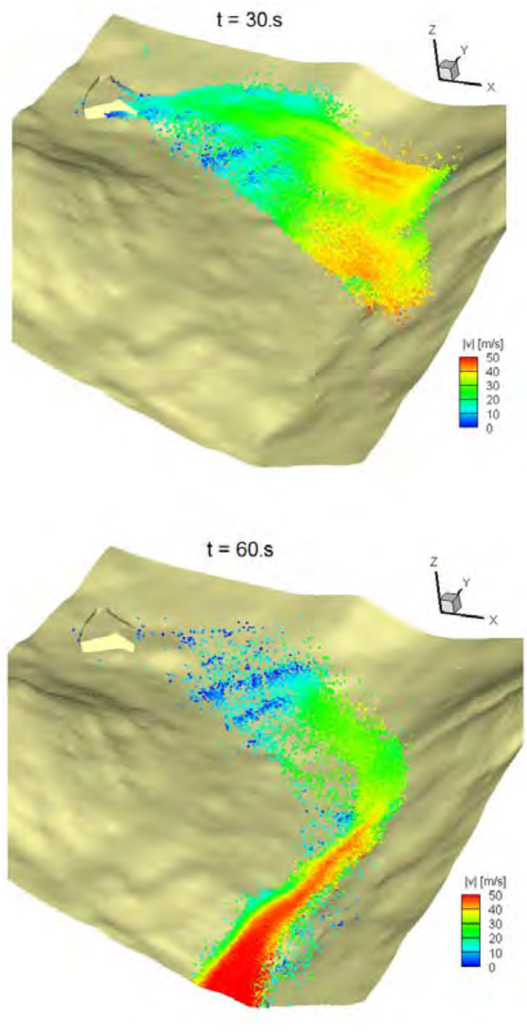

Figure 6: *Numerical solutions at time t=30s (on the top) and 60s (on the bottom). The colour represents the velocity.*

The propagation of the wave front after the failure has been analyzed by Takahashi [14,15] which has interpreted the seismograph data recorded at Cavalese, located 3.7km from collapsed tailing dams. This provides a reasonable estimate of the velocity of the mudflow. After 30s the mudflow impacts against the cliff around the village Stava, located in the curve. The velocity of the wave front reaches about 37m/s. The maximum value of the SPH velocity exceeds the actual one. This can be due to have not implemented any turbulence model. Moreover, no interactions with the vegetation, such as trees, that partly covered the bottom in the valley Stava have been taken into account in our SPH model. They were actual obstacles able to reduce the speed and the destructive power of the mudflow. The resistance effects are particularly significant before the impact against the village Stava along the curved path. Also the crashed buildings were reduced to ruins and the impacts evidently decreased the flow energy. The lack in the numerical simulations of trees and buildings also causes a larger wave front after 30s in the SPH solution.

However, the numerical results provided by our SPH method to compute challenging complex phenomena on large scale are satisfactory, especially when compared with aerial photographs.

6 Conclusions

In this paper the new SPH method proposed in [1] has been successfully applied to simulate free surface non-hydrostatic flows of weakly compressible fluids. Moreover, it does not require careful calibrations of numerical parameters. The SPH results are accurate, as proven by the comparison with experimental measurements, obtaining also a better agreement than the SWE model.

High numerical efficiency has been also achieved through the MPI implementation that has led to high performance computing. That is an essential requirement to simulate large scale phenomena, such as the realistic mudflow computed in this paper.

7 Acknowledgments

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Transition Control Using Dielectric-Barrier Discharge Actuators

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Introduction

Dielectric-barrier discharge (DBD) plasma actuators have obtained more and more attention in the last ten years. The reasons for the increasing interest are the ease of use, the simple integration in surfaces and the fast response time of the force production. DBD actuators are the only actuators that create a body force above a surface without electrodes or any other obstacles above the surface. The force is directed tangentially to the wall and can be turned on and off without changing the smoothness of the surface. They do not need big chambers or pipes below the surface to burry piezo actuators or transport the fluid necessary for blowing or suction. They do not involve moving parts or any other mechanical device. No other device can create a body force without mass addition or removal in air. The only equivalent are Lorentz force actuators that are operated in water but not in air. All mentioned advantages make the plasma actuator the ideal flow control device in aircraft applications. The one big drawback the actuator has today is the limited amount of force, which prevents the application of plasma actuators for the separation control at higher Reynolds numbers. Many experiments and investigations were published that demonstrate the plasma actuators authority for controlling different flow situations in a convenient and comfortable way. Most of the investigations involve the control of flow separations on bluff bodies, cylinders, airfoils or wings. A small number of investigations aims at different flows like jets or just an actuator in quiescent air. Very little applications use plasma actuators for boundary layer control. The only effect on laminar boundary layers demonstrated up to now is the tripping the feasibility of tripping a laminar boundary layers to trigger the transition. Boundary-layer control offers a wide range of possibilities for the reduction of skin friction or other contributions to the drag of vehicles or fluids in internal flows. The passive control of boundary layers has been performed since the beginning of fluid dynamics and has reached a state of perfection that does not leave much room for further improvements. Active methods offer further way to reduce drag and/or the weight of systems, both leading to a reduced fuel consumption, increased energy efficiency and eventually reduces CO_2 emission. The present work investigates the the applicability of plasma actuators for active control of a laminar boundary layer. The objective is to perform a delay of the transition of the boundary layer in order to reduce the drag that a body experiences as it moves through the air.

Methodology

The investigations were performed in a wind tunnel test section equipped with a horizontal flat plate on which the boundary layer to be investigated evolves. A specially designed displacement body is mounted under the ceiling of the test section to create a constant positive pressure gradient on the flat plate. The pressure gradient amplifies the instability of the laminar boundary layer and promotes the transition to establish a base flow with the transition point on the plate at lower velocities. Additionally to the pressure gradient Tollmien-Schlichting (TS) waves are excited artificially to have a controlled flow situation with a transition due to the growth of two-dimensional perturbations and not a mixture of bypass and natural transition. The TS waves are excited using a vibrating bar flush mounted in the surface at the position where the positive pressure gradient starts. The vibration frequency is adjusted to yield the strongest amplification of the induced waves downstream of the exciter.

Both, the amplitude of the exciter and the pressure gradient are adjusted to yield a transition roughly 250mm downstream of the excitation at 8-10m/s for the base flow. The base flow and the controlled flow were captured and measured using hot-wire measurements as well as laser-doppler anemometry. Full boundary-layer profiles were measured at 19 downstream positions in order to capture the transition process and its downstream position. The boundary-layer shape factors were calculated to determine the position of the transition to turbulence. The boundary-layer profiles and the profiles of the velocity fluctuations provided further insight into the involved processes. The plasma actuators were operated using a new and innovative high-voltage generator providing an AC voltage of $5-12KV_{pp}$ at a $6-8KHz$ plasma operating frequency. The high voltage generator was driven by a control signal produced by a computer. The operating signal comprises the plasma operating frequency as well as a modulation frequency that turns the AC-frequency on and off in the case of the pulsed operation. The flat plate was additionally equipped with a set of surface hotfilms that captured the oscillations in the boundary layer to provide data for the closed-loop control circuits involved in the wave cancelation experiments. All equipment, programs and software, procedures and post processing concerning the usage of plasma actuators and the conducting of such experiments were developed during this PhD thesis and were newly established at the institute. No such experiments were performed at the institute before.

Results

The experiments can be divided in two parts: the stabilization of a laminar boundary layer and the active wave cancellation. In both cases a noteworthy transition delay could be achieved. The experimental setup for the boundary-layer stabilization is shown in Figure 1. The actuators are positioned 100mm and 200mm downstream of the exciter. They are oriented in spanwise direction producing a force in downstream direction. They are operated continuously resulting in a deformed boundary-layer profile for a short distance downstream of the actuators. This deformation results from the momentum addition in the lower regions of the boundary layer and leads to a more round profile with a lower shape factor and higher stability against oscillations. This is the region where the artificially induced TS-waves are attenuated. A convenient way to present the results of the measurements at all 19 downstream positions is to plot the shape factors at all positions. Figure 2 shows a plot of the shape factors of the boundary-layer profiles at all positions with and without control. The circles show the shape factor development of the unstabilized flow and the asterisks show the results of the stabilized flow. It is apparent that the transition could be delayed by approximately 200mm.

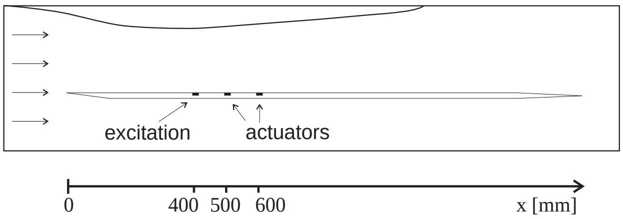

Figure 1: *Experimental setup.*

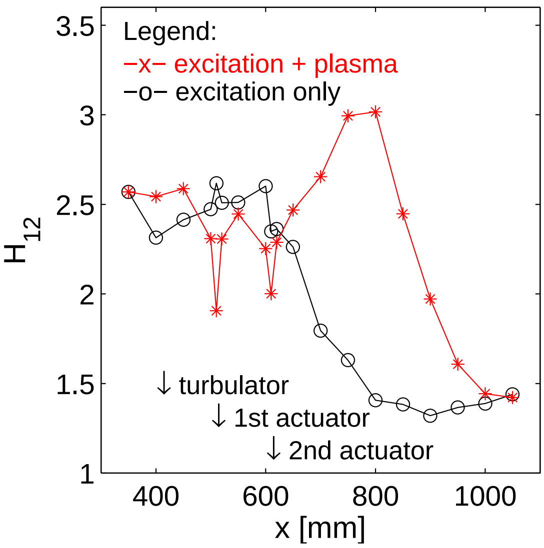

Figure 2: *Shape factor development with and without control for the LDA measurements.*

The shape factor decreases at $x = 500mm$ and $x = 600mm$ compared with the uncontrolled case due to the acceleration and deformation of the boundary layer for a short distance. The mechanism of the damping effect consists of two parts: 1. The body force created by the actuators accelerates the flow and alters the velocity profile to become a more stable profile leading to a much higher critical Reynolds number; 2. The second effect is the thinning of the boundary layer by the actuators, which leads to lower local Reynolds numbers. The actuators separate the local Reynolds number and the critical Reynolds number which leads to the delay of transition. The setup for the active-wave cancelation is similar to the first one but consist of only one control actuator and two sensors upstream and downstream of this actuator, Figure 3.

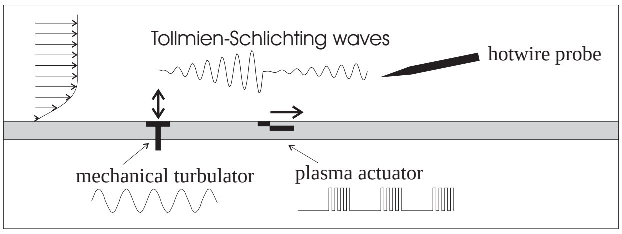

Figure 3: *Details of the actuator placement.*

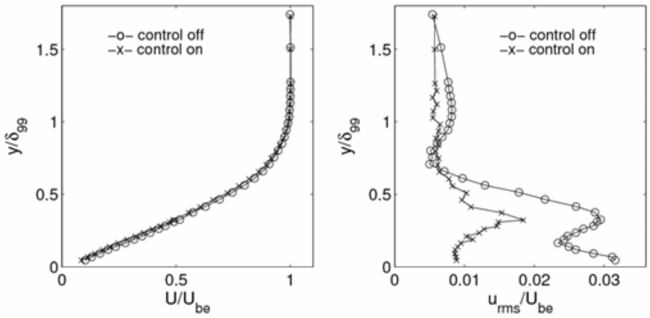

Figure 4: *With and without wave cancellation.*

This time the plasma actuator is operated in a pulsed mode in which the high plasma operating frequency is turned on and off with a modulation frequency. It could be shown that by a precise adjustment of the involved parameters such as modulation frequency, duty cycle length and body force magnitude the artificially introduces TS waves can be attenuated efficiently. Figure 4 shows the result of such a cancellation. Here strong TS waves with 3-dimensional components are attenuated considerably by the pulsed actuator. It could also be shown in this work that this attenuation is effective enough to lead to a delayed transition by about 50mm. The high sensitivity of the adjusted parameters to slight changes of the flow conditions especially of the tunnel speed, make the integration of the actuator into a closed-loop control circuit necessary.

Therefore two simple but efficient control circuits have been developed and successfully implemented into the setup. The plot at the top of Figure 5 shows the velocity of the wind tunnel. It is abruptly altered manually in several steps. The control circuit has to react on these changes of the external operation conditions and to readjust the controlled parameters. The second and third diagrams show the phase and the duty cycle, which are both controlled by the circuit. The bottom diagram shows the amplitude of the waves measured by the downstream sensor. The control circuit is activated at the time $t = 5\,$s. Before that time the amplitude diagram shows the amplitude of the not influenced TS waves.

Quickly after the activation a minimum of the amplitude is found by the automated adaption of the phase and the duty cycle. Each time the tunnel velocity is changed manually the amplitudes of the waves increases rapidly but the circuit reestablishes the low amplitudes by a precise wave cancellation.

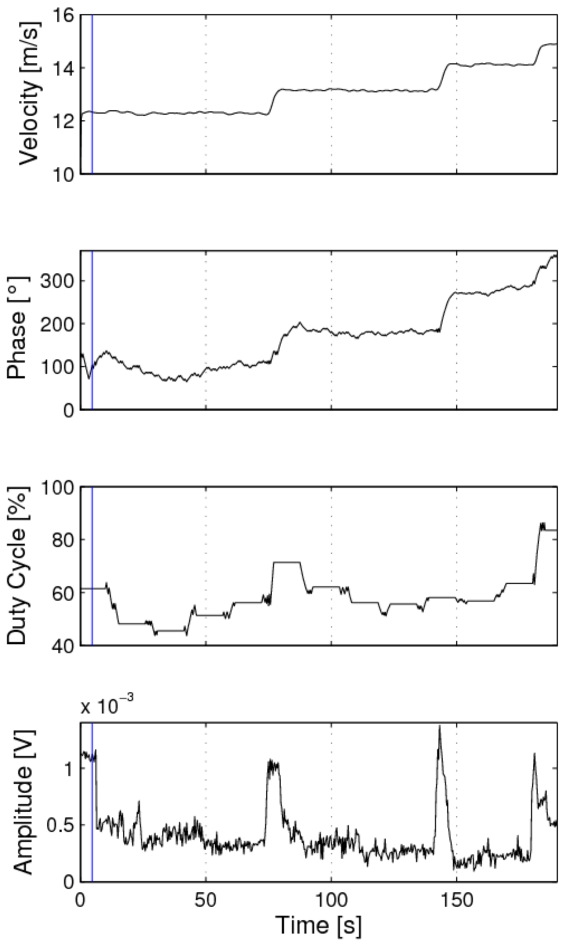

Figure 5: *Cancellation results obtained with the phase control circuit.*

Both sets of experiments show for the first time the large potential of plasma actuators for boundary-layer control applications. The even pave the way for high Reynolds number experiments since it was shown that only small forces are necessary for the wave cancellation. The whole work is the basis of now 6 further PhD theses that are currently further developing the boundary-layer control technology using plasma actuators.

Outlook and Ongoing Work

The results obtained in this work initiated several projects concerning plasma actuators for transition control. New results of the ongoing experiments show the applicability of plasma actuators for active-wave cancellation at higher velocities up to 28m/s on the same setup as used in this work. A further increase of free-stream speed up to 40m/s will be achieved on a new and smoother experimental setup. In the meantime preparations are going on to transfer the experiment from the flat- plate wind tunnel setup to a glove for the wing of a motorized glider. After conducting the experiments at flight conditions in the wind tunnel, real in-flight experiments will be conducted. In parallel to these efforts higher sophisticated control algorithms are being developed. Some of the new control algorithms are based on algorithms known from optimization theory, such as the Nelder-Mead Method. Additionally our new algorithms are capable of using an in-situ measured TS-wave frequency instead of using the driving frequency of the wave excitation.

As well as the active-wave cancellation experiments the boundary-layer stabilization experiments are being continued. The usage of streamwise actuator arrays instead of single actuators and new types of plasma actuators will make this transition control method more reliable than the first versions and easier to apply than the active-wave cancellation. Eventually a combined wave-cancellation and stabilization setup might yield the longest lasting laminar boundary layer on the wing glove of our motorized glider plane.

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Efficient and Robust Uncertainty Quantification for Computational Fluid Dynamics and Fluid–Structure Interaction

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Motivation

Numerical errors in computer simulations have shown a tremendous decrease over the last decades due to the increased availability of computational resources. The effect of not exactly known initial and boundary conditions nowadays dominates the accuracy of numerical predictions. Also uncertainties in multi–physics modeling result in a large spread of fluid–structure interaction simulation results. Inherent physical variations can in these applications even trigger an earlier onset of unstable flutter behavior, which can lead to unexpected fatigue damage and structural failure. On the other hand, the effect of this physical uncertainty cannot be quantified by a Monte Carlo simulation of performing a large number of random computations due to the already high computational costs of a single deterministic simulation.

The Stochastic Collocation approach [1] has been proposed in the context of structural mechanics as a more efficient uncertainty quantification method based on Gauss quadrature sampling of the Polynomial Chaos expansion [2]. However, its recent utilization in computational fluid dynamics and fluid–structure interaction applications [3] has revealed a number of important shortcomings of the approach. It is widely acknowledged in literature [4,5,6] that the two central open problems in uncertainty quantification are currently the accurate approximation of discontinuous responses and unsteady behavior, which are both encountered in the highly sensitive problem of the stochastic bifurcation of transonic aero-elastic systems.

Developed methods

For discontinuous response surfaces the global polynomial interpolation of Stochastic Collocation results in unphysical oscillatory predictions. As a robust and efficient alternative approach a piecewise polynomial approximation is proposed based on Newton–Cotes quadrature sampling in an adaptive simplex elements discretization of probability space [7]. This formulation is the first uncertainty quantification method that satisfies the total variation diminishing and extrema diminishing robustness properties extended to probability space, which assure that no non–zero probabilities for unphysical realization are predicted due to overshoots at discontinuities [8]. Due to the hierarchical location of the Newton–Cotes quadrature points the samples are reused after refinements, which enables the monitoring of a convergence measure in the stochastic grid refinement until a robust convergence criterion is reached.

In unsteady simulations, uncertainty quantification methods usually result in a fast increasing number of samples to maintain a constant accuracy in time. This problem is especially profound in problems with oscillatory responses of which the frequency is affected by the random parameters. It is, therefore, practically impossible to resolve the asymptotic stochastic behavior, which is of practical interest in post–flutter simulations. Two original approaches for unsteady oscillatory problems are developed which maintain a constant accuracy in time with a constant number of samples. The methods are based on time–independent parameterization of the oscillatory samples [9,10] and interpolation of scaled samples at constant phase [11]. The latter formulation is proven to results in a bounded error in time for periodic and non–periodic responses [8]. The framework is extended to multi–frequency responses of continuous structures by employing a wavelet decomposition pre–processing step [12]. The thesis also contributes to the advancement of uncertainty quantification for nonlinear problems [13] and arbitrary input distributions [14].

Results

The developed uncertainty quantification methodologies enable for the first time the reliable high–fidelity numerical simulation of multi–disciplinary problems including the effect of uncertainties. The robustness of the novel approach is demonstrated in Figure 1 for the transonic flow over a NACA0012 airfoil for a random angle of attack α with a beta distribution in domain $\alpha \in [1^o, 3^o]$. The standard deviation field of the static pressure indicates a local production of standard deviation in the shock region above the airfoil at 70% of the chord. This is caused by the sensitive shock wave location with respect to variations in free stream angle of attack as illustrated by the mean and 99% uncertainty interval for the pressure on the upper surface. The uncertainty band shows an amplification of the 2^o range of α to a variation of shock wave location of approximately 20% of the chord. The robustness of the extrema diminishing property is proven by the 99% uncertainty interval falling within the range of the extrema of the samples.

In the fluid–structure interaction simulation of the transonic NACA0012 airfoil in Figure 2 the combined effect of randomness in the ratio of structural natural frequencies $\bar{\omega}$ and free stream velocity U_∞ on the post–flutter behavior is resolved for a uniform and beta distribution with a coefficient of variation of 10% and 1%, respectively. The developed method resolves the highly oscillatory response surface of the pitch angle α as function of the random parameters using only $n_s = 9$ samples. The pitch angle standard deviation σ_α shows a fast oscillatory increase until the unsteady system reaches a steady asymptotic stochastic behavior with $\sigma_\alpha = 1.6^o$, which is a factor 16 larger than the initial pitch angle $\alpha(0) = 0.1^o$. The discretizations with $n_s = \{9, 13, 25\}$ samples are uniformly converged up to $6.2 \cdot 10^{-3}$, which demonstrates that the convergence and accuracy of the method are also in practice constant in time.

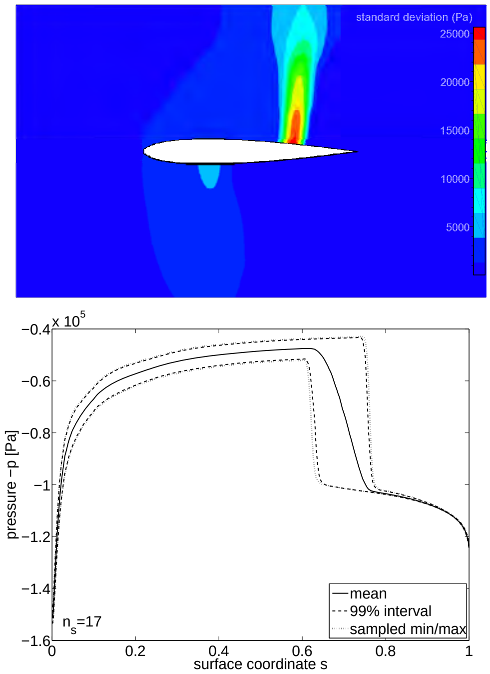

Figure 1: *Transonic airfoil flow problem: (left) standard deviation of the static pressure field; (right) pressure distribution over the upper surface.*

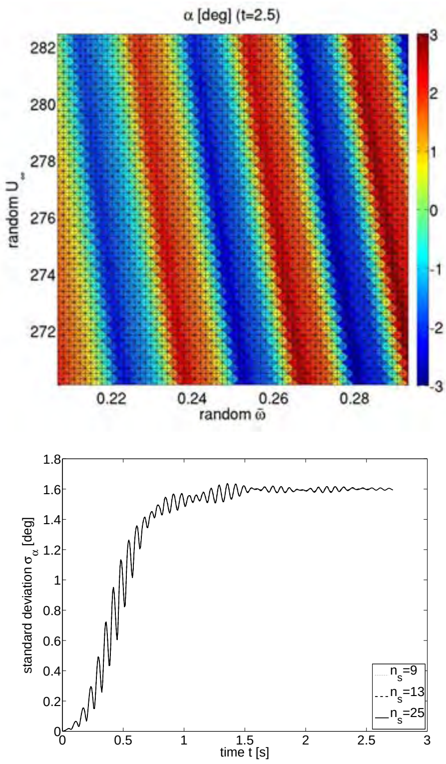

Figure 2: *Transonic airfoil flutter problem: (left) pitch angle response surface at $t = 2.5$; (right) pitch angle standard deviation as function of time.*

The effectiveness of commonly used design safety factors to account for uncertainty is compared in Figure 3 with the developed uncertainty quantification methodology for the three–dimensional transonic AGARD 445.6 aero–elastic wing benchmark. To that end the mean of the random free stream velocity U_∞ with a beta distribution and coefficient of variation $cv_{U_\infty} = 3.5\%$ is fixed at a realistic safety margin of 5% below the actual deterministic flutter speed. The non–zero flutter probability of 6.19% predicted using $n_s = \{9, 11\}$ samples demonstrates that the presented uncertainty quantification approach forms a more reliable design practice than using safety margins in combination with deterministic simulation results. Additional applications of uncertainty quantification to challenging nonlinear stochastic stall flutter problems are presented in [15,16,17]. In conclusion, the examples illustrate that the developed methods have the potential to advance uncertainty quantification in computationally intensive problems with discontinuities and unsteadiness from practically impossible to a routine analysis.

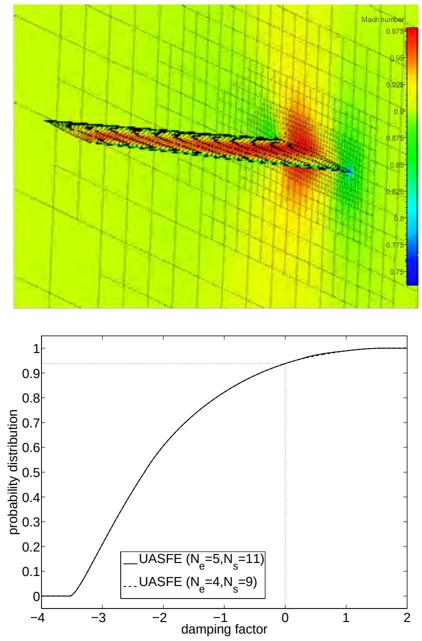

Figure 3: *3D transonic AGARD 445.6 wing: (left) initial condition; (right) cumulative PDF of the damping factor.*

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1^{st} SIG43 Workshop on Fibre Suspension Flows

2-3^{rd} April, 2009, VTT Technical Research Centre of Finland, Finland.

Jari Hämäläinen

Department of Physics, University of Kuopio, Finland.

Introduction

ERCOFTAC Special Interest Group on fibre suspension flows (SIG43) was established in 2008. The first workshop organized by the group was held April 2-3, 2009, at the Technical Research Centre of Finland (VTT), in Jyväskylä, Finland. Local workshop arrangements were carried out by Dr. Janne Poranen and Mr. Juha Salmela from VTT. The workshop collected together researchers from five countries: Finland, Sweden, Norway, Poland and France. There were also participants from industry (Metso Paper, Tamfelt) and from SME's who are offering CFD services to industry (Numerola, Process Flow). Altogether 25 persons took part in the first SIG43 workshop.

Scientific programme

The workshop consisted of 12 presentations dealing with CFD and experiments for fibre suspension flows:

- Opening, Janne Poranen, VTT and Jari Hämäläinen, University of Kuopio.
- *Modelling of fibre suspension flows in papermaking processes by combining Non-Newtonian fluid dynamics and turbulence*, Juha-Pekka Huhtanen, Tampere University of Technology.
- *CFD study of refining hydraulics*, Dariusz Asendrych, Czestochowa University of Technology.
- *Simulations of long particles in turbulent flows*, Lihao Zhao, Norwegian University of Science and Technology.
- *Modelling of fibre suspensions in papermaking process*, Heidi Niskanen, University of Kuopio.
- *Experiments on the development of the fibre orientation distribution in elongational base flow*, Hannu Eloranta, Tampere University of Technology.
- *Application of ultrasound anemometry for measuring filtration of fibre suspensions: Effect of fibre and pulp properties*, Sanna Haavisto, VTT.
- *Experimental study on the transition from dilute fibre suspension to fibre network*, Gabriele Bellani, KTH.
- *Filtration of Fibre Suspension in a Shear Flow*, Mika Laitinen, Numerola Oy.
- *Fibre suspension modelling at Process Flow*, Hannu Karema, Process Flow Ltd Oy.
- *Flow of pulp in pipes*, Salaheddine Skali-Lami, Nancy University.
- *New experimental results on the flow regimes in closed channel flows of wood fibre suspensions*, Ari Jäsberg, University of Jyväskylä.
- *UDV measurements and CFD simulation of two-phase flow in a stirred vessel*, Sanna Haavisto, VTT.

Tour of the experimental facilities in the Jyväskylä region

There are several fibre suspension research units in the Jyväskylä region which were visited during the workshop. The tour started from the Metso Paper's pilot paper machine, which is the main research unit of the world leading paper machine supplier. The experimental laboratory of University of Jyväskylä, Department of Physics, was visited next. Also the experimental laboratories at VTT were introduced.

Workshop material

An abstract booklet and a CD-ROM consisting of all the presentations are available. Full papers have not been written. For further information on the SIG43 and the 1st workshop, please, contact the SIG43 coordinator, Professor Jari Hämäläinen (jari.hamalainen@uku.fi).

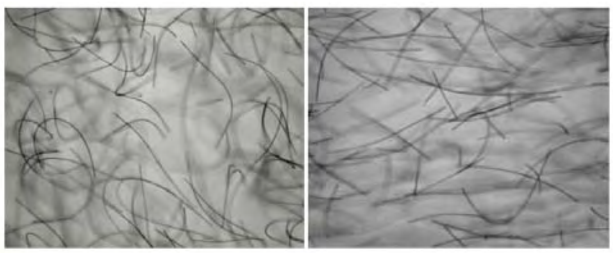

Figure 1: *Random and oriented fibres (experiments by Hannu Eloranta, TUT).*

Workshop on Turbulent Combustion of Sprays

7th June, 2009, Corsica, France.

Organised by

- Bart Merci, Ghent University, Belgium.
- Dirk Roekaerts, Delft University of Technology, The Netherlands.
- Amsini Sadiki, Darmstadt University of Technology, Germany.
- Reni De Meester, Ghent University, Belgium.
- Albert Simeoni, Università di Corsica, France.

Background and objectives of the meeting

The aim of this workshop was to stimulate progress in the understanding of turbulent spray combustion by organising focused discussions on open problems and promising new initiatives and collaborations in this area. The workshop will link recent developments in studies of dispersed multiphase flow and combustion.

The intention is to have interactive discussion between experts and young researchers. Two invited lectures, given by experts in the field of turbulent spray combustion (one experimental and one computational), will initiate discussions, whereas participants will have the opportunity to present their work in contributed poster presentations. An important aspect of this workshop will be round-table discussions, which will focus on the assessment of state-of-the-art and on initiation of future collaboration in experimental as well as computational techniques in spray combustion. It is the intention to define some 'target test cases', for which experimental databases will be developed and on which modelling and numerical algorithm issues will be tested.

Summary of the event

On 7 June 2009, the first Workshop on Turbulent Combustion of Sprays ('TCS 1') took place in Porticcio - Ajaccio (Corsica). The workshop started with a lecture, given by Prof. Assaad Masri (University of Sydney, Australia), on detailed experiments in spray combustion. After the lunch, Prof. Eva Gutheil (University of Heidelberg, Germany), provided an excellent overview of existing models in numerical simulations of turbulent spray combustion, pinpointing weaknesses and strengths. Throughout the workshop, and specifically during the poster session following the invited lectures, there was intensive discussion amongst the participants. This confirmed the hope of the organizers and invited speakers that this workshop can be the start of a series of workshops. A start was made with the identification of target test cases for comparison of numerical simulation results and for model development, to be discussed in future workshops. An extended organizing committee has been established for that purpose.

The participants have been encouraged to submit their work presented at the workshop to Flow, Turbulence and Combustion or to contribute a chapter in a book to appear in the ERCOFTAC book series.

Invited lectures

- A. Masri (University of Sydney, Australia): Experimental studies of turbulent spray combustion - State-of-the-art and databases
- E. Gutheil (University of Heidelberg, Germany): Issues in computational studies of turbulent spray combustion

Poster contributions

- Experimental and numerical study of a two-phase turbulent flame. C. Letty, S. Saengkaew, B. Renou, G. Gréhan and J. Réveillon
- Real gas effects in mixing-limited spray models. C. Kurvers and C.C.M. Luijten
- Multiphase Flow Modeling: From Micro- to Macro-Scales. A. Özel, D. Wunsch, M. Maglio, Z. Zeren
- Two phase autoignition considering complex chemistry: evaporating droplet mass and heat transfer influence. Z. Bouali, C. Pera, J. Réveillon
- Development of Numerical Tools for Spray Combustion in Aero-engines. B. Franzelli, J.M. Senoner, C. Silva, F. Jaegle, B. Cuenot, T. Poinsot
- Modeling Engine Spray Ignition with Igniting Flamelets. C. Bekdemir, L.M.T. Somers, L.P.H. de Goey
- Influence of Evaporation on the Prediction of the Kerosene Spray Combustion. M. Chrigui, A. Sadiki, and J. Janicka
- Flame Propagation Regimes in Turbulent Hydrogen Jets. A. Veser, M. Kuznetsov, A. Friedrich, N. Kotchourko, G. Stern, G. Fast, M. Schwall, W. Breitung
- United PDF Formulation of Turbulent Evaporating Sprays. G. Anand and P. Jenny
- Entrainment and Evaporation Degree of Kerosene in the ESA-Configuration: Effects of gas phase temperature and pre-vaporisation length. M. Chrigui, A. Wahid, A. Sadiki and J. Janicka
- Simulation of Interaction between Pool Fire and a Water Mist Spray. A. Coghe, G. Manzini, L. Araneo, L. Iannantuoni
- Reynolds Stress and PDF Modeling of Two-way Coupling and Vaporisation Interaction in Turbulent Spray Combustion. N. Beishuizen, D. Roekaerts
- Spark Ignition and Flame Propagation in Sprays. A. Neophytou and E. Mastorakos and R. S. Cant
- Simulations of spark ignition of a swirling n-heptane spray flame with conditional moment closure. P. Schroll and E. Mastorakos and R. W. Bilger
- Laser ignition of spray flames. C. Letty and E. Mastorakos

5^{th} Workshop on Synthetic Turbulence Models

1-3th July, 2009, Warsaw University of Technology, Poland.

Andrzej Nowakowski[1], Jacek Rokicki[2], Konrad Bajer[3], Franck Nicolleau[1] and Claude Cambon[4]

[1] *Sheffield Fluid Mechanics Group, University of Sheffield, UK.*
[2] *Institute of Aeronautics and Applied Mechanics, Warsaw University of Technology, Poland.*
[3] *Institute of Geophysics, University of Warsaw, Poland.*
[4] *Laboratoire de Mécanique des Fluides et d'Acoustique, École Centrale de Lyon, France.*

www.sig42.group.shef.ac.uk/SIG42-05.htm

Introduction

The conference on Synthetic Turbulence and Vortex Flow was organized at Warsaw University of Technology under the auspices of ERCOFTAC. It was the fifth workshop on Synthetic Turbulence Models organised by SIG42 Special Interest Group and for the first time attracted participants from outside the European Union. On this occasion, the SIG 35 was involved too. The three days event was attended by 32 people including 17 participants with scheduled presentations. The presenters were affiliated to 10 different institutions, from which 8 represented institutions from 4 European Union countries and 2 were from the American continent. This was the first SIG42 workshop with such a scope. The venue enabled the participants to exchange ideas or initiate collaborative links outside the European community. The meeting was also a good opportunity to visit the fluid mechanics laboratories and strengthen the links with scientists working in prominent Polish Universities: Warsaw University of Technology, the University of Warsaw and Wroclaw University of Technology. Young scientists took this opportunity to present their work (seven young scientists are eligible for ERCOFTAC scholarships). The discussions were fruitful in particular there were interesting inputs from Charles Meneveau (Johns Hopkins University) and Carlos Rosales (Technical University Federico Santa Maria) on Eulerian synthethic turbulence models. The first time that topic was introduced during SIG42 meeting.

Abstracts of Talks

Turbulence in superfluid helium

H. Bajer, Institute of Geophysics, The University of Warsaw, Poland.

The new topics developed by Konrad Bajer's research group at the University of Warsaw have been presented. In particular the subject of superfluid turbulence and its explanation in terms of vortex dynamics was discussed. The physical analysis was based on careful analytical considerations. Superfluid helium offers dynamical properties that challenge classical turbulence models and test fundamental turbulence theories.

Vorticity and geometrical statistics in isotropic helical turbulence

Y.Li, Sheffield Fluid Mechanics Group, University of Sheffield, Department of Applied Mathematics, UK.

Helicity is defined as the scalar product between velocity and vorticity. It is an invariant of the Euler equation, and has been observed to play important roles in magnetohydrodynamics, geophysical flows. Recent results indicate that it also has effects on the regularity of the solutions to the NS equations. In this talk, a recent study of isotropic helical hydrodynamic turbulence fields is presented. The helical turbulence fields are generated by direct numerical simulations of the NS equations with constant helicity input. The helicity cascade from large scales to small scales is studied using a filtering approach. The emphasis is on the effects of helicity on the geometrical statistics of the vorticity field. It is shown that helicity cascade is related to the symmetric part of the gradient of the vorticity field, which is a symmetric tensor. It is found that, in helical turbulence, the eigenvalues of this tensor show skewed distribution, so that the intermediate eigenvalue of the tensor is more probable to be negative. It is also shown that, in helical turbulence, the vorticity tends to align more closely with its increasing direction, and that these properties of the vorticity field in helical turbulence are one of the mechanisms to generate helicity cascade.

Vortex Particle Method. Boundary Conditions and Boundary Layer Eruption

H. Kudela and T. Kozlowski, Wroclaw University of Technology, Poland.

The fundamentals of the vortex in cell (VIC) method were presented. The usefulness of the method was demonstrated by the solution of several well known and well-documented problems. Especially the method is very well suited for the problems that are governed by the vorticity dynamics. The authors focused on the problem of the flow over the cylinder and thin ellipse (the external problems) and also on unsteady viscous flow past oscillating and translating ellipse that mimics aerodynamics of the fly of insects and the falling paper problem. The numerical studies related to the eruption of boundary layer from the wall were also presented. It was shown that eruption of boundary layer takes place in the wake of the flow past a cylinder for very high Reynolds numbers.

Synthetic turbulent-like flows realisable in the laboratory

M. Priego Wood and J. C. Vassilicos, Aeronautical Department, Imperial College London, UK.

The spectral and particle dispersion characteristics of steady multiscale laminar thin-layer flows are investigated through numerical simulations of a two-dimensional layer-averaged model. The model assumes a semiparabolic velocity profile and is solved using a semi-Lagrangian spline method. The main features of the flows are turbulent-like and consistent with previous experimental studies. The Eulerian wavenumber spectra and the Lagrangian frequency spectra oscillate around power laws that reflect the self-similarity of the forcing. In the weak forcing regime, the exponents of these power laws can be related to the multiscale geometry and the intensity scaling of the forcing. The Lagrangian spectra also show low-frequency plateaus, which arise from the slow motions far away from the applied forces. The absolute dispersion of tracer particles in these steady planar flows presents a ballistic stage followed by a diffusive regime, which results from the decorrelated motions of particles lying on streamlines of different period. Relative dispersion shows an additional intermediate stage consisting of several separation bursts, which originate from the intense strain regions imposed by the different forcing scales. While these bursts can cause locally superquadratic mean square separation, the trapping by steady recirculation regions rules out an intermediate relative dispersion power law, regardless of the number of scales in the flow.

Synthetic Turbulence via the Multiscale Lagrangian Map Approach

C. Rosales, Technical University Federico Santa Maria, Chile.

A simple method is proposed to generate synthetic vector fields as surrogates for turbulent velocity fields. The method is based on the minimal Lagrangian map, by which an initial Gaussian field generated using random-phase Fourier modes is deformed. The deformation is achieved by moving fluid particles of a sequence of low-pass filtered fields at their fixed velocity for some scale-dependent time interval, interpolating onto a regular grid, and imposing the divergence-free condition. Statistical analysis shows that the resultant non-Gaussian field displays many properties commonly observed in turbulence, ranging from skewed and intermittent velocity gradient and increment probability distributions, preferential alignment of vorticity with intermediate strain-rate, and non-trivial vortex stretching statistics. Differences begin to appear only when interrogating the data with measures associated with intense vortex tubes that are conspicuously absent in the synthetic field. To explore the dynamical implications of these observations, the synthetic non-Gaussian fields are used as initial conditions in DNS and LES of decaying isotropic turbulence, and results are compared with initializations using Gaussian fields. The non-Gaussian synthetic fields yield more realistic results with significantly shortened initial adjustment periods.

Minimal map synthetic turbulence: Intermittency and anomalous scaling

C. Meneveau, Mechanical Engineering, Johns Hopkins University, USA.

A simple method, the Multiscale Minimal Lagrangian Map (MMLM) approach to generate synthetic turbulent vector fields was introduced (Rosales and Meneveau, Physics of Fluids 2006). It was shown that the synthesized fields reproduce many statistical and geometric properties observed in real, isotropic, turbulence. In this paper we investigate if this procedure, which applies a minimal Lagrangian map to deform an initial Gaussian field, can produce also anomalous scaling in the inertial range. It is found that the advection Lagrangian Map time-scale is crucial in determining anomalous scaling properties. With the sweeping time- scale used in MMLM, non-Gaussian statistics and realistic geometric features are reproduced at each scale, but anomalous exponents are not observed, i.e. we observe nearly Kolmogorov 1941 scaling. Conversely, if the appropriate Kolmogorov inertial-range turnover time-scale is used in a modified approach (the Multiscale Turnover Lagrangian Map - MTLM - method), fields with realistic anomalous scaling exponents are reproduced. Remarkably, the intermittency and multifractal nature of the energy dissipation is also found to be quite realistic. Finally, the properties of the pressure field derived from the MTLM velocity field are studied and found to be quite realistic also. The results shed new light on what are minimal dynamical requirements for the generation of anomalous scaling and intermittency in turbulent flow: at least one turnover time for small eddies to be sufficiently deformed, as well as the accumulation of spatially correlated deformations across scales. We also review the advected delta-vee system (Li and Meneveau 2006, Journal of Fluid Mechanics) as well as the JHU turbulence database cluster (Li et al. 2008, Journal of Turbulence).

Synthetic models and DNS for MHD turbulence with external magnetic field and rotation

B. Favier, Laboratoire de Mécanique des Fluides et d'Acoustique, École Centrale de Lyon, France.

Interactions between a turbulent velocity field of a rapidly rotating electrically conducting fluid and a magnetic field occur in many astrophysical and geophysical systems. We propose here a comparison between direct numerical simulations (DNS) and a synthetic model of rotating magnetohydrodynamic (MHD) turbulence. Kinematic simulations (KS) have already been used in many contexts from particle dispersion to aeroacoustics and small-scale dynamo.

We consider an incompressible initially isotropic turbulence submitted to an uniform magnetic field in a frame rotating with a constant angular velocity. In a first approach, we focus on a large interaction parameter and low Rossby number regimes, in which the anisotropy due to both Coriolis and Lorentz forces are of prime importance.

Concerning the synthetic model, the turbulent velocity field is synthesized as a random superposition of incompressible Fourier modes, including linear dynamics. The main originality of the present work is to compute both the velocity field and the magnetic field using KS.

The Eulerian dynamics, as well as the dispersion properties of rotating MHD flows are discussed. Comparisons between KS and DNS results are also proposed, with an emphasis on anisotropy in such flows.

Axisymmetric turbulence: towards a theory for both statistics and dynamics
C. Cambon, Laboratoire de Mécanique des Fluides et d'Acoustique, École Centrale de Lyon, France.

Anisotropic turbulence until the smallest scales can be found in incompressible and (statistically) homogeneous turbulence, especially when the conventional cascade is altered by anisotropic waves (rotating inertial turbulence, MHD Alfvénic turbulence). Stably stratified turbulence offers another example, in which strong turbulence mediated by non-propagating modes (e.g. toroidal motion) can coexist with gravity wave-turbulence. Rotating turbulence at low Rossby number and high Reynolds number gives a good example of anisotropic (inertial) wave-turbulence: it is shown, or reminded, how a spectral formalism, with the energy/polarization/helicity decomposition, gives the optimal description of anisotropy with a minimal number of scalars. One of the finest information, without equivalent in physical space (e.g. SO(3) symmetry group applied to structure functions), is provided by angle-dependent spectra. This information can be extracted from DNS and anisotropic theory, ranging from wave-turbulence to generalized EDQNM; it could be prescribed too in an improved KS. It is important to stress that the anisotropy can increase at increasing wavenumber, until a possible maximum, more or less related to an Oszmidov-type threshold wavenumber, but re-isotropization at the smallest scales remains a complex, not completely understood, process. A theory for axisymmetric turbulence can be constructed, based on the anisotropic spectral description, but also supported dynamically by exact generalized Lin's equations. New insight to MHD turbulence with and without rotation is finally presented, in close connection with the talk by Benjamin Favier, dealing with analytical results, incorporation in KS (+RDT) and high resolution DNS.

Stratified Decaying 2D Flows: Experiments in Non-Rotating and Rotating Conditions
A. Matulka and J. Redondo, Universidad Politecnica de Catalunya, Barcelona, Spain.

Two sets of turbulence decaying experiments have been studied in the middle of a density interface. Experiments were divided in two categories: a) Stirring (Non- Rotating) Decaying 2D Turbulence, and b) Rotating Decaying 2D Turbulence. In the first category, the whole group of stirred experiments were a compilation of five sets of total mixing experiments, dependent on the initial Richardson number. The Total time mixing was between 53 and 72 minutes. The density of fluid after the total mixing was in the limits between 1027 and 1037. For the other category, the boundary conditions from all the rotating experiment conditions related to Reynolds Re, Rossby Ro, Ekman Ek and Richardson gradient Rig numbers are reported; moreover parametric spaces of Rig, Re and Ro are analyzed.

Wake behind a sphere - Experimental research
K. Gumowski, Institute of Aeronautics and Applied Mechanics, Warsaw University of Technology, Poland.

The experimental setup, the analysis and the results of laboratory investigation of the flow behind the sphere were discussed. The experiments have been conducted using a new test rig (a low velocity water channel) at the Institute of Aeronautics and Applied Mechanics of Warsaw university of Technology. It was found that after a first stationary transition where the flow breaks the axisymmetry, controlled experiments allow the definition of a threshold for the second transition from stationary to unstable flow. The transition includes three-dimensional peristaltic oscillations of the two trailing vortices prior to hairpins shedding. The scenario has been proposed to explain the hairpin formation, as pieces of a counter-rotating longitudinal vortex. Hairpin shedding is suggested to be the result of oscillations, which are powerful enough, and reconnection of the trailing vortices.

Low-Reynolds-number instabilities of channel flows
J.Szumbarski, Institute of Aeronautics and Applied Mechanics, Warsaw University of Technology, Poland.

The presentation consists of two parts. In the first part, a brief account on recent results concerning stability of the channel flows is provided. It is shown that wall waviness oriented transversely with respect to the main unidirectional flow can lead to radical reduction of the critical Reynolds number (down to 58 compared to 5772 of the reference Poiseuille flow) while keeping the flow resistance basically unchanged or even slightly reduced. Geometric properties of the unstable mode have been also discussed. In the second part, numerical simulations of laminar flows behind polygonal contours confined between parallel walls are presented. The numerical method based on spectral element discretization and using the "do nothing" approach to the inlet/outlet conditions is proposed.

Sheffield Fluid Mechanics Group

The last session was organised by the Sheffield Fluid Mechanics Group. There was a series of four talks linked to F. Nicolleau's group in the Sheffield Fluid Mechanics Group and Paris 6.

In the context of synthetic turbulence, particularly for Kinematic Simulations, the turbulence energy spectrum appears as the models' main input. In order to understand better the links between Eulerian and Lagrangian properties we propose some studies of fractal forcing of turbulent flows (see also Martin Priego Wood contribution). The first presentation of this group was by F. Nicolleau and presents experimental results from fractal orifice flows. These orifices can be seen as a systematic way to monitor turbulence inner structure and play with the flow spectral properties. The experiment is then modelled using Detached Eddy Simulation by Hongwei Zheng (second presentation). Some theoretical background results are proposed by Thomas Michelitsch in the third presentation of this group. The last talk demonstrated the capabilities of the newly developed numerical code for multicomponent flows. It is expected that this development will lead us to investigate the fractal geometries for mixing in two-phase flow environments.

Turbulence generated after a fractal orifice
F. Nicolleau, Sheffield Fluid Mechanics Group, University of Sheffield, UK.

Fractal-shaped orifices are thought to have a significant effect on the flow mixing properties downstream a pipe owing to their edge self-similarity shape. Here, we investigate the pressure drop after such fractal orifices and measure the pressure recovery at different stations downstream the orifice. A direct comparison is made with the pressure drop measured after regular circular orifices with the same flow area. Our results show that the pressure drop measured across the fractal-shaped orifices is lower than that from regular circular orifices of the same flow areas. This result could be important in designing piping systems from the point of view of losses. It looks promising to use the fractal-shaped orifices as flowmeters as they can sense the pressure drop across them accurately with lower losses than the regular circular shaped ones. The main reason for the lower pressure drop across a fractal orifice in found in its ability to create a wider distribution of velocity scales.

DES of fractal orifices
H. Zheng, Sheffield Fluid Mechanics Group, University of Sheffield, UK.

This contribution presents the simulation of DES results on the flows after the two special multi-scale fractal shaped geometry (SF2 and SF3) orifices and the normal orifice in a pipe. As compared to the normal circular orifice, more mixing structures are generated after the fractal shape orifice. The numerical mean velocity profiles along the pipe show a good agreement with the experiment values obtained by hotwire anemometry.

DES of fractal orifices
T. Michelitsch, CNRS Institute Jean Le Rond d'Alembert University of Paris VI, France.

Many systems in nature have arborescent and bifurcated structures such as trees, fern, snails, lungs, the blood vessel system, etc. and look self-similar over a wide range of scales. Which are the mechanical and dynamic properties that evolution has optimised by choosing self-similarity? How can we describe the mechanics of self-similar structures in the static and dynamic framework? Physical systems with selfsimilarity as a symmetry property require the introduction of non-local particle-particle interactions and a (quasi-) continuous distribution of mass. We construct self-similar functions and linear operators such as a self-similar variant of the Laplacian and of the D'Alembertian wave operator. The obtained selfsimilar linear wave equation describes the dynamics of a quasi-continuous linear chain of infinite length with a spatially self-similar distribution of nonlocal inter-particle springs. The self-similarity of the nonlocal harmonic particle-particle interactions results in a dispersion relation of the form of a Weierstrass-Mandelbrot function which exhibits self-similar and fractal features. We deduce a continuum approximation that links the self-similar Laplacian to fractional integrals and which yields in the low-frequency regime a power law frequency dependence for the oscillator density. For details of the present model we refer to our upcoming paper (Michelitsch et al., in press, Phys. Rev. E).

Computing the evolution of interfaces using multicomponent flow equations
A. Nowakowski, Sheffield Fluid Mechanics Group, University of Sheffield, UK.

A multicomponent flow model is investigated for liquid and gas interface modelling. The hyperbolic problem is tackled using a high-resolution HLLC scheme on a fixed Eulerian mesh. The scheme for the nonconservative terms is derived in order to fulfil the interface condition. The results are demonstrated for several one and two-dimensional test cases including bubble explosion under water test.

Pilot Centres and SIGs involved

- ERCOFTAC label and scholarship are gratefully accepted
- Institute of Aeronautics and Applied Mechanics, Warsaw University of Technology.
- Centre Henri Bénard, French ERCOFTAC Pilot Centre.
- ERCOFTAC SIG42 and SIG35

Quality and Reliability of Large-Eddy Simulation II

9-11th September, 2009, Pisa, Italy.

Maria-Vittoria Salvetti*, Bernard J. Geurts, Johan Meyers, Pierre Sagaut

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Context and Objectives

The second Workshop on 'Quality and Reliability of Large-Eddy Simulations', QLES2009, was held at the University of Pisa from September 9 to September 11, 2009. Its predecessor, QLES2007, was organized in 2007 in Leuven (Belgium). The focus of QLES2009 was on issues related to predicting, assessing and assuring the quality of LES. The development of computational resources and the corresponding tendency to apply LES-methodologies to turbulent flow problems of significant complexity, such as arise in various applications in technology and in many natural flows, makes the issue of assessing and optimizing the quality of LES predictions a timely challenge. Different error sources are present in LES, which are mainly related to physical modeling (especially of subgrid scales), to numerical discretization techniques, to boundary-condition treatments, and to grid resolution and design. These errors may interact in a complex non-linear manner, eventually leading to unpredictable and unexpected effects on LES results.

To establish the credibility of LES as a tool for the innovation of industrial flow applications and for the study of complex-physics problems, clear standards and criteria to assess and predict the quality and the reliability of the simulation results should be devised. To this aim, an understanding of the nonlinear accumulation and interaction of the different errors arising in large-eddy simulations, and of their dependence on the different simulation parameters, is required. This is also crucial for the development of methodologies and techniques aimed at controlling the different errors and, hence, at optimizing the quality of LES results.

The main goal of QLES2009 was to enhance the knowledge on error sources and on their interaction in LES and to devise criteria for the prediction and optimization of simulation quality, by bringing together mathematicians, physicists and engineers and providing a platform specifically addressing these aspects for LES.

Participation

In total 64 participants from 12 countries registered for this workshop. The majority of participants was from academia and research institutes. In addition, several companies and consultancy agencies were represented.

Content of the workshop

QLES2009 gathered 7 invited lectures, held by speakers from different scientific fields: Lars Davidson (Chalmers University, Sweden), Jean-Luc Guermond (Texas A&M University, USA), Andreas M. Kempf (Imperial College London, United Kingdom), Johan Meyers (Katholieke Universiteit Leuven, Belgium), Marc Parlange (Ecole Polythecnique Fédérale de Lausanne, Switzerland), Thierry Poinsot (Institut de Mécanique des Fluides de Toulouse, CNRS, France), Philippe Spalart (Boeing Commercial Airplanes, USA).

Johan Meyers presented an overview of recent developments of the 'error-landscape' methodology, aimed at investigating the quality and reliability of large-eddy simulations by constructing a full response surface of the LES error behavior. Thierry Poinsot illustrated the application of LES to the simulation of complex reacting flows and discussed issues related to the reliability and the repeatability of LES results for such applications. Philippe Spalart drew the attention to a careful grid generation and optimization as a key issue to obtain accurate and reliable LES predictions for external flows. Marc Parlange and Chad Higgins reported recent a-priori tests of models for subgrid-scale processes in stable and unstable atmospheric boundary-layers carried out by using data from field experiments. Jean-Luc Guermond reviewed the mathematical properties of the 3D incompressible Navier-Stokes equations and their relation to LES. He also illustrated how the notion of suitable weak solutions can be used to devise LES closure models. Andreas Kempf discussed quality issues and the possibility of using quality indicators and error-charts in combustion LES, for which the presence of a wide range of chemical and mixing scales makes the assessment of simulation quality and reliability even more challenging than for "fluid-flow only" LES. Finally, Lars Davidson addressed the issue of how to estimate the resolution of LES simulations of recirculating flows.

Next to the invited lectures, 33 contributed presentations were selected by a Scientific Committee of 14 experts. These contributions were divided in the following main topics: (i) Modeling and error assessment of near-wall flows; (ii) SGS modeling and discretization errors; (iii) Assessment and reduction of computational errors; (iv) Mathematical analysis and foundation for SGS modeling. Ample time for discussions was available between presentations, during coffee breaks, lunches and at the conference dinner.

A book of abstracts was prepared including the invited lectures as well as the contributed papers. A final volume of proceedings will be published by Springer in the ERCOFTAC Series and a selected number of papers will be included in a special issue of the Journal of Scientific Computing.

From the presentations and the discussions held during the workshop, it was clear that the tendency to apply LES to various, very complex industrial and environmental problems, already observed during the previous QLES workshop, further enhanced in the last two years. Several examples of such complex applications were shown during the workshop for which LES is able to give accurate results. It was also made clear that this requires a profound knowledge of the problem and a careful combination of physical modeling, numerics, grid resolution and quality. Although SGS modeling is still felt as the most critical issue in LES, several contributions were given at the workshop to the investigation of the sensitivity of the quality of LES results also to numerical methods, boundary conditions treatments and grid resolution. Recent developments and applications of methodologies aimed at understanding, predicting and minimizing error dynamics in LES were also presented.

In the spirit of the QLES series, this workshop gave a stimulating contribution to the development of higher standards for the assurance of quality and reliability of large-eddy simulations. Critical and open issues remain in order to increase the accessibility of LES to non-specialist users. In this perspective, a third meeting of the QLES series will be organized at Ecole Polythecnique Fédérale de Lausanne (Switzerland) in 2011.

Acknowledgments

On a European scale financial support was provided by COST Action P20 'LESAID' (LES-Advanced Industrial Design) and ERCOFTAC (European Research Community on Flow, Turbulence and Combustion). Locally, the University of Pisa supported the workshop. This support was essential for the organization of this event and is gratefully acknowledged.

The Swiss
'Leonhard Euler Centre'
Pilot Centre Report

EPFL-LTCM: Laboratory of Heat and Mass Transfer

Post Station 9, CH-1015 Lausanne, Switzerland.

The main research fields at the LTCM 'Heat and Mass Transfer Laboratory', under the directorship of Prof. John R. Thome are:

- Single and two-phase heat transfer in microchannels
- Theoretcial and numerical modelling of two-phase flows and flow regime transitions
- Falling film evaporation and condensation
- Quantitative multiphase flow visualisation

CMOSAIC - 3D Stacked Architectures with Interlayer Cooling

Madhour, Rabello, Szczukiewicz, Borhani, Thome

Several indicators show that the speed of transistor density and performance improvement that drove the IT industry for the last 50 years is slowing down. With its scaling engine slowing, the industry is scrambling to find new packaging alternatives to maintain the overall pace according to Moore's law. While 2D scaling has been used in high performance processors for several decades, the third dimension has not yet been tackled. Recent progress in the fabrication of through silicon vias has opened new avenues for high density area array interconnects between stacked processor and memory chips. Such three dimensional integrated circuits are attractive solutions for overcoming the present barriers encountered in interconnect scaling, thus offering an opportunity to continue the CMOS performance trends over the next decade.

This project is a genuine opportunity to contribute to the realization of arguably the most complicated system that mankind has ever assembled: a 3D stack of computer chips with a functionality per unit volume that nearly parallels the functional density of a human brain. The aggressive goal is to provide the necessarily 3D integrated cooling system that is the key to compressing almost 1012 nanometer sized functional units into a 1cm^3 volume with a 10 to 100 fold higher connectivity than otherwise possible. Even the most advanced air-cooling methods are inadequate for such high performance systems where the main challenge is to remove the heat produced by multiple stacked dies with each layer dissipating 100-150W/cm^2. Therefore, state-of-the-art single phase liquid and two-phase cooling systems are being developed, using specifically designed microchannel arrangements. The employed coolants range from liquid water and two-phase environmentally friendly refrigerants to novel engineered nano-fluids. To this aim, *CMOSAIC* has brought together a multi-disciplinary team of internationally recognized experts to jointly conduct research into the underlying physics of the proposed cooling mechanisms through experiments and theoretical modelling. This team, coordinated by the LTCM, includes: EPFL-LSM, EPFL-ESL, EPFL-LTCM, ETHZ-LTNT, ETHZ-FML and IBM Zürich Research Laboratory. The team will also develop all the necessary modelling and design tools needed to simulate 3D integrated circuits stacks during their operation in order to mitigate hot spots, and test various prototype stacks with the goal of identifying and bringing into reality novel methods for heat removal in these high performance systems.

CMOSAIC was scientifically evaluated by the Swiss National Science Foundation and is financed by the Swiss Confederation's Nano-Tera.ch fund.

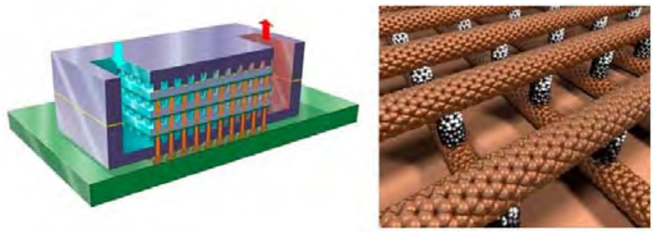


Figure 1: *Schematics of (left) a 3D-IC architecture incorporating liquid cooling channels, and (right) the through silicon vias (TSV).*

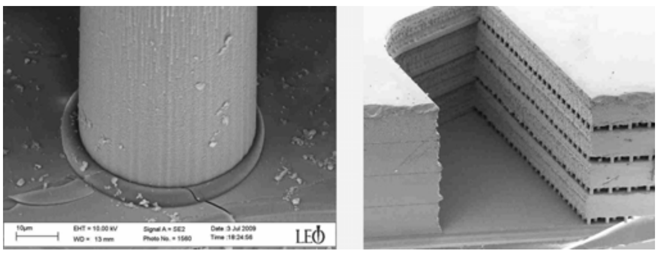


Figure 2: *(left) SEM close-up of a pin-fin pillar bonded with polyimide to a flat surface, and (right) a cross-section through the silicon stack showing the fluid cavity structures bonded with polyimide.*

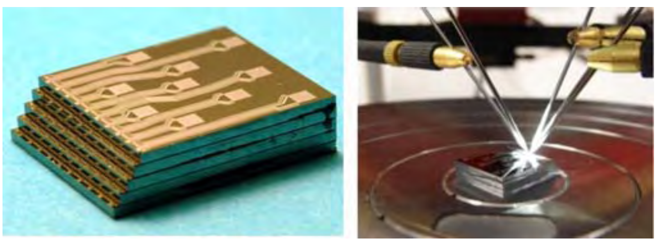


Figure 3: *(left) 5-tier thermal stacks, and (right) measurement of their temperature profiles using a probe station to create an RC thermal library.*

Micro-Evaporation Cooling for Microprocessor under Uniform, Non-Uniform and Transient Heat Flux

Costa-Patry, Olivier, Thome

Thermal management of computers is becoming more and more challenging. Several authors have shown that two-phase flow evaporation in microchannels could raise the ceilings for the performance of computers. The available results for two-phase cooling are concentrated on uniform heat flux test sections, whereas microprocessors produce an uneven and transient heat flux over their two-dimensional footprint. Therefore, in order to better understand the true operational characteristics of micro-coolers, micro-evaporators made of silicon and copper with hydraulic diameters varying between 100 and 300μm, are tested on a thermal package with 35 independent heating zones and 35 temperature sensors. Data acquisition can be performed up to 1kHz and the system reaction heat flux up to 3.5MW/m^2 can be studied. These results will be of interest the future design of micro-evaporators. This research is carried out in partnership with IBM and funded by the Swiss KTI.

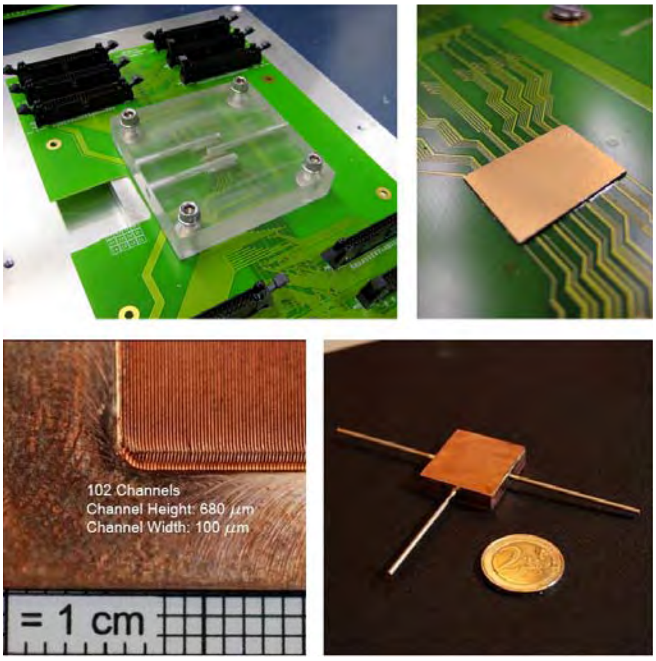


Figure 4: *The micro-evaporator is 12x18 mm in size with 5 channels/mm. It has 35 local heaters and 35 local temperature sensors to model non-uniform heating and hot spots.*

Fundamental Study on Adiabatic Annular Two-Phase Flow in Micro and Small Diameter Channels

Milan, Borhani, Thome

The aim of this fundamental project is to investigate adiabatic annular two-phase flow inside small diameter vertical circular channels. The channels will range from minichannels, with diameters from 10mm to 3mm, down to microchannels with diameters as small as 1mm. We will focus in particular on the liquid entrained fraction, the void fraction, the time-averaged velocity profile in the liquid film, and the interfacial waves; four of the most important flow parameters in annular two-phase flow. The proposed research is intended to fill the gap in the existing literature regarding annular two-phase flows inside micro and small diameter channels which are of great interest to numerous emerging microscale technologies. In particular, extending knowledge of the entrained liquid fraction and the void fraction all the way down to the microscale will allow a sound theoretical model of microscale annular two-phase flow to be developed. This is of great importance since it will provide a strong basis for the development of more sophisticated heat transfer prediction models for such geometries and flow regimes using our database obtained in previous studies. This project is funded by the Swiss National Science Foundation.

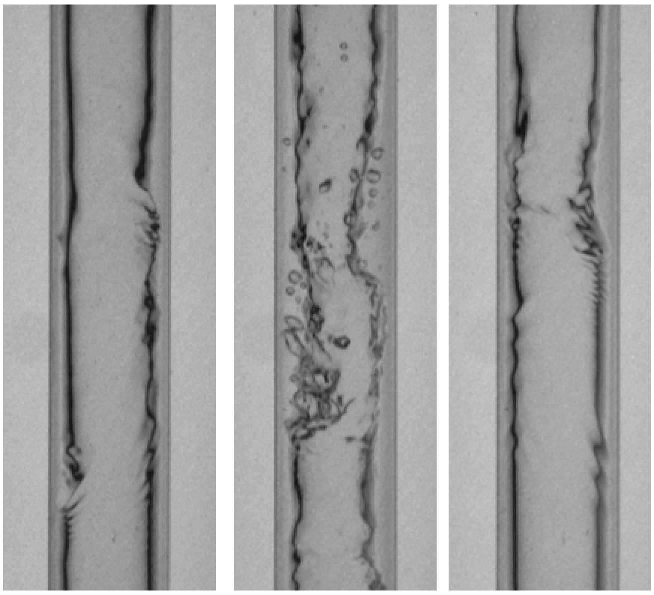


Figure 5: *Annular and churn flow regimes for vertical air-water co-downflow in a 9mm tube.*

Macro to Microscale Transition in Two-Phase Flow and Evaporation

Ong, Thome

This fundamental research program focuses on investigating the confinement effects of channel dimension and refrigerant fluid properties on flow boiling heat transfer, two-phase flow patterns, pressure drop, critical heat flux and film stratification in a single channel. Flow boiling experiments have been conducted for three refrigerants, R134a, R236fa and R245fa in single circular channels with 1.03, 2.20 and 3.04mm internal diameters. In particular it focuses on determining the key mechanisms and flow characteristics that control the transition process from macro-to-microscale flow regimes for two-phase phenomena. This project is funded by the Swiss National Science Foundation.

Visualization of falling film evaporation on a tube bundle

Christians, Thome

In previous work performed at the LTCM, the heat transfer characteristics of falling film evaporation and condensation on tube arrays and tube bundles for both smooth and enhanced tubes have been studied. This research not only resulted in a large experimental database from which prediction models have been developed, but also indicated significant discrepancies between the heat transfer characteristics of tube array and bundle evaporators. This difference is thought to be heavily dependent on the inter-tube flow pattern. As such, the proposed aim of this study is to expand the evaporation experimental database for single tube, tube arrays and bundle test sections to include the new tubes provided by LTCM's industrial partners, and to perform a detailed visualization study for falling film evaporation inside the tube arrays and tube bundles.

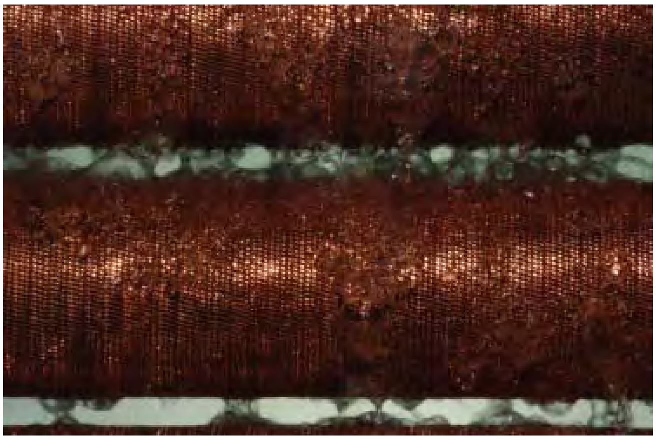


Figure 6: *R-134a falling between horizontal enhanced tubes of a 1 x 10 single-array at* $q = 20kW/m^2$, $Re_{film} = 700$ *and* $T_{sat} = 5C$.

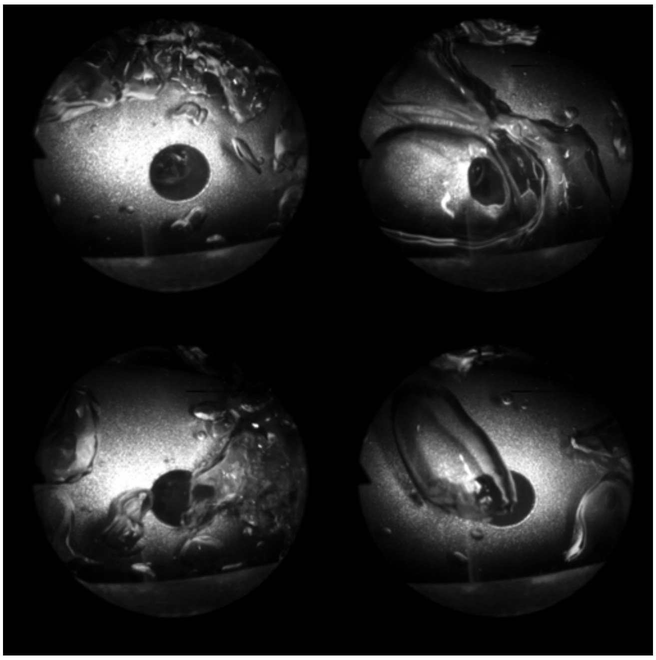


Figure 7: *Image sequence of R134a at mass flux of* $4kg/m^2s$ *and a vapour quality of 20% flowing through a tube bundle. Images are taken in the adiabatic section of the bundle, with a bore scope camera, and show a bubbly type flow.*

Enhanced Boiling on a Tube Bundle: Heat Transfer, Pressure Drop and Flow Patterns
van Rooyen, Thome

The tests will cover a wide range of refrigerant mass velocities, heat fluxes, vapour qualities and different refrigerants in order to obtain a representative database of conditions common in applications. The planned experimental work has the following objectives: (i) to link each flow regime and its specific physical behaviour to the heat transfer and pressure drop observed in the bundles, and (ii) to use the results database to further improve our understanding of the mechanisms active inside tube bundles during evaporation. To this aim, we will develop phenomenologically based prediction models from the observations made of the two-phase flow structures.

Numerical modelling of two phase flows
Nichita, Thome

In the present study we focus on the *one* fluid methods, namely level set and volume-of-fluid, for the modelling of two phase flows. More precisely, within the framework of the volume of fluid method we define a level set function which will be used to calculate the curvature and normal to the interface, since volume of fluid provides a rather poor calculation of these two values. The general CFD code Fluent is used, which already contains the volume of fluid method. The level set method and the method of Brackbill have been coded into Fluent as User Defined Functions. Another objective is to implement for the first time a model for a dynamic contact angle into Fluent, which will be very useful in simulations of bubbles that break-up at T-junctions. It is believed that the present 3D code when finished and validated will constitute one of the most advanced two phase flow modelling tools available. In parallel, validations of the new code are being implemented versus published experimental data on classic flows.

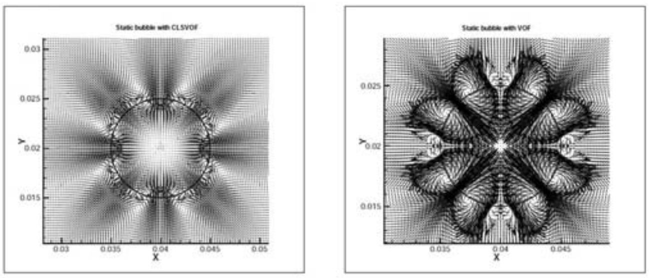


Figure 8: *Velocity field around a static bubble: (left) CLSVOF and (right) VOF.*

Numerical Modelling of Annular Film Condensation in Circular and Non-Circular Channels under Normal and Micro-gravity
Nebuloni, Thome

The objective of this research is to investigate the process of laminar annular film condensation in circular and non circular channels of pure substances, for different operative conditions: mass flow, saturation temperature, average vapour quality, gravity intensity and test section inclinations. Particular care has been dedicated to the effects of surface tension which become important especially when the inner perimeter of the channel has a strong curvature and it is not uniform. This phenomenon is known as the *Gregorig effect*. The channel shape and size can also strongly influence the mean heat transfer coefficient and pressure drop. Normal gravity and microgravity conditions have also been analyzed with special attention to the effects of residual and unsteady (g-jitters) contributions. This work is funded by the European Space Agency.

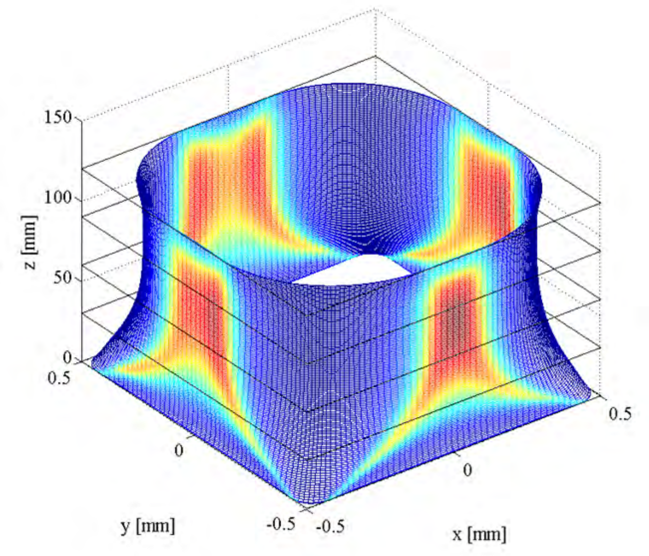


Figure 9: *Example of calculated liquid vapour interface and regions of high heat transfer coefficients for a square mini-channel.*

Experimental Evaluation of Two-Phase Pressure Drops and Flow Patterns in U-Bends

Da Silva Lima, Thome

Curved channels in the form of bends are encountered in many industrial two-phase flow applications, such as U-bends in air-conditioning and refrigeration evaporators and condensers. For engineering design purposes, the evaluation of the pressure loss in two-phase flows is necessary. Basically, for the same flow conditions the pressure loss is higher in a U-bend than in a straight pipe with an equal cross flow section and mean length. Moreover, the curved tube causes a perturbation that propagates up- and downstream of the U-bend itself, modifying the typical straight tube pressure loss at the vicinity of the U-bend. From an energetic viewpoint the investigation of U-bends on two-phase pressure drops (in the bend and before and after the bend) are particularly important in energy-efficient designs of evaporators and condensers coils. Such units utilize small temperature approaches and hence accurate prediction of the local saturation pressures and temperatures are imperative. Thus, the objectives of this project are defined in two axes: (a) observations of the flow pattern modifications induced by the U-bend and (b) measurements of (i) the axial variation of the frictional pressure drops in the straight tubes up- and downstream of a U-bend and (ii) the frictional pressure drop in the U-bend itself. This study in being carried out in a test section specially developed for this purposes. This work is funded by ASHRAE.

Theoretical modelling of microscale and macroscale annular two-phase flows for adiabatic and diabatic flow conditions

Cioncolini, Thome

Annular two-phase flow, characterized by the presence of a continuous liquid film flowing on the channel wall and surrounding a central gas core laden with entrained liquid droplets, is one of the most frequently observed flow patterns in practical applications involving gas-liquid two-phase flows. The objective of the research project is to develop annular flow closure relations and models that are required in most thermal-hydraulic predictions, including the onset of dryout in boiling channels and the heat transfer effectiveness below the dryout. In particular, the turbulent structure in the annular liquid film in both adiabatic and diabatic flow conditions is currently being investigated, and new closure relations for predicting the wall shear stress and the entrained liquid fraction are currently being developed. This work is funded by the Swiss National Science Foundation.

Two-phase cooling system with micro-evaporator applied to high performance microprocessors: Theoretical and experimental analysis

Wu, Marcinichen, Thome

The cooling of data centers presents an estimated annual cost of 1.4 billion dollars. Nowadays, the most widely used cooling strategy is refrigerated air cooling of the data centers' numerous servers. When making use of this solution, nevertheless, 40% or more of the refrigerated air flow typically by-passes around the racks of servers in datacenters, according to recent articles published at ASHRAE's Winter Annual Meeting at Dallas in 2007. This behaviour motivates the search for a green two-phase cooling solution to the future generation of higher performance servers that consume much less energy to cool them.

The goal of this work is to propose and develop a new novel hybrid two-phase cooling system with multi microchannel evaporator elements for direct cooling of the chips and memory on the IBM blade server boards. The main focus is to work with two-phase flow of dielectric refrigerants, using a compressor or/and liquid pump to drive the fluid, a micro evaporator for cooling of the chip and a micro condenser for heat recovery, which can reduce the demand of cooling energy by up to 50%. A mathematical model to thermally simulate and evaluate the performance of the hybrid cooling system at steady and transient conditions will then be developed. Our partners in this Swiss KTI funded project are IBM and Embraco.

Figure 10: *An IBM Blade board*

EPFL-LIN: Laboratory of Computational Engineering

Post Station 9, CH-1015 Lausanne, Switzerland.

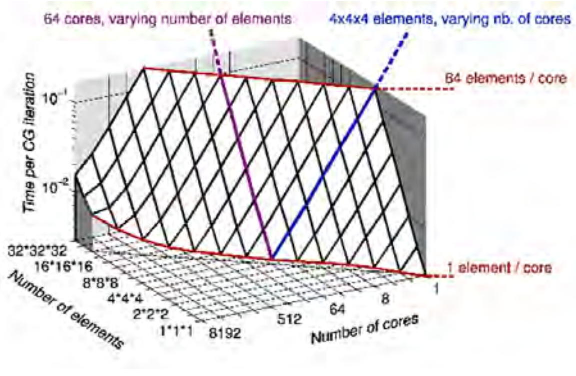
The Laboratory of Computational Engineering (LIN) is a research and teaching laboratory within the Institute of Mechanical Engineering (IGM) of the School of Engineering (STI) at the Swiss Federal Institute of Technology - Lausanne (EPFL). The LIN is involved in a wide range of basic and applied research in computational science and engineering with an emphasis on numerical fluid mechanics.

Fundamental and applied research, as well as teaching, are undertaken within three main themes:

- Physical and numerical modelling
- hardware and software resources
- complex multiphysics applications

Physical modelling activities are focussed on the understanding of complex (e.g. unsteady, turbulent, 3D, reacting) compressible and incompressible flows, including non-Newtonian fluids and particulate flows. The numerical simulation of these flows is performed using a variety of numerical methods (e.g. finite element, spectral element, lattice Boltzmann and discrete element methods). To perform state-of-the-art simulations, attention is given to the hardware and software resources required; the LIN is thus strongly involved with the Pleiades cluster, grid computing initiatives and scientific visualization. Finally, these basic aspects are employed for complex multiphysics simulations, often involving the coupling of different methodologies (fluid-structure, fluid-particle, plasma-aerodynamics, etc.).

The spectral activities of the LIN are focussed on the study of the instabilities of viscoelastic fluid flows. A first approach is performed on the matrix logarithm for the conformation tensor (Azadeh Jafari) while the second one investigates grid filter models and carries out Fourier pseudo spectral calculations (Marc-Antoine Habisreutinger). The software toolbox Speculoos has been completely parallelized and runs of the 8192 processors of the EPFL BlueGene/P. The achieved speedup that is almost linear is given on the next figure:



DNS and LES computations are tackling the turbulent convective flow Inside a cubical cavity that is differentially heated. Furthermore a Lagrangian particle tracking is computed to check the deposition mechanisms. This research is sponsored by the Paul Scherrer Institute and is related to nuclear safety problems. The doctoral students are R. Puragliesi and Christoph Bosshard.

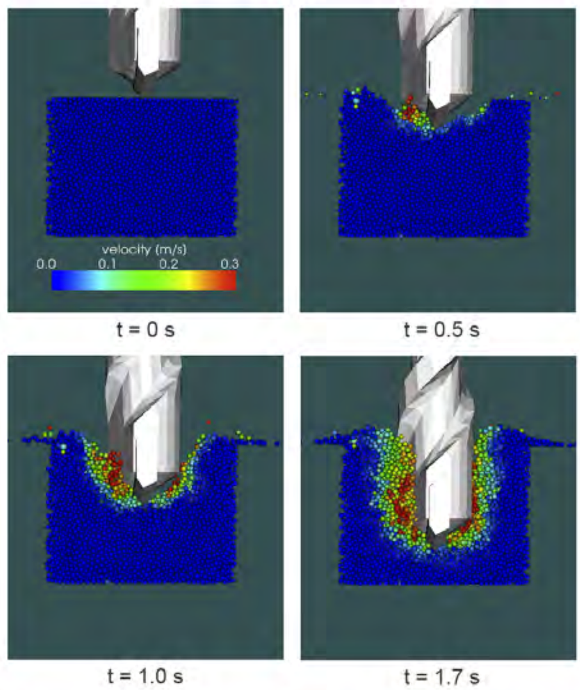
The thesis presented by Orestis Malaspinas in October 2009 is entitled "Lattice Boltzmann method for the simulation of viscoelastic fluid flows". The thesis provides new insights into the capabilities of the LB method to simulate complex flows and rheologies.

Other research activities include:

The Discrete Element Method and it application to drilling agglomerate solid materials

Sawley, Schenkel, Binggeli

The Discrete Element Method (DEM) is based on the resolution of Newton's equations for a collection of particles and their interactions. By considering different models for the inter-particle forces, DEM can be applied to the numerical simulation of a wide range of physical behaviour, such as free-flowing granular materials, particulate-fluid mixtures, rheologically-complex flows and agglomerate solid materials. An in-house software package has been specifically developed to provide flexible force modelling, treat particle interactions with complex surrounding geometries, and enable efficient computation of systems having a large number of particles (> 100,000).



In collaboration with an industrial partner, detailed DEM simulations have recently been undertaken of the drilling of agglomerate materials produced by bonding aggregate particles of different sizes. Drilling involves two separate processes: the breakage of the solid material (characterized by its strong adhesive microstructure) into small individual particles by the tip of the drill bit, and the extraction of these individual particles (which form an essentially freely-flowing material, termed "bore dust") by the spiral shaft of the drill bit. These two processes are coupled: the efficiency of breakage by the drill bit tip determines the quantity of material to be transported, while the efficiency of extraction determines the presence of bore dust jamming that can affect the breakage process. The goal of the study is to obtain an increased understanding of each of these two processes, and hence the possibility of optimizing the drill bit shape and the drilling operation.

Aerospace activities
Leyland, Gaffuri, Casagrande, Potter, Sobbia, Savajano, Joshi, Goekce

A broad number of activities have been performed in the context of HISAC, an EC-FP6 project on environmentally friendly high speed aircraft. Work includes: emission analyses, acoustic shielding (with LEMA-STI-EPFL and SMR Bienne), plasma actuators for sonic boom mitigation (with LTT-STI-EPFL and CRPP-SB-EPFL), study of vortical structures and high lift devices over novel leading edge technologies, multi-disciplinary optimisation (with LENI-STI-EPFL), and aerodynamic assessment of wind tunnel and flight shapes.

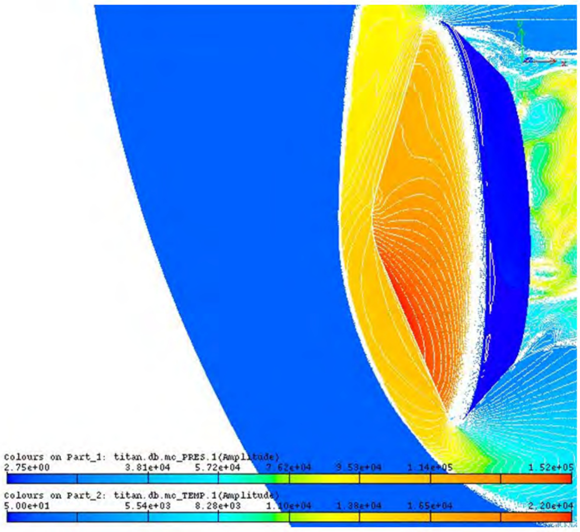


Figure 11: *Titan probe simulation in experimental conditions corresponding to flight aerocapture conditions of the Titan entry.*

In ESA related projects, an aero-thermodynamic campaign was achieved for the IXV project with different degrees of modelling. An aerodynamic and aero-thermodynamic database has been made. Currently, modelling of radiating aero-chemistry flows with gas-surface interaction is being undertaken within ESA-NPI activities. In particular, we are comparing flight and experimental data.

Figure 12: *Vortical structures over experimental model of high speed wing shape at landing conditions.*

Other aerospace projects include: the development of Langmuir probes for shock tube experiments, a continuation of research on radiation probes with University Queensland, Australia, and collaboration with LTT and CRPP on plasma-flow interaction. Furthermore, research on parallel mesh adaptation respecting the geometrical surfaces has recently finished with the PhD Thesis of A. Casagrande.

Developments of tools for the simulations of non-Newtonian flows with the lattice Boltzmann method
Fiétier

A software based on the lattice-Boltzmann Palabos (for Parallel Lattice Boltzmann Solver) tool box (and with former version Open LB) has been developed by Orestis Malaspinas during his Ph.D. Thesis to study the flows of Newtonian, generalized Newtonian (Carreau and power-law fluids) and viscoelastic fluids. Emphasis has been put on the definition of consistent boundary conditions for the various types of fluids and on the implementation of an efficient algorithm for serial and parallel computations. For both types of inelastic and viscoelastic non-Newtonian fluids, the computational model has been validated against various relevant benchmarks (e.g. 4:1 contraction, Poiseuille flow, Taylor-Green vortex, Four-roll mill). Palabos is a free library for lattice Boltzmann simulation written in C++, providing a variety of lattice Boltzmann models, offers a framework for high performance computing with efficient parallelization (good scalability) using the MPI extension and is shared by an increasing community of researchers (http://www.openlb.org/). For viscoelastic fluid flow simulations, a decoupled algorithm using a classical lattice Boltzmann solver for the generalized Navier-Stokes equations and a modified advection-diffusion scheme for the constitutive equation is used. Although only two types of equations have been implemented (Oldroyd-B, FENE-P), extension to other rheological models is straightforward. Members of our laboratory (Jonas Lätt and Orestis Malaspinas) are very active developers of this package. A module enabling one to simulate multi-phase flows with the Open LB package has also been developed by Joris Verschaeve during his Master's thesis. The capability of several models proposed in the literature has been tested on several benchmarks involving the motion of individual drops.

EPFL-LTT: Turbomachinery Laboratory

Post Station 9, CH-1015 Lausanne, Switzerland.

The research scope of LTT includes efforts to increase reliability, efficiency and power output of gas turbines and aero engines. The following research areas are the most important at LTT:

- Fluid-structure interaction at forced response and flutter for turbine and compressor,
- boundary layer control by aspiration in compressors,
- cooling techniques for gas turbine blades,
- blade row interaction,
- shock/boundary layer interaction control using plasma.

Since the retirement of Prof. A. Bölcs in 2002, LTT has been managed by Dr. Peter Ott. On going research projects are summarised below.

Flutter Investigations in Turbines and Compressors

Chenaux, Zanker, Ott

Flutter refers to an interaction between the air flow and the turbomachinery blades that induces structural vibrations. These vibrations can damage and eventually destroy the blading. LTT has investigated the aeroelastic behaviour of several axial turbine and compressor bladings on annular cascades under forced and free vibration. The long-term objective is to be able to identify which flow conditions are susceptible to flutter, as well as which physical mechanisms contribute to this instability. The results are also used to build up the databases of validation cases for the numerical developments.

Through the ERCOFTAC visitors program close contacts with DLR (Deutsches Zentrum für Luft und Raumfahrt) in Göttingen have been established. A model cascade with a special blade suspension for free flutter was designed and manufactured by DLR (Göttingen) and is being tested in the annular test facility of LTT. Unsteady measurements close to and also inside the flutter region were conducted with success. Within the European Research FP7 research project FUTURE one turbine cascade and one compressor cascade will be investigated close to and under flutter conditions.

Boundary Layer Control

Colombo, Charbonnier, Deslot, Ott

Modern gas turbines tend to work with higher temperature and pressure levels in order to obtain a higher overall efficiency. Consequently a higher pressure ratio has to be delivered by the compressor. In order to limit its size, the stage pressure ratio has to be augmented. This implies to increase the load by increasing the deflection and lowering the blade number. The consequently higher pressure gradients tend to make the flow separate.

The presently performed investigation within the FP6 research project NEWAC has the objective to control the boundary layer in order to avoid separation from the airfoil for a maximum range of flow conditions. This is done in the present study via a suction slot on the suction side of the airfoil. The tests are done in the non-rotating annular cascade facility of the laboratory.

Three kinds of blade sets are tested: one baseline set without suction, a second with boundary layer suction and a third one with a reduced number of blades and boundary layer suction. The reference measurements on the cascade without boundary layer control were performed in 2008 in the laboratory's annular cascade with subsonic inlet conditions. During 2009, the cascade with boundary layer suction was tested successfully. In the beginning of 2010 the last cascade will be investigated. Several publications were presented on this subject, e.g. [7].

Heat Transfer and External Cooling of Turbine Blades

Jonsson, Charbonnier

The problem of heat transfer in gas turbines is a central issue of research in turbomachinery. Operating conditions are pushed towards higher pressure and temperature levels, which is favorable for the specific power output and thermal efficiency. Consequently, flow temperatures found at the turbine inlet exceed by far the temperatures supported by the material of the structure. This requires an effective and reliable cooling of all critical components, such as first stage vanes, blades, and end walls. One investigated technique is called film cooling or external cooling. It consists in ejecting coolant air onto the surface through a series of discrete holes. Classical flow measurements (pressure taps on the blading and platforms) are complemented by heat transfer measurements on the blades using the Transient Liquid Crystal Technique. For the platforms, heat transfer measurements can be performed in a steady state manner, but with a limited resolution. Better spatial resolution is achieved by applying a newly developed transient method using electrical heater foils. The method has been validated on a flat plate and compared with numerical results. After that, this new technique has been used for measurements on a contoured film cooled platform and showed good quality results. These tests are performed in the Linear Cascade Test Facility of the laboratory. Different blade and channel geometries have been investigated with several film cooling arrangements at sub- and transonic flow conditions. In collaboration within a European Project (TATEF2) a turbine vane cascade with intensively cooled vanes and platforms was tested [2], [3], [6]. CFD was carried out in order to analyze the obtained results and in order to study the accuracy of different codes. [1], [4], [8]. The following figure shows a comparison between measurement and computation for the film cooling effectiveness.

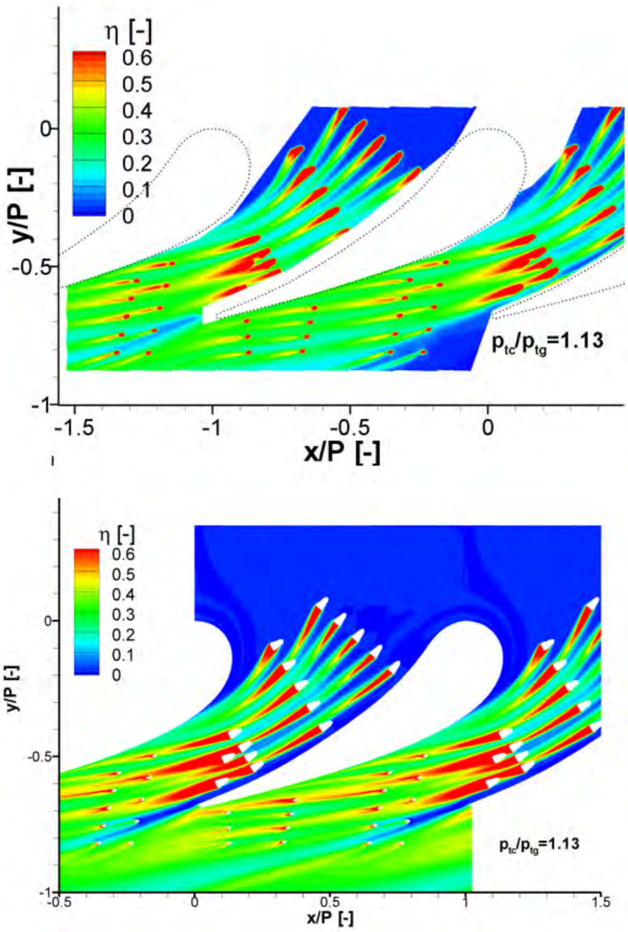


Figure 13: *Measured (top) and computed (below) film cooling effectiveness on platform.*

Pressure Sensitive Paint (PSP) Measuring Technique
Jonsson

This experimental method was developed for turbomachinery applications at the laboratory by a former ERCOFTAC fellow (Dr. P. Steiner). This method allows non-intrusive direct measurement of the 2D surface pressure distribution.

Another development based on Pressure Sensitive Paint is the application onto a model for the determination of the film cooling effectiveness. Further investigations were carried out for combining the Transient Liquid Crystal Technique and PSP techniques in order to improve the accuracy of film cooling measurements.

Blade Row Interaction
Kristukat, Bölcs

In transonic axial compressors the interaction between the bow-shock and the highly loaded Inlet Guide Vane (IGV) introduces an additional loss source: the shock induced boundary layer separation on the IGV.

A project on the rotating axial compressor test facility of the LTT investigated this interaction. Depending on the axial spacing between the IGV and the rotor, the influence of the upstream propagating bow shock on the upstream flow field varies and even acts as a source for forced vibration of the upstream blade row.

The test facility is equipped with a measurement system for the acquisition of unsteady pressures at high frequencies up to 100 kHz. Further on, the test facility provides possibilities for measurements with steady pressure taps, aerodynamic probes and a torque meter.

A PhD thesis comparing both experimental and numerical results was accomplished in 2008 [10].

Influence of a Weakly Ionized Boundary Layer on Transonic and Supersonic Air Flows
Pavon, Goekce, Peschke, Ott

The formation of strong shocks on bodies in transonic and supersonic air flows (for example around aircraft wings) is a large source of energy loss. In this last decade, a new area in science has emerged, which proposes the use of plasma fields as a way to modify airflow properties. There is evidence that weak ionization of gas can influence shock waves around test objects. In this joint LTT, LIN (Numerical Engineering Laboratory, EPFL) and CRPP (Plasma Physics Research Center, EPFL) project, the objective is to investigate the effects of a surface Dielectric Barrier Discharge (DBD) on the shape, strength and absorption of the shock envelopes, and to model the physical phenomena involved. The developments of the system aim at sonic boom alleviation and drag reduction on aircraft.

A PhD work was successfully finished in 2008 [11] demonstrating that a DBD can be formed and sustained in a transonic air flow up to Mach numbers of at least 1.1. The interactions between these high speed air flows and the plasma have been studied in detail [5], [9]. The results offer new perspectives for the use of DBD in transonic and supersonic gas flows and their applications to flow control on aircrafts and to plasma-assisted combustion. Presently a follow-up project is running financed by the Swiss National Funds, and also the European FP7 project PlasmAero was recently started.

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ETHZ-CSE: Computational Science and Engineering Laboratory

CAB H 69.2, Universitätstrasse 6, CH-8092, Switzerland.

We develop computational tools for the study of complex scientific and engineering problems. Research areas in the laboratory include multiscale particle methods and derandomized optimization algorithms applied to areas of Life Sciences, Fluid Mechanics, Nanotechnology and their interfaces. We emphasize the parallel development of algorithms,software, hardware and applications while we consider indispensable the interactions with our collaborators.

Particles for multiphysics simulations

The simulation of the motion of interacting particles is a deceivingly simple, yet powerful and natural, method for exploring physical systems as diverse as planetary dark matter and proteins, unsteady separated flows, and plasmas. Particles can be viewed as objects carrying a physical property of a system, that is being simulated through the evolution of the trajectories and the evolution of the properties carried by the particles.

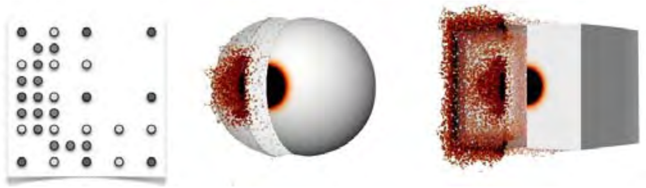

Figure 14: *(left) Principle of wavelet based adaptation in 2D: after the data is compressed on a regular grid, particles are created with appropriate core sizes. (middle and right) Particle-Wavelet method as extended to the simulation of transport problems on implicit geometries: the particles adapt to small scales in both the function and the geometry on which it is defined.*

Lagrangian descriptions of discrete and continuum systems

Simulations of continuum and molecular phenomena can be formulated by following the motion of interacting particles that carry the physical properties of the flow. In a continuum, these properties can be macroscopic, e.g. density, momentum, vorticity. for a discrete system, such as atoms, we will consider mass, velocity and electric charge.

Continuum systems, particle methods and computational challenges We study Lagrangian, multiresolution, particle methods for the simulation of continuous systems with an emphasis on fluid mechanics applications. Particle methods, such as Smoothed Particle Hydrodynamics and Vortex Methods enjoy the inherent robustness and adaptivity of Lagrangian methods. At the same time though, uncontrolled particle distortion leads to degraded accuracy and the computation of of spatial differential operators on the particles is highly inefficient. For these reasons, we develop hybrid particle-mesh methodologies which periodically reinitialize the particle positions through high order, moment conserving interpolation and use the mesh for efficient computations of differential operators.

Wavelet Particle Methods

We combine the adaptivity of Lagrangian particle methods with the multiresolution capabilities of wavelets. The goal is the achievement of high accuracy while minimizing the amount of computational elements. We rely on the remeshing of the particle methods in order to introduce multiresolution capabilities in a systematic framework. We utilize grids of variable resolutions as dictated by the wavelet analysis of the fields carried by the particles. The key computational challenge for this formulation is the processing and the communication patterns between the computational elements.

Accelerated Stochastic Simulation Algorithms

Stochastic simulations of reaction-diffusion processes are frequently used for the modeling of physical phenomena ranging from biology and social sciences to ecosystems and materials processing. In this work we focus on the stochastic modeling and simulation of spatial dynamics of chemical kinetics intrinsic to physical phenomena ranging from morphogenesis and pedestrian traffic to epitaxial growth and epidemics.

Atomistic-Continuum Coupling for Liquids

Nanofluidics deals with the study of fluid flows inside and outside nanostructures. Nanoscale flows are often embedded in larger scale systems, when for example nanofluidic channels interface microfluidic domains. Despite the success of atomistic simulation models (like Molecular Dynamics (MD)), their limitations in accessible length and time scales are stringent and allow only the analysis of elementary systems and for short times. As fully atomistic simulations are prohibitively expensive, purely continuum approaches are not possible due to the lack of the correct boundary conditions for the continuum solver (no-slip boundary condition may be not valid at the nanoscale)

Hybrid atomistic-continuum simulations are necessary to study large systems for reasonable times. We develop novel computational concepts based on dynamic control theory for the exchange of information between atomistic and continuum descriptions

Derandomized Evolution Strategies and Local Learning

We develop Evolution Strategies (ES) for Optimization coupled with Local Learning models to tackle problems with expensive cost functions. ES are a class Bioinspired optimization Algorithms that mimic natural processes to find optimal designs. In the successful translation of the natural evolution process into efficient and robust computer algorithms, model building plays a central role. Local meta-models are used to replace costly evaluations of the objective function by cheap estimates. We investigate and enhance ESs and we apply them to challenging real world problems.

Virus Traffic

All known cellular cargos including protein, vesicles, organelles and pathogens are bidirectionally transported by molecular motors on microtubules to the cell center and periphery. However, it is unknown if the motor activity is regulated or works stochastically. Viruses are simple cargos, and their replication requires dynein and kinesin mediated transport. Here we carried out live cell microscopy, single virus tracking and trajectory segmentation as a basis to computationally model bidirectional transport of human adenovirus type 2 on microtubules.

Systems Biology of the Drosophila Wing

The genetic program that directs the growth and precise shape of an organ is not known. Developmental genetics has provided us with the toolkit (morphogens, transcription factors etc.) that is used to make an organ but we do not know how this toolkit is used to make a Drosophila wing of reproducible size and form. The answer to this question requires the quantitative description of wing development at a systems level and the ability to simulate the process at the molecular, cellular, and tissue level.

Tumor Induced Angiogenesis

Tumor induced sprouting angiogenesis is the process of new capillary growth from an existing vasculature, induced by tumor cells that have the Şangiogenic switchŤ turned on. Vascular endothelial growth factors (VEGF) released by tumor cells diffuse through the extracellular Matrix and stimulate endothelial cells lining existing vessels in the proximity of the tumor to form sprouts. As the newly formed sprout tips migrate through the ECM, defining the morphology of the gradients determine their migration paths.

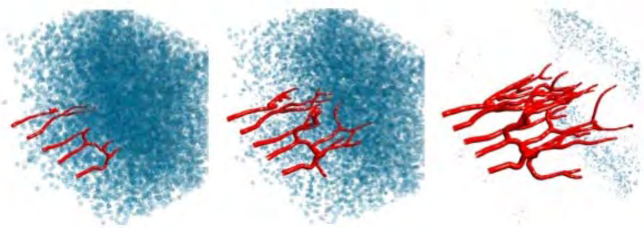

Figure 15: *Simulation of blood vessel growth (red) in the presence of matrix-bound VEGF (blue).*

Vortex dynamics

Hurricanes, tornadoes, water swirling down a drain are all examples of vortices. Vortices are needed to close the valves at every beat of our heart, to mix fast milk and coffee and they are responsible for bird and airplane flight.

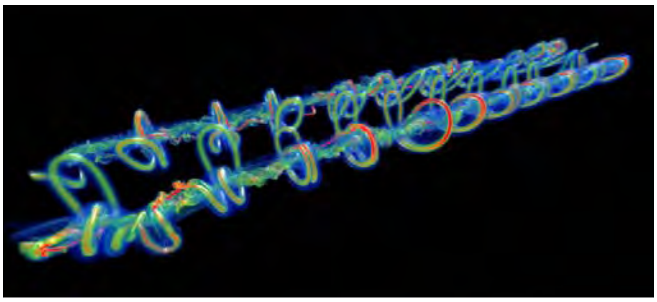

Figure 16: *Simulation of a medium-wavelength instability in a 4-vortex wake: vorticity magnitude.*

Bio-Inspired Flying and Swimming Devices

We study archetypal types of flyers and swimmers found in nature ranging from the microscale (pollen and bacteria) to the macroscale level (birds and eels). These forms serve for inspiration of engineering devices that can be in turn optimized using bioinspired algorithms.

Cavitation

Cavitation is defined as the breakdown of a liquid medium and occurrence of cavities and is of high importance in a wide range of applications from engineering (turbomachinery) to medicine (lithotripsy).

In collaboration with the Laboratory for Hydraulic Machinery (Prof. Avellan, EPFL) we conduct a computational/experimental study of cavitation in hydraulic turbomachinery responsible for operating instabilities, erosion, noise and vibration. Under the so-called static conditions, vapor is formed when the pressure drops below the vapor pressure. Hydrodynamic cavitation is the onset of such cavities inside a liquid flow as the local high velocities induce low pressure. The pressure threshold under which the liquid cohesion is no longer guaranteed would ideally be defined from a microscopic point of view although in practice, it is more convenient to use macroscopic fluid properties. Cavitation-induced bubbles collapse and generate jets, shock waves and pressure oscillations when subjected to high pressures.

Fullerenes in liquids

Fullerenes are a family of carbon allotropes, molecules composed entirely of carbon, which form hollow spheres, ellipsoids, tubes, or planes. Their unique physical properties make them excellent candidates for applications ranging from gas sensors to targeted drug design and delivery. We focus on the interaction of fullerenes with fluids as we are interested in the design of nanosensors and actuators. Of particular interest is the interaction of fullerenes with water and biomolecules for bio-nanotechnology applications.

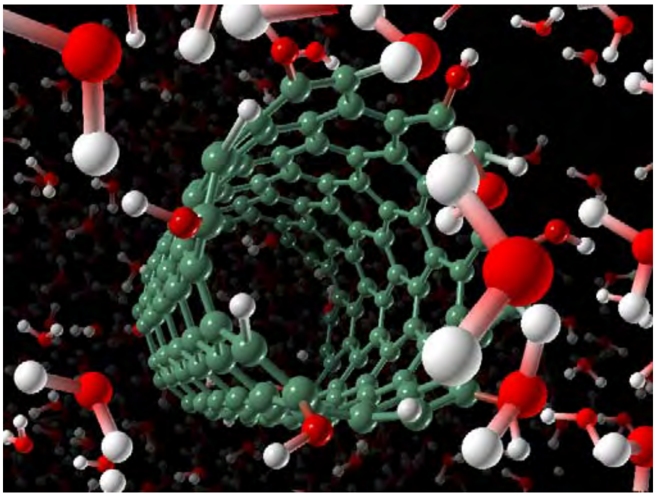

Figure 17: *Water Transport in CNTs.*

Nanoscale Heat Transfer

The transport processes of mass, momentum, and heat in nanoscale systems are dominated by the large surface-to-volume ratio inherent at this length scale. To understand these processes we have to extend our macroscale models to include the effect of the micro structure eg.: surface chemistry, atomic scale corrugation, and fluid- and and solid impurities. In this research we study nanoscale heat transfer and we apply temperature gradients to drive solid and fluid nanoparticles.

ETHZ-IPE: Institute for Process Engineering

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This report summarizes the present research activities of the laboratory for Transport Processes and Reactions at the ETHZ's Institute of Process Engineering under the directorship of Prof. Ph. Rudolf von Rohr. As far as the topics of ERCOFTAC are concerned, the research involving fundamental and applied studies on multiphase flows, and turbulent mixing, are of particular interest.

Transport mechanisms and large-scale structures in narrow channels

Zenklusen, Rudolf von Rohr

Flow situations in process and chemical engineering are often characterized by high Reynolds numbers, complex wall geometries, transport of scalars and by the presence of multiple phases. Most of the resulting transport problems are still described by empirical correlations, which lack in generality. On the other hand, computation of these transport problems is often not possible due to enormous computational costs or the lack of appropriate models. Fundamental understanding of the present transport mechanisms is an absolute necessity for product quality, reduction of by- products and for ecological and cost arguments.

In previous works [1-4] of our institute, flows over wavy walls with additional scalar transport (mass and heat transfer) were studied as flow situations. Flows over wavy walls reveal coherent, large-scale structures, which govern heat and species transport in such flows. Furthermore these coherent, large-scale structures are sensitive to alterations in the structure of wavy walls.

In our institute, continuous mini reaction systems in the millimetre scale are investigated, with the purpose of combining the advantages of micro-reactors (narrow residence time distributions, uniform temperature distributions) with the advantage of batch reactors (throughput).

Based on the knowledge of the above described large-scale structures and the industrial relevance of continuous mini reaction systems, simultaneous momentum and mass transport in narrow channels in the millimetre scale with complex surfaces are studied within this project. First a narrow channel with a wavy bottom is investigated, which provides information about the influence of side walls and top wall on coherent, large-scale structures observed in flows over wavy walls. In a next step the channel is adapted to geometries which correspond to the mentioned continuous mini reaction systems. The findings of these configurations allow describing transport mechanisms and large-scale structures in narrow channels.

Non-intrusive measurement techniques (particle image velocimetry (PIV) and planar laser-induced fluorescence (LIF)) are used to get spatio-temporal information on simultaneous momentum and mass transport. Besides experiments, numerical computations are used to provide more information.

We acknowledge financial support from ETH Zurich and the Swiss National Science Foundation (SNF)

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[2] N. Kruse, PhD thesis, ETH Zurich, (2005)
[3] C. Wagner, PhD thesis, ETH Zurich, (2007)
[4] S. Kuhn, PhD thesis, ETH Zurich, (2008)

Extraction in Microreactors: Enhanced Mass Transfer by Adding an Inert Gas Phase

Assmann, Desportes, Rudolf von Rohr

On-chip separation of liquids is an essential step in order to realize the continuous operation of microreaction systems. However, it remains challenging, as surface forces dominate over body forces on these length scales ($Bo \ll 1$), so that conventional separation techniques based on gravity cannot be transferd to the microscale. Therefore, novel separation principles have to be exploited, such as separation by capillary forces [1], extraction [1,2,3], and distillation [4].

The efficiency of extraction is influenced by the flow pattern, which determines the prevailing mixing principle [2]. Segmented flow provides a faster mixing, whereas stratified flow is easier to separate [3]. In this work we will apply a novel flow pattern to the liquid extraction of vanillin by adding an inert gas phase to the immiscible liquid phases, such establishing a three-phase flow within a rectangular microchannel. An improved mass transfer between the liquid phases will be demonstrated.

Experiments are being carried out in microstructured devices made of polydimethylsiloxane (PDMS) and glass with a channel cross section of 300 μm x 180 μm. The extraction of vanillin with toluene as organic solvent was selected based on previous experiences in our lab [3]. The extraction efficiency is being determined by GCMS measurements of the toluene phase and UV Vis measurements of the water phase. Due to the hydrophobic wall properties, toluene builds the continuous phase, whereas water and the inert gas are dispersed.

The flow pattern is being determined by stereomicroscope measurements. Therefore the organic phase was colored with Sudan III (red) and the water phase with fluorescein (yellow). Since the continuous phase is distributed as a liquid film on the wall, the three-phase flow pattern provides a larger surface area between the liquid phases, which is one reason for the enhanced mass transfer. Additionally, recirculation within the water slug also improves mixing of the two liquid phases. The μ-PIV result for one water slug is exemplarily shown in the following figure. The slug velocity was subtracted to visualize the secondary flow pattern.

The enhanced mass transport will be demonstrated by applying the novel three phase flow pattern to the extraction of vanillin dissolved in water. The residence time is varied by adjusting the volumetric flow rates. Different reactor designs with different inlet designs, as well as separation strategies for the three phases will be examined. Preliminary experiments at a residence time of 0.55 s and separation by capillary forces provided a $k_L a$-value of 3.5 for segmented two-phase flow and of 4.5 for the presented three-phase flow pattern, supporting our previous statements.

We acknowledge financial support from E. Barell Foundation, Basel, Switzerland.

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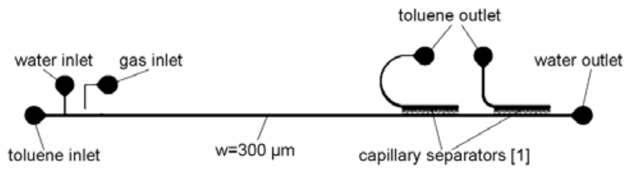

Figure 18: *Channel design of microchemical device used for extraction.*

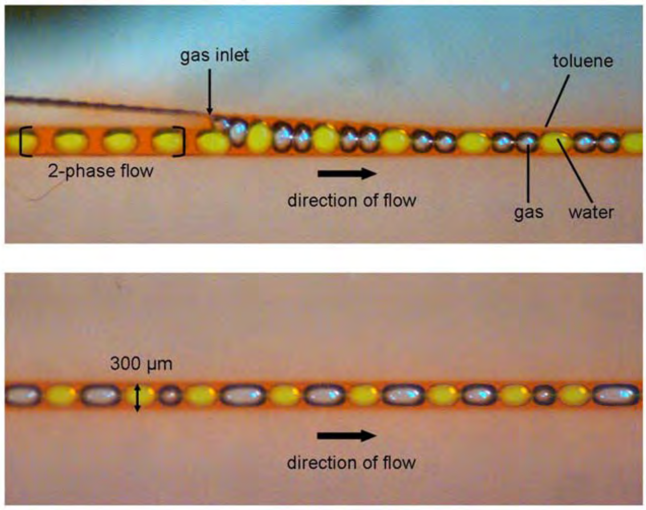

Figure 19: *Stereo microscope images of the liquid-liquid-gas flow pattern. Toluene (red, colored with Sudan red) builds the continuous phase, water (yellow, colored with fluorescein) and the inert gas are dispersed.*

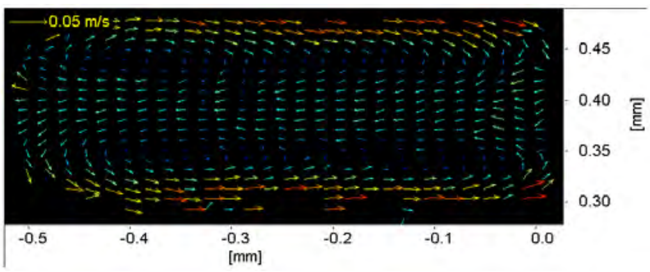

Figure 20: *μ-PIV measurement of the water-slug. Slug velocity was subtracted to visualize the secondary flow pattern. Direction of flow is indicated by arrow in the upper left corner.*

Synthesis of Rubrene Organic Nanocrystals in a 3D Hydrodynamic Focusing Device
Desportes, Rudolf von Rohr

We investigate the synthesis of organic nanocrystals in a 3D hydrodynamic focusing. This reactor is based on the microfabrication of a T or Y-type crossing microchannel molded in PDMS and covered by a glass substrate. A glass capillary, with an outer diameter equal to the channel dimension, is inserted in an open channel. This technique allows to get a 3D focused stream observed from Confocal Laser Scanning Microscopy (CLSM) technique, see following figure. The reaction performed is the non-solvent crystallization of the rubrene. Such fluorescent molecule was chosen because of its fluorescence properties, which allows previous investigations by Fluorescence Lifetime Imaging Microscopy [1]. The results obtained by FLIM have shown a strong kinetic effect of the operating conditions (flow rate conditions) on the crystallization process.

The aim of this project was to check how these operating conditions entail a control of the organic nanoparticles size. The crystallization process and the nanocrystals size are linked to the mixing controlled by diffusion of the water solution flowing from the side channels in the focused stream containing the rubrene dissolved in ethanol/THF mixture solution. The mixing efficiency by diffusion and the mixing uniformity of the aqueous solution within the focused stream were determined from Confocal Laser Scanning Microscopy (CLSM 5 Pascal, Zeiss). To quantify this mixing level the same amount of fluorescein ($1.5\text{x}10^{-4}$ mol.L^{-1}) were dissolved in the water solution with CTACl as a stabilizing agent (10^{-2} mol.L^{-1}) and in the organic solution (THF/ethanol (30/70 vol. fraction)). By flowing separately these two solutions in the microreactor, the fluorescence intensity measured for the aqueous solution of fluorescein is 10 times higher than those of the organic solution. Due to the different fluorescence intensity the dye will act like a label of the mixing degree of water into the organic focused stream. The aqueous solution flows from the side channels with a volumetric flow rate (Qs) chosen from 5 to 30 μL.min^{-1}. The organic solution flows from the capillary with a volumetric flow rate (Qc) in the range of 1 to 3 ţL.min-1. The excitation of the fluorescent dye, fluorescein, is done by an Argon ion laser at 488 nm wavelength and a high pass filter allows the detection of the emitted light. A 1 μm thick optical slice was imaged by scanning the channel perpendicularly to the cross section over the width of the channel and over 30 μm along the channel. The resolution of each slice was 3.3 μm^2 per pixel. The acquisition time for one pixel was 3.6 μs and eight measurements per pixel were averaged for better representation of the focused stream. All the slices obtained from the PDMS top to the glass substrate at the bottom are stacked up. Those stacks were built up at different positions along the main channel. Each stack allows us to reconstruct at each position a picture of the cross section with the intensity averaged over the 30 μm length of the stack.

The efficiency of the diffusion process was quantified within a ROI which fits the shape of the focused stream at the channel intersection. This ROI was kept at different position along the main channel. From the fluorescence intensity measurements, the average water fraction (X_{mean}), and its standard deviation (σ) are determined over each analyzed ROI. The minimum intensity (I_{min}) and the maximum intensity (I_{max}) were determined by flowing in the channel respectively the organic solution (ethanol/THF mixture) and the aqueous solution), both containing the dye. The maximum water fraction (X_{max}) is deducted from the I_{max}. From those data the mixing efficiency (M.E) and the mixing uniformity or mixing index (M.I) were then determined. Experimental results showed that the mixing efficiency and a high mixing quality (M.I=0.1) are reached faster by increasing the side flow rate to the capillary flow rate ratio.

Furthermore, the synthesis of rubrene crystals were performed under a variety of flow rates conditions. We showed that, by increasing the focusing ratio (from 5 to 40), the mean size of nanocrystals is decreasing (from 100 nm to 45 nm). Characterization of mixing allowed a better understanding of the nanocrystals synthesis: a fast supersaturation (high mixing efficiency in a short time) induces the generation of numerous nuclei, which limits the crystal growth. The 3D hydrodynamic focusing microreactor was efficient to produce, without clogging, organic nanoparticles with controlled size [2].

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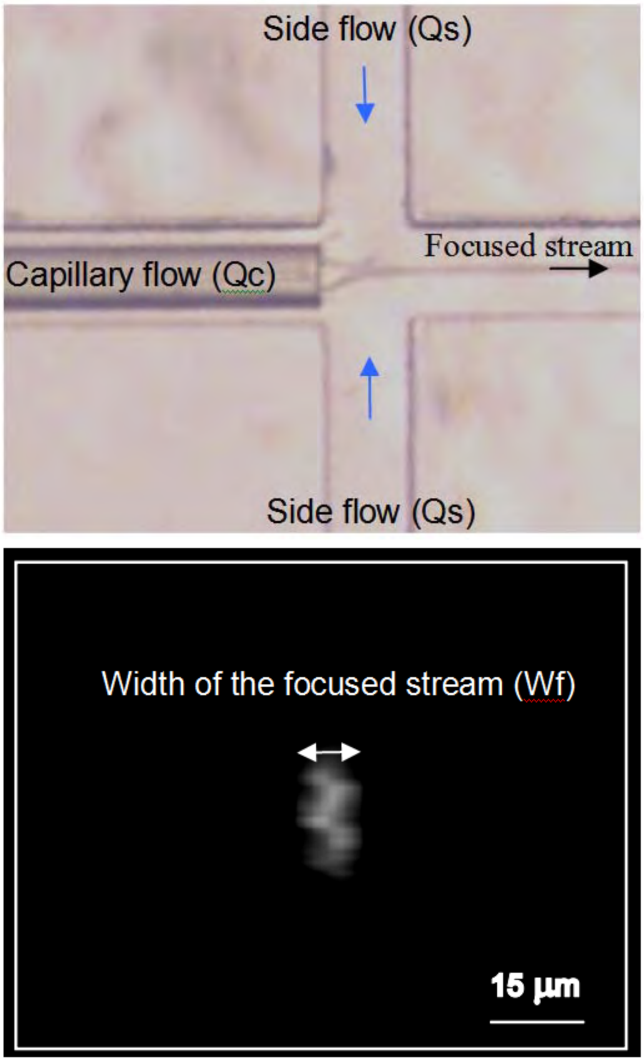

Figure 21: *(top) T-type microdevice coupled with capillary. The focused stream appears in the middle on the main channel. (bottom) Sample image from CSLM of the cross section of the main channel. The focused stream labelled by a fluorescent dye and the two side flow are water. The rectangle with full white lines represents the microchannel walls.*

New plug flow reactor concept for fast mixing and enhanced heat transfer

Hutter, Rudolf von Rohr

In the industry large scale equipments, predominantly dis- or semicontinuous batch processes are still used due to the economy of scale. For chemical plants the investment costs are in general proportional to the capacity to the power of 0.5 to 0.7. The growing need of energy saving and sustainable production leads to a demand on small scale continuous devices as the recuperation of energy is more efficient and mass and heat transfer is strongly enhanced. In micro reaction systems the scale up is mostly realized by numbering up individual micro reactors. For a large-scale production this is not an economical solution. But beside the huge pressure drop and the predominant laminar flow within Microsystems the small scales offer many advantages. Our approach is to use high porous micro structured inserts for plug flow reactors in the millimeter range. The system has to offer the possibility of high throughput (liquid flow rate up to 2.5 l/min) at comparable small pressure drop. A huge potential arises from open cell metal foams. Their outstanding thermal properties led us to the design of a new plug flow reactor concept in cooperation with the industrial partners DSM Nutritional and Premex Reactor AG. The system, which complies with a so called heat exchanger reactor [1], offers an alternative approach to discontinuous processing. The porosity of metal foam is typically larger then 85%. This property combined with a high specific surface of up to the order of $10^4 \mathrm{m}^2/\mathrm{m}^3$ is a major advantage compared to common packing materials and fixed beds. In contrast to the excellent heat transfer characteristics of open celled metal foam [2] the mass transfer [3] and the hydrodynamic flow behavior [4] was investigated only by few researchers. Within this study we ascertain metal foam from m-pore GmBH (Germany) of 20, 30 and 45 ppi concerning mixing efficiency in an application-oriented assembly with respect to the use as static mixing elements in continuous plug flow reactors.

In the first investigated design the reactor consists of a pipe with an inner diameter of 7mm and commercially available metal foam inserts with different pore sizes of 20, 30 and 45 ppi. Simultaneous PIV and LIF measurements were performed in orthogonal planes normal to the radial and axial direction downstream of a foam element of 50mm length. The investigated Reynolds numbers range from 600 to 7600 based on the empty tube diameter. We investigated the influence of the pore sizes on the scalar mixing efficiency and compared the results to the reference empty tube case. An increased turbulence intensity caused by the metal foam was observed over the whole range of Reynolds numbers. The increased radial velocities lead to an enhanced mixing performance. Coefficients of variation in the order of 0.1 were achieved.

In a second design the idea of metal foam was developed further to a reactor with a clearly defined geometry manufactured by Selective Laser Sintering which is a common method in the field of rapid prototyping. The reactor has the advantage of a fixed connection of the periodic structured porous media with the tube wall as it is sintered as one single part. This results in an enhanced heat transfer which was shown in different experiments. The possibility of Simulations and the comparison to experimental results allows optimizing the geometry for a given application. To perform optical measurements the reactor was also build up by stereo lithography using a transparent material. We could show that the turbulent kinetic energies measured downstream the porous element were strongly increased compared to the commercial metal foam. The influence of the geometry is in addition investigated by means of a Large Eddy Simulation and will be compared to experimental results.

We gratefully acknowledge financial support from the Swiss Confederation's innovation promotion agency (CTI) in cooperation with DSM Nutritional Products and Premex Reactor AG.

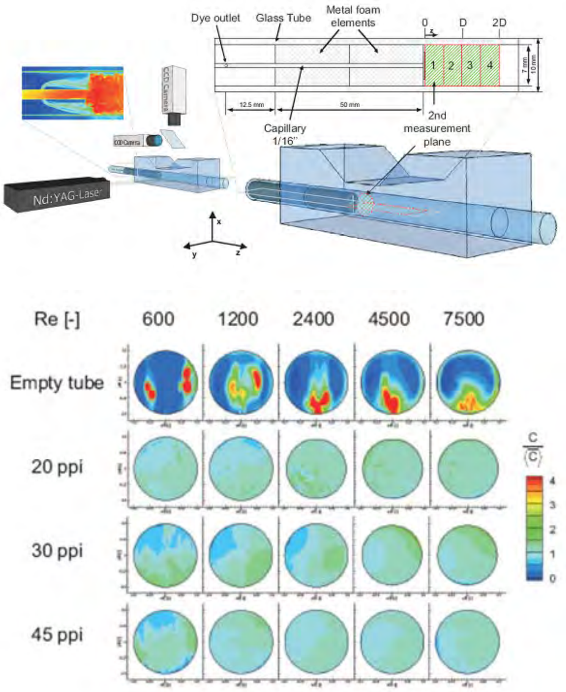

Figure 22: *Experimental Setup (top) for simultaneous PIV/PLIF measurements and mean concentration fields (bottom) of an aqueous Rhodamine B tracer dye downstream metal foam elements of different pore sizes in comparison to the empty tube reference cases for different Reynolds numbers.*

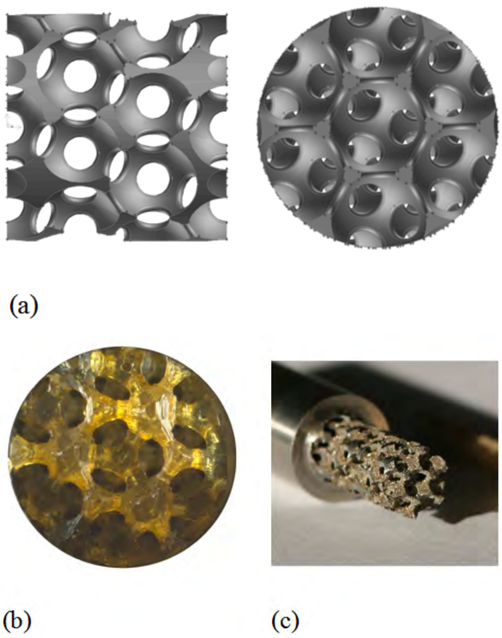

Figure 23: *CAD view of structured porous media (a) in comparison to the transparent reactor manufactured by stereo lithography (b) and the laser sintered stainless steel reactor (c).*

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ETHZ-LAV: Aerothermochemistry and Combustion Systems Laboratory

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The computational work at the Aerothermochemistry and Combustion Systems Laboratory (LAV) is directed towards the direct numerical simulation of reactive flows using a spectral element low Mach number solver co-developed in collaboration with the Argonne National Laboratory, U.S.A, the computational reactive fluid dynamics (CRFD) of a broad range of combustion related applications, and the development and application of lattice Boltzmann models and tools.

The *engine CRFD group* of the Aerothermochemistry and Combustion Systems laboratory (LAV) is tackling a broad range of combustion related phenomena. These include upstream processes such as atomisation and breakup of liquid fuel jets, evaporation and mixture formation and spray evolution; combustion model development with emphasis on turbulence-chemistry interaction; mechanism development/reduction for designer fuels specifically tailored to HCCI-type processes and, finally, modelling of exhaust gas after-treatment systems employing selective catalytic reduction (SCR).

Some of the current research activities of LAV are summarised below:

Autoignition of a hydrogen jet in co-flowing hot turbulent air

Further development of next generation low-emission devices in terms of enhanced performance and efficiency and reduced pollutant emissions can be significantly aided by the ability to better understand and predict autoignition in the presence of fluctuations of velocity, temperature and composition. Recent experiments of axisymmetric fuel plumes in turbulent co-flows of hot air in a duct have shown that autoignition kernels appeared at random locations and instances. Unsteady flamelets propagated from these locations into the surrounding unburned inhomogeneous mixture either (a) extinguishing in the neighborhood of the original autoignition site (*random spots* regime), (b) propagating upstream to create a lifted flame (*lifted flame* regime) for high enough co-flow velocities and/or low enough temperatures of the incoming streams, or (c) a non-premixed flame propagating to the nozzle rim to create an anchored (*flashback* regime) for low enough air velocities/high enough temperature.

Guided by the experimental work, direct numerical simulations with detailed chemistry and transport are used to study autoignition spot characteristics in the presence of strong convection and the balance between autoignition and flame propagation that sometimes results in overall flame establishment, see figure below.

The project is funded by the Swiss Federal Institute of Technology (ETH grant number TH-21-06-3).

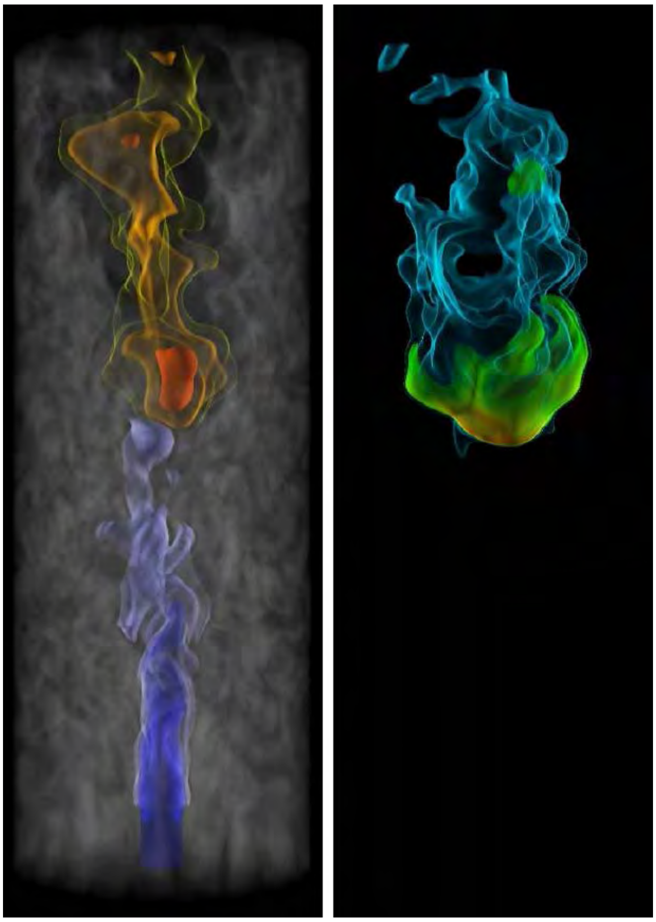

Figure 24: *Autoignition of a hydrogen jet in a hot turbulent air co-flowing stream . Volume renderings of (left) temperature showing the fuel stream (T=857K, blue), the hot air stream (955K, gray) and two ignition kernels (orange) (right) mass fraction distribution of the hydroperoxy radical (HO2).*

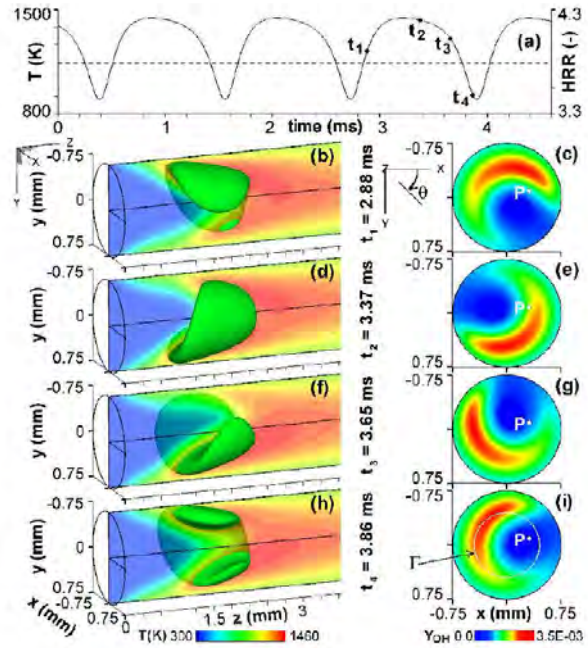

Figure 25: *Clockwise spinning flame at inflow velocity 150 cm/s in a d = 1.5mm tube: (a) time history of temperature (solid line) at the reference point P = (0.3, 0.1, 2.06) mm, and integral heat release rate HRR (dashed line); (b, d, f, h) iso-surfaces of OH mass fraction $Y_{OH} = 1.7x10^{-3}$, and temperature iso-contours on the y-z plane at the four times t_1 to t_4; (c, e, g, i) iso-contours of Y_{OH} on the $x-y$ plane at $z = 1.5mm$ at t_1 to t_4.*

Dynamics of premixed flames in inert and catalytic channels and ducts

Combustion at the micro- (sub-millimeter range) and meso-scale (millimeter range) has attracted increased interest during the last few years in attempts to harness the high specific energy of fuels in miniaturized devices for portable power generation. Progress in the fundamental knowledge of combustion at these scales and in the understanding of reactor thermal management is essential for the further development of such systems.

The dynamics of lean premixed hydrogen flames was studied using numerical simulations with detailed kinetics and transport in two- [1, 2] and three-dimensional [5] geometries. The possibility to suppress the instabilities by covering the walls with a predetermined catalyst load was also addressed [3].

In 3-D tubes, and depending of the tube diameter, axisymmetric and non-axisymmetric, steady and and unsteady combustion modes are observed in the narrow tube. As the inflow velocity of the incoming mixture is increased, these modes include steady mild combustion, oscillatory ignition/extinction, steady closed and open axisymmetric flames, steady non-axisymmetric flames, and azimuthally spinning flames, see figure below. Some of the modes are found to co-exist over extended ranges of inflow velocities.

The effect of channel height, inflow velocity and wall temperature on the dynamics and stability of unity Lewis number premixed flames in channels with specified wall temperature was also investigated with steady and transient numerical simulations using a two-dimensional thermo-diffusive model. The simplified model was capable of capturing many of the transitions and the combustion modes observed experimentally and in direct numerical simulations in micro- and meso-scale channels, indicating that the thermal flame/wall interaction was the mechanism leading to the observed flame instabilities [4]. The project was funded by the Swiss National Science Foundation (SNF project number 200021-109398).

Three-dimensional simulations of cellular non-premixed jet flames

The formation, dynamics and structure of cellular flames in circular non- premixed jets were examined with three-dimensional numerical simulations incorporating detailed descriptions of chemistry and transport. Similar to experiments reported in the literature, CO2-diluted hydrogen in diluted or pure oxygen co-flowing streams in the proximity of the extinction limit were considered. As in the experiments, several preferred cellular states were found to co-exist with the particular state realized depending on initial conditions as well as on the jet characteristics, see figure below. The simulations provided additionally the temporal transitions to different stationary or rotating cellular flames, their detailed structure, and the dependence of the scaling of the realized number of cells with the vorticity thickness [6]. The project was funded by the Swiss National Science Foundation (SNF project number200021-101976).

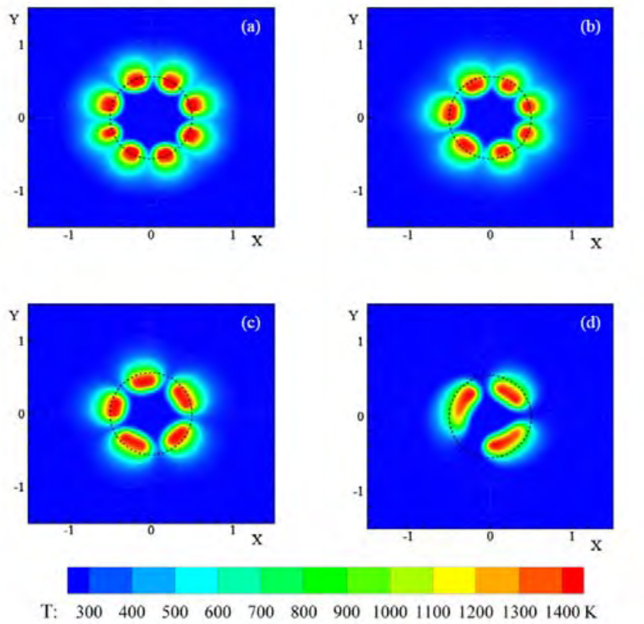

Figure 26: *(a) to (d): Temperature iso-contours on the plane 0.5d_j above the nozzle for the inlet velocity profiles P_1 to P_4, respectively. (Jet: $u_j = 37.7 cm/s$, $X_{H2} = 0.19$; co-flow: $u_c = 4.66 cm/s$, $X_{O2} = 1.0$). Nozzle location marked by the dashed circle.*

Lattice Boltzmann method for simulations of fluid turbulence

A new theory of higher-order lattice Boltzmann (LB) models is proposed and elaborated in detail. A general theory of the construction of lattice Boltzmann models as an approximation to the Boltzmann equation is presented. New lattices are found in all three dimensions and are classified according to their accuracy. The efficiency and accuracy of the new lattices is demonstrated via simulations in all three dimensions.

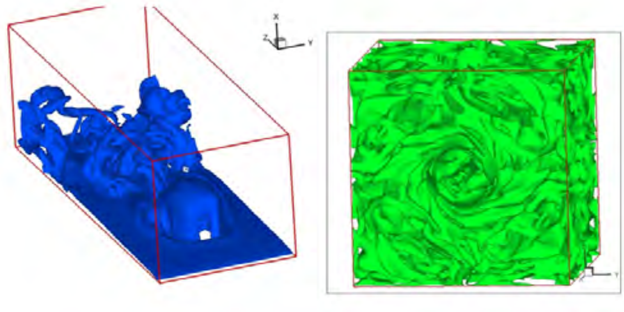

Figure 27: *Lattice Boltzmann (Left) simulation of flow past a cube placed on a surface and (right) simulation of turbulent Kida Vortex flow.*

Generalized Maxwell distribution function is derived analytically for the lattice Boltzmann method. All the previously introduced equilibria for LB are found as special cases of the generalized Maxwellian. The generalized Maxwellian is used to derive a different class of multiple relaxation-time LB models and prove its entropy principle (H theorem).

Three-dimensional numerical simulations of benchmark turbulent Kida Vortex flow, using a new high-order lattice Boltzmann models were performed. Extensive comparisons of the results obtained using LB with results from a reference spectral element method simulations are reported. It is demonstrated that the lattice Boltzmann method can be an efficient alternative as it quantitatively captures the most important features of fluid turbulence and compares well with results from high order direct numerical simulations.

Development of *lumped* mechanism for HCCI and *designer* fuels

In the framework of the large FVV cluster project *Kraftstoffkennzahlen*, involving 15 Universities and a number of automotive and energy companies, the activities are directed at defining fuel indices to describe the suitability for a defined range of standard fuels as well as tailored designer fuels for use in homogeneous charge compression ignition (HCCI) engine operation. Under such engine conditions, the low temperature and negative temperature dependence of fuels exhibiting two-stage ignition are of particular interest. Therefore, several existing detailed, skeletal and reduced mechanisms are analysed and a comparison with more phenomenological approaches is carried out. Experimental data from a shock-tube operated at one of the partner Universities is used for validation; variations in the operating conditions include pressure, temperature, fuel type, equivalence ratio as well as the rate of exhaust gas recirculation (EGR). Developments towards a lumped, universal phenomenological description which can be used for the large number of fuels of interest, and which has the potential for inclusion in 3D-CRFD have been presented in [7]. Good agreement has been demonstrated for individual conditions as well as for a wide range of conditions.

Modelling of catalytic channels for selective catalytic reduction of NOx

In an effort to lower NOx exhaust emission from Diesel engines, the reduction of NO by means of SCR is a very promising technique. This sub-task of the *CCEM-NEADS* project - a larger collaboration involving several laboratories of PSI, EMPA and LAV - aims at modelling the flow inside single catalytic channels and the processes occurring on the catalyst surface, viz. adsorption/desorption of species, intraporous diffusion and heterogeneous chemistry. A broad range of experimental data provided by the PSI Exhaust Gas Aftertreatment group for steady and transient operation has been used to develop and validate a 1D+1D channel model [8]; the following figure shows an example for the response in the conversion rates of NO and NO2 to transient ammonia inlet conditions.

In mobile applications, difficulties associated with the storage of the volatile ammonia have resulted in the common adoption of storage of an aqueous urea solution instead. Therefore, following a first study in [9], in a next step the accurate dosing, atomisation, evaporation as well as the modelling of thermolysis and hydrolysis processes will be investigated in more detail.

This project is funded by the Swiss Competence Centre for Energy and Mobility (CCEM project NEADS) and by the Swiss Federal Office of Energy (BfE grant no. 102859).

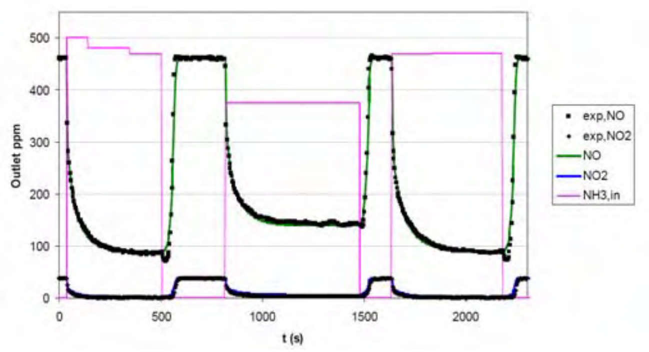

Figure 28: *NO and NO2 reduction at a hourly gas space velocity of 50000 at 300C.*

Assessment of spray models for injection configurations with marine engine dimensions and conditions

Task 2.1 of the *HERCULES beta* project, in the sustainable surface transport of the seventh framework programme (FP7) of the EU, seeks to improve simulation tools for large marine engine development. Experimental data from a combustion chamber with marine engine dimensions is used to validate models for spray atomisation, droplet secondary breakup, combustion and, finally, emission models.

In a first step, the existing models which have been developed over the years for injection configurations of much smaller dimensions are assessed, in a first stage with special emphasis on the evolution of the spray morphology (as shown in the following figure) [10] , which have been presented in [11]. Various short-comings have already been identified and developments are underway to address these issues [12].

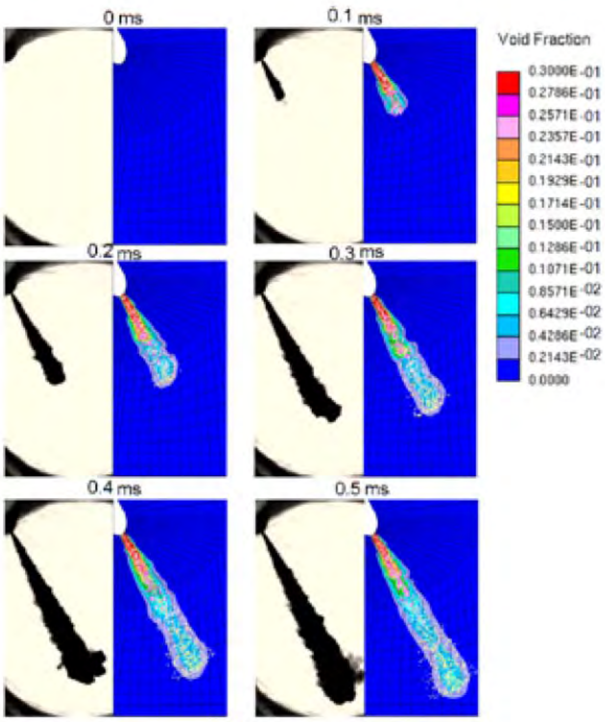

Figure 29: *Comparison of simulated vs. experimental spray penetration.*

Simulation of methane direct injection for turbocharged premixed engines

In the frame of the *CLEVER* project, which is a collaboration between LAV, the institute for dynamic systems and controls (ICSD) of ETH and EMPA. In an effort to reduce CO2 output of passenger car engines, a gasoline engine is converted to direct injection of methane and combined with turbo-charging, Miller valve timing and hybridisation. A broad range of turbo-chargers and valve timing strategies have been compared by employing process simulation tools, which have been presented in [13]. Deviations in cylinder-to-cylinder volumetric efficiencies and flow conditions inside the intake manifold have been studied by means of coupled 1D/3D CFD calculations. First 3D-CFD simulations of the complete engine geometry including moving valves have been carried out. Further efforts in this field will address in-cylinder mixing and the optimisation of timing and geometric orientation of the gas injection valve, aimed at improving the homogeneity of the charge.

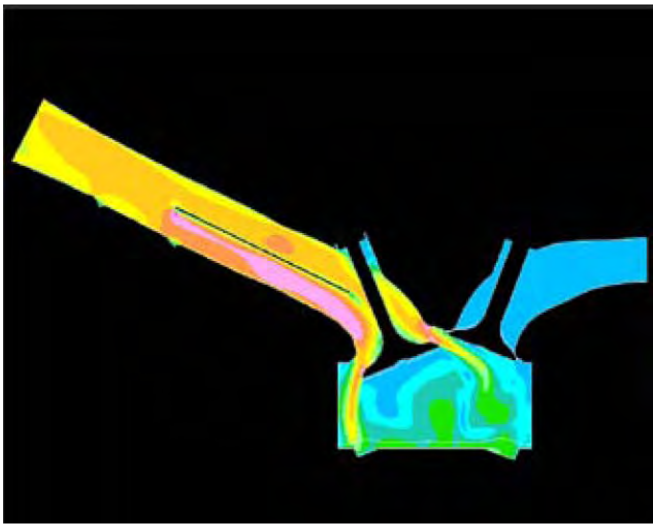

Figure 30: *Velocity magnitude at 430 degree crank angle with open tumble flap.*

The project is funded by a variety of Swiss Federal Agencies (BfE, BAFU, Novatlantis, energie-CH) and German automotive/energy companies (BOSCH, DVGW, Hoerbiger, VW, SVGW).

Mixture formation in Diesel piloted *dual-fuel* engines

Ignition of a homogeneous gas-mixture by injection and ignition of a small amount of liquid fuel (pilot injection), is a complex process which is not fully understood and still largely optimized by trial-and-error procedures. The main objective of this FVV-project, see e.g. [14], is to carry out a detailed analysis of the main processes of ignition and combustion induced by pilot injections of liquid fuels. Therefore, a systematic investigation of the ignition behaviour and the following homogeneous flame propagation by means of a detailed examination of the reaction kinetics is necessary.

Since the pilot spray is injected in an atmosphere containing hydrocarbons (lean premixed methane), knowledge concerning the state of mixing of the pilot fuel with methane is essential. A combined λ_{tot} for both the fuels can be determined for every cell of the computational domain thus providing time resolved information on the amount of fuel which can be burnt dependent on the ignition delay.

Combustion modelling with Conditional Moment Closure

Modelling efforts aimed at improving predictions for auto-igniting sprays have been further validated in terms of predictions of heat release rate and ignition location by means of a closed combustion chamber with optical access. The study also assesses the sensitivity with respect to the choice of the chemical mechanism as well as spray modelling options and have all been published in [15].

The same numerical platform has been used to study a broad range of operating conditions of a heavy-duty Diesel engine; validation criteria include pressure and heat release rate evolution as well as trends for NO engine out emissions as published in [16].

This project is funded by the Swiss Competence Centre for Energy and Mobility (CCEM project *CeLaDE*) and by the Swiss Federal Office of Energy (BfE grant no. 102688).

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PSI - Combustion Fundamentals Group

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Mesoscale modeling of transport phenomena in fuel cell systems and catalytic microreactors

Prasianakis, Mantzaras

The main goal is to develop an advanced numerical tool for modeling key microscale processes occurring in both thermochemical and electrochemical advanced energy conversion systems (solid oxide fuel cells, SOFCs, polymer electrolyte fuel cells, PEFCs, microcombustors, etc). In such systems, complex phenomena are acting at different time scales (from microseconds for the chemical time scales to seconds for thermal conduction in the solid) and length scales (from microns in the pores of a PEFC diffusion barrier layer or in the washcoat of a catalytic combustor, to centimeters in fuel cell stacks or microreactors). Moreover, the associated small sizes (porous electrode structures in fuel cells, porous catalytic layers in combustion systems, etc.) necessitate the construction of specialized models since classical continuum approaches (using Navier Stokes flow equations) are not valid at very small scales. The lattice Boltzmann (LB) method is the appropriate candidate for this kind of micro/meso scale problems. The development of an advanced LB model accounting for multicomponent, reacting, non isothermal and complex geometry flows is highly desirable.

Lattice Boltzmann method

The lattice Boltzmann method (LB) is based upon the solution of the Boltzmann equation not in its full continuous form, but in a discrete representation through the use of a conveniently selected minimal set of fictitious particles.

Lattice Boltzmann methods have proven suitable to correctly describe slip velocity effects in microflows due to their kinetic origin. Apart form their inherent advantage in the microflow regime, LB methods compete with classical CFD solvers in macroscopic flow problems. The success of LB methods is mainly in the isothermal single component flow description. For non-isothermal flows, as well as for multi-component flows, new models have been recently developed [1-6]. Numerical simulations of a catalytic channel reactor and of the flow through specific structural components of fuel cell systems are presented next.

Catalytic reactor simulations

The study of catalytic micro-reactors is of high importance with applications in portable power units using hydrocarbon fuel. Numerical investigation concerning the ignition and transient response of methane-fueled catalytic micro-reactors is studied by the LB method. Comparison in a regime, wherein the standard CFD methods are valid, has been presented in the following Figures.

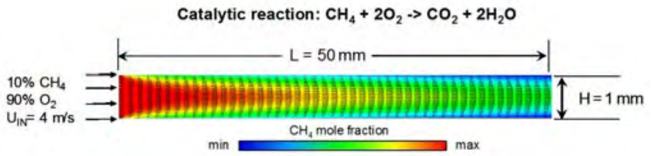

Figure 31: *Flow of Oxygen-Methane mixture through a channel with catalytic reactions at the walls. Contours of the methane mole fraction are plotted [4].*

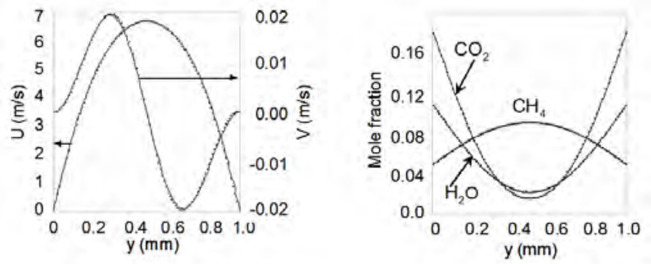

Figure 32: *Comparison of transverse species and velocity profiles at a fixed axial position (x=25mm) using: a) multi-component D2Q9 lattice Boltzmann model (symbols), b) classical CFD (solid lines) [4].*

Fuel cell systems

The numerical study of the flow in a fuel cell system allows an a priori optimization and prediction of its working efficiency. Both in solid oxide fuel cells (SOFC) and polymer electrolyte fuel cells (PEFC), there is a multitude of phenomena occurring in the micro-scale. A part of the SOFC, which can be studied with the LB method, is the porous anode. In the following Figure, preliminary results of the flow of a mixture through a complex geometry domain are plotted. Validation of the algorithm, for macroscopic flows is conducted in collaboration with the LTNT group at ETH-Zürich [7]. By decreasing the characteristic length scale of the domain, microflow effects that cannot be described by the standard formulation of the Navier-Stokes are observed.

The new algorithm will be used to address key issues in PEFCs, by comparing measured and predicted permeabilities and diffusivities in the diffusion barrier layer (DBL) of the cathode. The results will be used to test macroscopic models used in such systems. The general applicability of the numerical tool extends to advanced engineering applications that include chemically reacting flows, which are of great significance in the field of combustion.

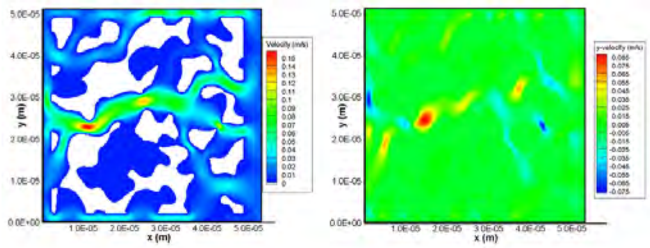

Figure 33: *A mixture of CH4 and H2O enters from the left side and exits from the right side of the domain. The velocity contours are plotted. Magnitude of velocity is in m/s, and magnitude of the y-component of the velocity is in m/s.*

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PSI - Modelling and Analysis Group of the Thermal Hydraulics Laboratory

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The activities within the laboratory as a whole are concerned with the application of state-of-the-art technologies to the heat/mass transfer processes and hydraulics relevant to the safety and efficiency of current and future nuclear reactors. The large-scale, integral test facility PANDA was originally conceived in the early 1990s to provide confirmation of the characteristics of passive safety systems for advanced Light Water Reactors (LWRs), but more recently has focused on investigations of fundamental flow phenomena, such as bubble plumes, mixing and stratification. A number of additional small- and medium-scale, single-effect test facilities are now also operating. At all three scales, experimentation is accompanied by the development and application of novel instrumentation techniques able to measure the distributed parameters characteristic of 3D flow fields.

ARTIST is the other main test facility, reproducing at reduced scale aerosol deposition behaviour during a postulated severe accident initiated by a steam generator tube rupture. The associated iodine chemistry is also studied.

The experimental programme is balanced by the development and validation of numerical models, the overall theme being aimed at replacing the existing empirical models by mechanistic modelling, using CFD in particular, but including also system and component studies as well as multi-scale modelling approaches to basic phenomena such as boiling.

The Modelling and Analysis Group, presently consisting of six staff members plus one post-doc, has four principal research areas:

- Modelling of 3D flow behaviour (single-phase and two-phase) using the CFD codes FLUENT and CFX
- Simulation of LWR containment behaviour and primary circuit analysis using the *CFD-like* code GOTHIC and the system code RELAP5, respectively
- Validation of CFD models, especially single-phase turbulence models and two-phase closure relationships
- Fundamental studies of nucleate boiling

Research within the group is carried out within a multi-project environment, the projects being at both national and international levels, and generally supported by external funding to a level of 50%. In addition, *in-kind* contributions are made to the OECD Nuclear Energy Agency in the field of international promotion of CFD applications to nuclear reactor safety. The different fields of research carried out are summarised below.

STARS

Under this project heading - an activity financially supported by ENSI, the Swiss Federal Nuclear Safety Inspectorate - investigations are made using the commercial CFD code ANSYS-CFX of in-vessel mixing of inlet coolant streams in a typical Pressurized Water Reactor (PWR) geometry. A heterogeneous mixture - i.e. hot/cold or of different boron concentration - entering the core region would be detrimental to reactor performance. CFD modelling is used to determine the degree of mixing at the core inlet. Experimental data are available from scale-model tests to evaluate different turbulence models. Both steady-state and transient situations are considered.

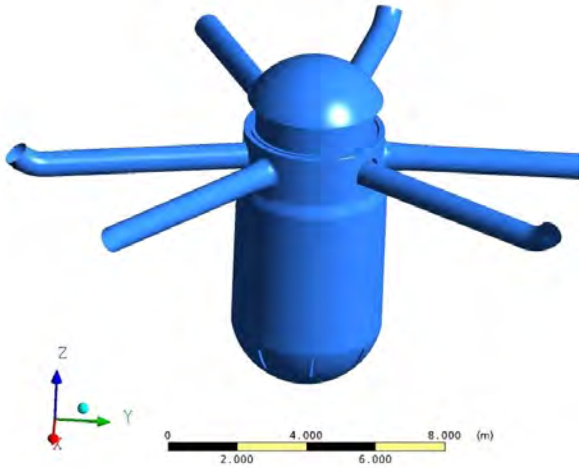


Figure 34: *PWR vessel simulation using CFD to determine boron-dilution concentrations using hexahedral grid with 6.7 million cells.*

PLiM

There are many examples in industrial plant in which fluids at different temperatures mix in a T-junction, the ensuing turbulent oscillations inducing high-cycle thermal fatigue in nearby pipework. With financial support from Swissnuclear, the issue is being investigated, both experimentally and numerically. The experimental setup consists of Plexiglas main and branch lines in a horizontal configuration. Ionized and de-ionized water are used to represent the hot and cold streams, and to map the flow field measurements of conductivity are made using a wire-mesh sensor (WMS) device in at cross-sections downstream of the junction.

In parallel, numerical simulations have been carried out using RANS, SAS and LES turbulence models. Only LES has been successful in capturing the concentration profiles. Simultaneously, numerical simulations of other T-junction configurations based on experiments in France, Germany and Sweden are also being undertaken, and, under the sponsorship of the OECD Nuclear Energy Agency, an international blind benchmark exercise has recently been initiated, attracting participation from 21 countries.

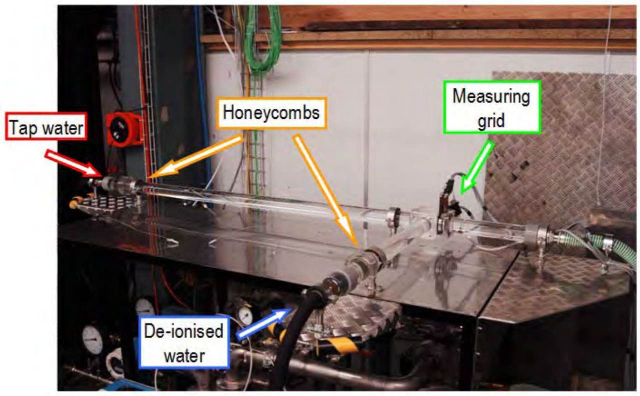


Figure 35: *PLiM experimental facility.*

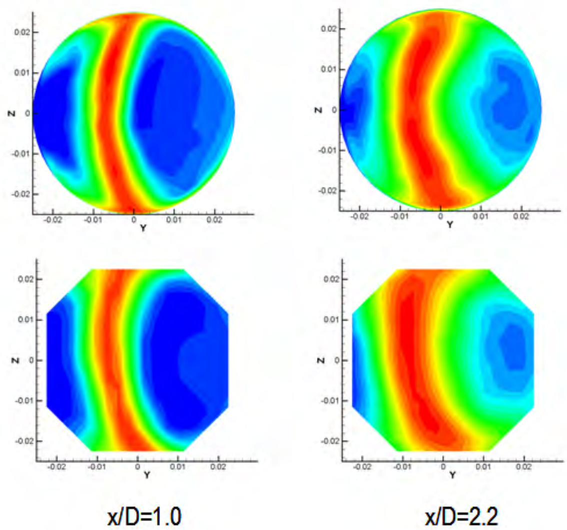
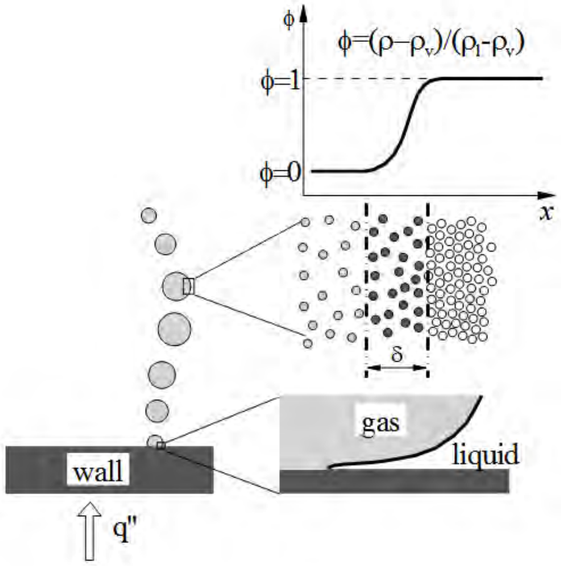


Figure 36: *Average RMS values of the fluid conductivity: calculated (top) and measured (bottom).*

MSMA

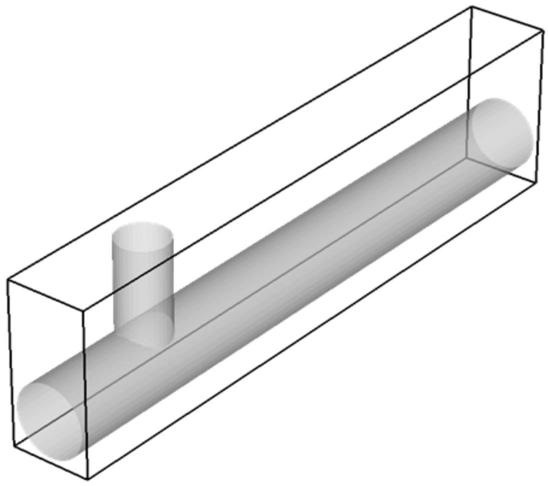
This project, financially supported by Swissnuclear, is concerned with Multi-Scale Modelling Analysis of convective boiling, and combines analyses at the molecular, nano- and micro- scales to develop meso-scale (i.e. CFD scale) closure laws. The initial phase of the project, which concentrates on low heat-flux conditions, is intended to initiate a long-term, combined experimental and theoretical programme leading ultimately to the reliable mechanistic prediction of the thermal crisis (Critical Heat Flux - CHF) in a rod bundle of a nuclear reactor core.



The liquid-vapour interface is not infinitely sharp (see Figure), but possesses a certain thickness, which varies with the saturation temperature. At relatively low temperatures, this thickness is of the order of a few molecular mean-free-paths, and so the properties of the fluid within this transition layer will change sharply from one phase to the other.

Molecular dynamics simulations have confirmed the smooth variation of the density across the interface for a range of temperatures below the critical point, and have provided clues concerning the relevant variables to be used to analyze the phase change process in a more fundamental way.

Central to the numerical analysis at the nano-, micro- and possibly also the meso-scale is the recently-developed, in-house computer program PSI-Boil. The spatial discretization is based on an orthogonal, staggered, finite-volume approach, an algorithm that is easily parallelized to run on high performance computers, achieving in most cases near linear speed-up with number of processors. The code runs in Direct Numerical Simulation (DNS) mode for micro-scale computations, but a Large Eddy Simulation (LES) option is available at the meso-scale. An interface tracking algorithm is also installed based on a Level Sets approach, enabling the movement of the bubble surface to be followed.



More recently, an Immersed Boundary Method procedure has been implemented by which internal geometric surfaces non-coincident with the computational grid lines are recognized, and the numerical algorithms appropriately adjusted in adjacent cells to account for the resulting polygonal mesh structure.

The procedure is fully automated, with the geometry imported directly from a CAD database. The Figure shows an example of how a T-junction geometry is imported into the computational box. With this technique, the use of PSI-Boil to perform CFD simulations at the meso-scale is being considered within the MSMA project.

WSL - Institute for Snow and Avalanche Research

Flueelastrasse 11, CH-7260 Davos Dorf, Switzerland.

Experimental environmental aerodynamics, micrometeorology and modelling are some of the many fluid dynamical research activities at the Institute for Snow and Avalanche Research SLF in Davos. The SLF experimental facilities include a suction-type boundary layer wind tunnel of 20 m length and 1x1m cross section and numerous alpine terrain field sites close to Davos. The SLF recently established one new field site (Wannengrat) equipped with dense networks of meteorological measurement stations. Recent wind tunnel studies of boundary layer flow over snow and vegetated soil surfaces are discussed below. Field research on wind erosion of sand and snow and eddy covariance measurements of wind and humidity are starting in winter 2009/10. Recent and ongoing research projects include:

Roughness Characterization of Snow Surfaces

Gromke, Manes, Guala, Lehning

Knowledge of the surface roughness is essential for understanding turbulent exchange processes within the lower part of the atmospheric boundary layer. A proper representation of the surfaces roughness is needed in every model of near surface mass, energy and momentum exchange processes. Considering the vertical profile of mean velocity in a turbulent boundary layer flow, this is done by assigning an aerodynamic roughness length z_0 to the surface. However, for snow surfaces a great uncertainty on the appropriate choice of z_0 exists. Literature data on z_0 for flat snow surfaces range from microns to several centimetres, spanning 4 orders of magnitude. Our aim is to improve the current knowledge of z_0 values for snow surfaces and to make those values available for model applications.

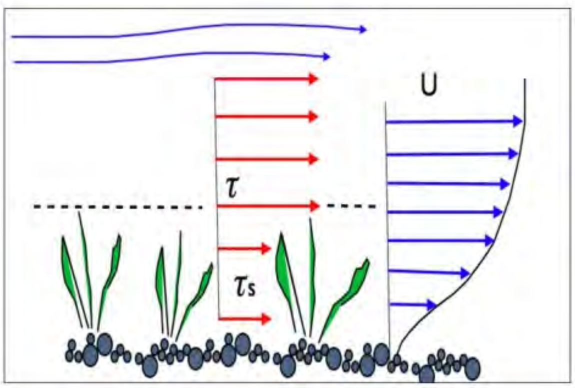
At the SLF, two procedures to describe the roughness of freshly fallen snow surfaces are followed. First, photographs of snow surfaces are taken and evaluated using digital image analysis resulting in snow surface contour line coordinates. Analysing second order spatial structure functions of the snow surface contour line coordinates, gives surface characteristic length scales which can be identified with typical snow particle and aggregate size scales. Second, aerodynamic roughness lengths z_0 are estimated from log-law fitting of velocity profiles over the snow surfaces measured in the SLF boundary layer wind tunnel.

A synthesis of both approaches suggests a linear relationship between the aerodynamic roughness lengths z_0 obtained from the wind tunnel measurements and the surfaces characteristic length scales. The correlation with the aggregate length scales is weak for the data analyzed thus far. This is an ongoing research project, and further study is needed to confirm the findings and establish a well-founded relationship.

Shear Stress Partitioning in Vegetation Canopies

Walter, Gromke, Manes, Lehning

The goal of this recently launched project is to understand and quantify the basic mechanisms governing the sheltering effect of vegetation against soil erosion and snow drift. In order to gain understanding of the physical mechanisms involved, the innermost layer of the atmosphere, the turbulent surface layer where wind forces are transferred to the ground by turbulent shear stress, is investigated. In vegetation covered surfaces, parts of the downward transferred shear stress are absorbed by the plants, resulting in reduced wind forces acting directly on the ground and diminished potential of erosion activity. The ratio of the total shear stress τ above the plants and the reduced shear stress acting directly on the soil surface τ_s quantifies the sheltering effect of the vegetation canopy. The novelty of the approach lies in the use of real living plants for the experiments. So far, abiotic imitations instead of real plants have been used in most wind tunnel studies. However, real plants display a highly irregular structure that can be extremely flexible and porous in contrast to the often rigid and non-porous artificial plant imitations.



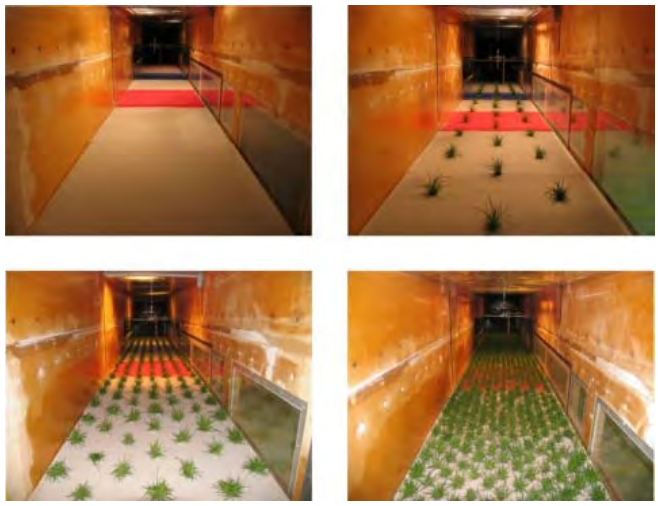
The final goal of the study is the development of a model which predicts the shear stress acting on the ground for given vegetation planting density and wind velocity. Such information can be used as an input for sediment, e.g. soil, sand or snow transport models as well as to develop suitable safety precautions to avoid wind erosion in arid regions.

Wind Erosion and Dust Concentration Reduction by Vegetation Canopies

Burri, Gromke, Graf

Wind erosion is the process by which soil is detached from the ground surface and transported by wind. All over the world, wind erosion causes huge annual soil losses and promotes the formation and spreading of deserts, thereby posing a threat to the livelihood of numerous people. Furthermore, wind erosion increases the content of fine mineral dust in the atmosphere. High concentrations of fine dust cause lung diseases and change the global radiation balance, which affects the Earth's climate.

In the SLF wind tunnel, experiments with grass canopies of four planting densities (no, low, medium and high) are currently conducted. Vegetation fetches of 8m length consisting of living grasses (Lolium perenne) with erodible sand grain layers are placed in the wind tunnel test section. At the end of the test sections, a sediment sampler is positioned to trap airborne sand grains at 60 height levels. Additionally, fine dust concentrations in the air above the vegetation fetch are measured. Colored quartz sand is used to visualize erosion and deposition patterns.



First results show that wind erosion activity decreases considerably for medium and high planting densities, whereas for low planting densities no reducing effect is found. A vegetation cover of $c_v = 15\%$ (corresponding to a frontal area index $\lambda = 0.11$) led to 93% and 50% reductions in total sediment mass flux and fine dust concentrations when compared to the non-vegetated reference case. A vegetation cover of $c_v = 55\%$ ($\lambda = 0.42$) inhibited wind erosion activity almost completely. Additionally, the vertical profiles of sediment mass flux vary with vegetation canopy density. For zero and low vegetation densities, exponentially decreasing mass flux profiles were observed, with a near-linear profile for the medium planting density and a profile showing a peak at around twice the canopy height for the high planting density.

The Netherlands 'JM Burgerscentrum' Pilot Centre Report

Gijsbert Ooms

General introduction

The JM Burgerscentrum (JMBC) is the Dutch research school for fluid mechanics. The Delft University of Technology is the coordinating university. The main goals of the JMBC are:

- Stimulation of co-operation of the participating groups with respect to their research efforts. It is the desire to be one of the leading institutes for fluid mechanics in the world.
- Organization of advanced courses for PhD-students. Researchers from industries and technological institutes also attend these courses.
- Co-operation with industries and technological institutes. The aim is to promote the use of up-to-date knowledge on fluid mechanics for solving practical problems.
- Strengthen the contacts between Dutch fluid mechanics research groups at universities and the international fluid mechanics community.

About 60 professors with their groups participate in the JMBC. These groups are located at the Delft University of Technology, Eindhoven University of Technology, University of Twente , the University of Groningen, the Radboud University of Nijmegen, Leiden University, Wageningen University and Utrecht University. They are from a number of disciplines; such as Civil Engineering; Mechanical Engineering; Maritime Technology; (Applied) Physics; Aerospace Engineering; Applied Mathematics and Chemical Technology. The professors with their senior staff form the council of project leaders, which meets twice a year. There are about 250 PhD-students in the JMBC.

The JMBC has a scientific director who is responsible for the management of the research school; the JMBC secretary assists him. Three times per year he justifies his actions to the Board of the JMBC, and asks the Board for advice with respect to proposed new activities. He is also assisted by the Management Team, which consists of the local directors from the Delft University of Technology (also responsible for the group at the University of Leiden), Eindhoven University of Technology (also responsible for the groups at the University of Nijmegen, Wageningen University, and Utrecht University) and the University of Twente (also responsible for the group at the University of Groningen).

The research projects carried out by the JMBC-groups have been ordered in a number of research themes. The reason for this ordering is to present in each theme a combination of projects which have coherence. The themes are:

- Complex dynamics of fluids
- Complex structures of fluids
- Mathematical and computational methods for fluid flow analysis.

The JM Burgerscentrum has many good contacts with industries and technological institutes in The Netherlands. For that reason there is an Industrial Board, in which participate Unilever, Gasunie, Corus, Philips, AKZO-Nobel, Teijin Twaron, Shell, DOW Benelux, ASML, DSM, NLR, NMI, TNO-Science and Industry, TNO-Defence and Safety, TNO-Oil - and Energy Industry, MARIN, Deltares, KEMA, ESTEC, Océ and ECN/NRG. The Industrial Board meets twice per year with the scientific director to discuss new activities of relevance to industries and technological institutes.

Each year (also in 2009) there are many scientific contacts with research groups in other countries. For that reason there are often external visitors to the JMBC groups. JMBC staff also regularly visits foreign fluid-mechanics groups, and presents their work at international conferences. The number of publications from JMBC staff in well-known scientific journals is considerable. The JMBC has attracted top-experts in different fields of fluid mechanics to the JMBC. These experts have been appointed as JMBC-professors at the three Technological Universities and are financed by the Boards of the Technological Universities or by the 3TU-federation. They contribute considerably to the achievements of the research school.

An important activity of the JMBC is the organization of the annual meeting of the research school (Burgersdag). This year about 200 persons attended the meeting. The theme of the meeting was research by JMBC PhD-students. Together with Engineering Mechanics the JMBC forms the Centre for Fluid Solid Mechanics. This Centre has been recognized as a centre of excellence in The Netherlands and has received significant funding by the Dutch Government for stimulating new research areas in fluid and solid mechanics.

The annual report of the JMBC provides an overview of the activities of the research school during the last year and a plan of action for the coming year. The core of the report consists of the description of the research projects, carried out by the JMBC groups. In each report the relevant information (title, theme, staff involved, project aim, achievements, publications, funding source, application, etc.) is given. Also some research highlights are presented. Besides the important progress in research the report describes the advanced graduate course program offered by the JMBC. Finally it provides information about the research school, such as goals, organization, relation with industries and technological institutes.

The annual day of the research school (Burgersdag) in 2009 was held at Eindhoven University of Technology. There were more than two-hundred participants. There was an excellent Burgers Lecture by Sankaran Sundaresan of Princeton University. Thereafter three parallel sessions were held during which JMBC PhD-students presented their projects via twelve minutes presentations. BendiksJan Boersma and Federico Toschi closed the day with interesting lectures. The many participants enjoyed this Burgersdag. There are, of course, some points for improvement. The next Burgersdag will be on 13 January 2010 at Twente University.

In the academic year 2008-2009 the course program was again a great success. There were courses on compressible flows, CFD II, fluid-structure interaction, PIV, biological fluid mechanics, turbulence, and wetting and capillarity-driven flows. The JMBC is grateful to the professors of the research school for their willingness and interest to organize these courses.

The distribution of the budgets for research projects of JMBC groups is now as follows: 1st money stream (universities) 25%, 2nd money stream (national science foundation) 50% and 3rd money stream (industries, institutes, EC) 25%. This is a significant change compared to the budget distribution of, say, five years ago, when the 1st money stream was still considerable. It shows the viability of the JMBC groups. The number of PhD students has never been so large.

Special JMBC events

JMBC/FOM meeting: 'Changing flows: Teaming up for new scientific challenges'. At the suggestion of the members of the Industrial Board a workshop was organized to discuss the relations between industries and institutes (GTI's and TNO) with JMBC groups. In a co-operation between FOM and JMBC this one-day workshop was held on 19 June 2009 in Utrecht. During the morning session special attention was paid to the needs of industries and institutes for advise/support/cooperation from university groups on topics in the area of fluid mechanics. Representatives from many industries and institutes gave brief presentations about these needs of their organizations. During the afternoon session topical workshops were held to discuss more focused topics for possible cooperation between industries, institutes and JMBC groups. At the end of the workshop there was ample time for further discussion of plans. Some conclusions of the workshop are given below:

- Almost all presentations showed that multiphase flow is the rule rather than the exception. There is a need for continued research in this area, both aiming at short-term improvements that can directly be implemented and applied (e.g. in the form of new industrial correlations) and aiming at long-term new fundamental insights that can replace the exhausted current engineering approaches.
- Another topic that was often mentioned was rheology. The research on rheology has received new interest in The Netherlands, in particular because a number of new groups with a more physical background study this topic.
- There was a considerable interest in mixing. There are two parts. The part "Flow and mixing in urban environments" is aimed at the growing need for accurate models for the dispersion of toxic gases in the urban environment. The part "Physics of mixing" aims at answering two questions. 1) How can a deeper insight in the physical processes and mathematical modeling of mixing (as developed by several academic groups) contribute to improved mixing processes for different industrial applications and in reverse order: 2) How can specific and fundamental questions from industries be translated into academic research programs.
- During the workshop developments of modern solvers for CFD problems and also particle-based simulation techniques were discussed. It is clear that these techniques are of crucial important for many applications.
- The Dutch industries and institutes have a great need for intensified co-operation with universities on research in the area of microfluidics, wetting and flow transport in thin layers. Possible topics are lab-on-a-chip applications, superhydrophobic surfaces, optofluidics, oil-recovery, chip cooling, two-phase flow in microchannels, coating flows, dynamic contact lines.

Research carried out by JMBC groups

Some research highlights are given below. The complete program of the research school can be found on our website: www.jmburgerscentrum.org

Internal wave patterns & their impact on mixing
Maas, Gerkema, Hazewinkel

The ocean's salinity and therefore its density increase with depth. This stratification supports subsurface waves, driven by tides. Periodic fluid motion over a shelf edge, or underwater mountain forces these internal gravity waves that appear as obliquely oriented, internal wave beams. Internal waves are of interest because they might explain observed strong mixing in the deep sea, one of the greatest unexplained mysteries of present-day oceanography. Experimentally, internal waves can be generated by periodically shaking a tank that is filled with a uniformly (salt) stratified fluid. Successive reflections of internal wave beams against inclined tank walls force the wave energy to collapse onto a closed orbit, the wave attractor. The wave attractor pattern depends on the precise shape of the tank and on wave frequency in combination with the stability frequency characterizing the stratification (Figures 1 and 2).

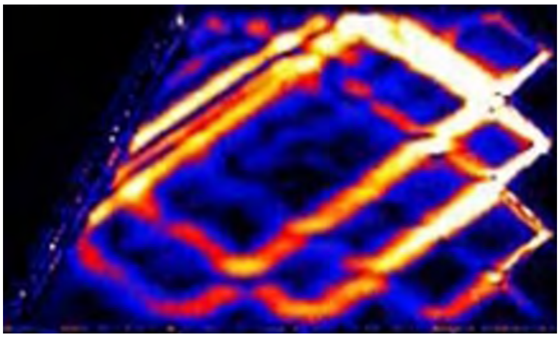


Figure 1: *Side view of the stationary internal wave energy distribution due to periodic, horizontal shaking of a trapezoidal tank having a vertical/sawtooth shaped right wall. Internal waves are focused and defocused by the sloping walls, but focusing dominates and energy propagates clockwise in the focusing direction. Colours indicate strong (white) or weak (blue) motion.*

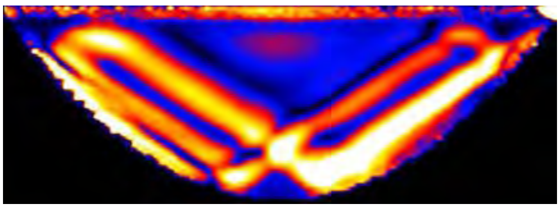


Figure 2: *Internal wave energy distribution in a parabolic channel.*

The long-term effects of wave attractors on stratification, current patterns and mixing, as well as their subsequent feed-back on these attractor patterns, are presently being studied. For this, a combination of theory and experiments is used. Initial investigations indicate that the wave attractors drive a net particle and fluid transport: first horizontally, towards the nearest attractor branch, and subsequently obliquely, along the attractor branches, in a direction opposite to the wave energy propagation direction. It turns out this can indeed provide an explanation for the elevated 'deep mixing'. The results described here were obtained under a FOM - 'dynamics of patterns' PhD grant. The work is a joint project between CWI (Amsterdam), DAMTP (Cambridge) and NIOZ (Texel).

Internal waves can also be trapped to density jumps. Such interfaces are regularly present in the ocean. The waves then appear as interfacial waves. Their interaction with the internal waves in the stratified layers adjacent to the interface may be responsible for sudden bursts of interfacial waves observed in the ocean and is currently being studied.

The structure of unsteady 3D sheet cavitation
Hoeijmakers, Engineering Technology, UT.

Cavitation describes the formation of vapor in a liquid in regions where the velocity is high and consequently the pressure is low, i.e. lower than the vapor pressure. Cavitation is an important phenomenon in hydraulic and hydrodynamic devices such as ship propellers, pumps and turbines, hydrofoils, valves, dams, spillways and bearings. Cavitation has detrimental effects such as erosion of the surface material, vibrations and noise radiation. Excessive cavitation deteriorates the efficiency of hydrodynamic devices.

In STW project TSF6170 "The Structure of 3D unsteady Sheet Cavitation" the Group Engineering Fluid Dynamics at the University of Twente cooperates with the Group Ship Hydromechanics and Propulsion at Delft University of Technology. In the project the most important form of cavitation in industrial applications is considered: Sheet Cavitation. In these applications mostly unsteady inflow occurs which is known to greatly affect sheet cavitation which becomes time-dependent.

The overall objective of the project is to determine a model for the description of the dynamics of 3D sheet cavitation on hydrofoils. The dynamics of sheet cavitation is important because it determines both the radiated pressure field and the erosive nature of the clouds of vapor shed from a sheet cavity. Furthermore, the sheet cavitation phenomenon is three dimensional in character. Ultimately, a better understanding of the interaction between unsteady inflow and cavitation will create the possibility of active cavitation control.

In the project at the University of Twente an unstructered-grid CFD method is developed for predicting the characteristics of unsteady cavitation in 3D. This method includes models for the transport of the vapor fraction in the cavitating flow regions. At Delft University of Technology an experimental investigation is carried out in their cavitation tunnel, with the ambition to measure simultaneously forces, surface pressures and flow field velocity distributions (PIV). This will result in data on the unsteady shape and volume of the cavity and on the structure of the flow in the closure region of the cavity. This data is used for the validation of the computational results and the underlying physical models of unsteady sheet cavitation.

Employing the computational method for cavitating flow employing a barotropic flow model, developed at University Twente, hydrofoils have been designed for testing in the Delft Cavitation Tunnel. The design is such that cavitation occurs in the mid-span region of the hydrofoil only, this to avoid the interaction of the cavity with the tunnel wall boundary layers as well as to create a cavitating flow that is representative for the flow occurring on a ship propeller. User Committee: Marin, Wärtsila, Flowserve, IHC, HRP, van Voorden, RNN, Shell, Twister BV.

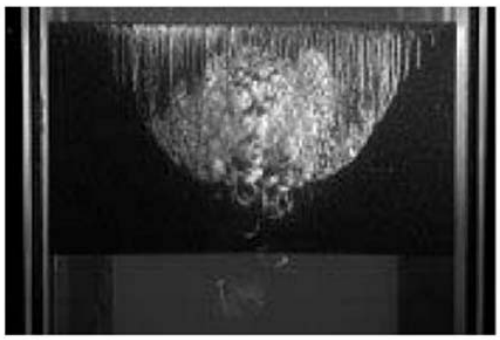


Figure 3: *Sheet cavitation on a hydrofoil. Top: Twist-11 hydrofoil designed to feature a mid-span triangular region with cavitating flow. Bottom: Sheet cavitation as observed in the Delft Cavitation Tunnel.*

Modelling enhanced heat transfer and surface reactions on the micro-scale
Nedea, van den Akker, Frijns, van Steenhoven
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Heat transfer on micro/nano-scale has become one of the major issues within many application fields, like micro-channel cooling for microelectronics and surface catalysis in micro reactors. In such miniaturized systems, the surface-volume ratio is large. This property can be used for example to increase the heat transfer considerably. The small-scale wall interactions affect the material properties up to the micro- and mini-scale level. Therefore, understanding the gas-wall or fluid-wall interactions thoroughly is indispensable for the temperature control and has to be studied on a molecular-scale. We developed a multi-scale hybrid method that combines the advantages of molecular dynamics (MD) and the stochastic direct simulation Monte Carlo method (DSMC): the accuracy of the interactions at the interfaces by MD, and DSMC in the bulk for low computational costs. The hybrid MD-DSMC method is coupling the MD and MC simulation domains using a buffer layer at the interface of these domains (see Figure 4). For instance, for the heat transfer between a cold and a warm wall, high picks and density oscillations appear near the wall boundary, and they are more pronounced near the cold wall. This wetting effect is studied with the hybrid method where the MD domain covers the entire oscillation region for accurate simulation of the interaction with the wall and MC in the bulk (see Figure 4). The results show that hybrid simulations give very accurate results compared to pure MD simulations, while MC simulations give higher deviations. The hybrid method is also five times faster than pure MD simulations and therefore also the simulation domains can be increased making the step towards real applications possible.

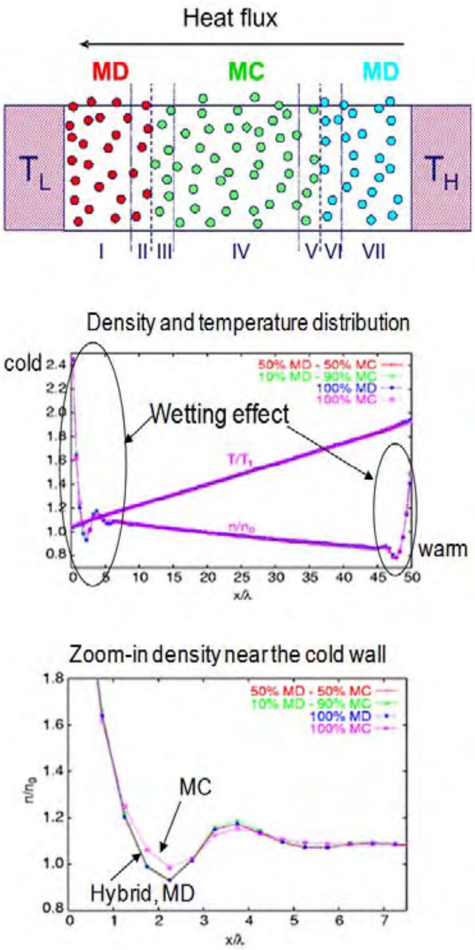

Figure 4: *Top: Heat flow between a cold (left wall) and a warm wall with MD domain near the cold wall and MC domain coupled via a buffer layer (II and III). Middle: Temperature and density distributions for a gas in between two walls with a prescribed temperature difference as calculated with MD, DSMC and the novel hybrid method. Bottom: zoom-in of the oscillation density region near the cold wall.*

In a two-phase flow, the phase transition between liquid phase and gas phase is important, since evaporation can dissipate a large amount of heat. It is important that in the MD simulations and in the hybrid MD-DSMC simulations, this phase transition is modelled thermodynamically correct. We simulated an equilibrium situation and compared the temperature profile, density profile, pressure profile and enthalpy with literature values (Figure 5). The thermodynamic properties agreed with experimental results from literature. Now we are describing the liquid-vapour phase transition at a heated solid wall.

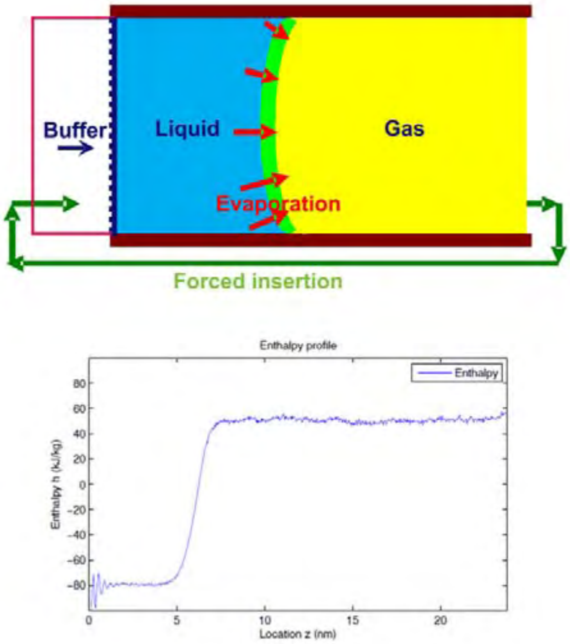

Figure 5: *Top: Schematic view of the MD simulation box with boundary conditions. Bottom: Enthalpy jump over the liquid-vapor interface ($x = 5 - 8nm$) for Argon molecules.*

A similar approach can also be used to study surface reactions where accurate boundary effects are computed from the molecular properties. From there boundary conditions for a continuum model can be derived. For instance, macroscopic values of diffusion, thermal and catalytic coefficients can be computed using hybrid MD - DSMC techniques and can be then integrated in the three dimensional Navier-Stokes equation solver. A direct coupling of the hybrid MD-DSMC method with the continuum model and also new kinetic models and scattering kernels describing the gas-wall interactions are investigated.

Computation of sound generated by turbulent flows

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Prediction of aerodynamic sound at moderate Mach numbers is difficult due to the low amplitude of the sound waves. An acoustic wave with a Sound Pressure Level (SPL) of 100dB, which corresponds to a pressure fluctuation of only 2Pa is already damaging for the human ear. In a turbulent flow, hydrodynamic pressure fluctuations in general scale with the velocity squared. These hydrodynamic pressure fluctuations are for flows with moderate Mach numbers of order 10000-50000. Thus roughly four to five orders larger than the aerodynamic sound we want to predict.

The large range of pressure that is required in the solution of the compressible Navier-Stokes equations places a severe restriction on the accuracy of the numerical method and resolution. In this research we use a 10th order compact staggered finite difference scheme to simulate a round turbulent jet flow, with $Re = 5000$ and $M = 0.8$ based on orifice quantities; Figure 6 shows the obtained vorticity magnitude.

The observer of the sound generally located far from the acoustic source and an extension to the far field is necessary. In this work we make use of the porous Ffowcs Williams & Hawkings equation to obtain the far field sound. In such a method pressure data is taken from the Navier-Stokes solution and by an analytical technique the far-field pressure is computed. A typical result obtained with this approach is also shown in Figure 6.

For the validation of the results an experimental setup has been build in which the simulated Reynolds and Mach could be matched exactly. The acoustic pressure fluctuations in the far-field obtained from the simulations are, in general, in good agreement with the observed experimental values.

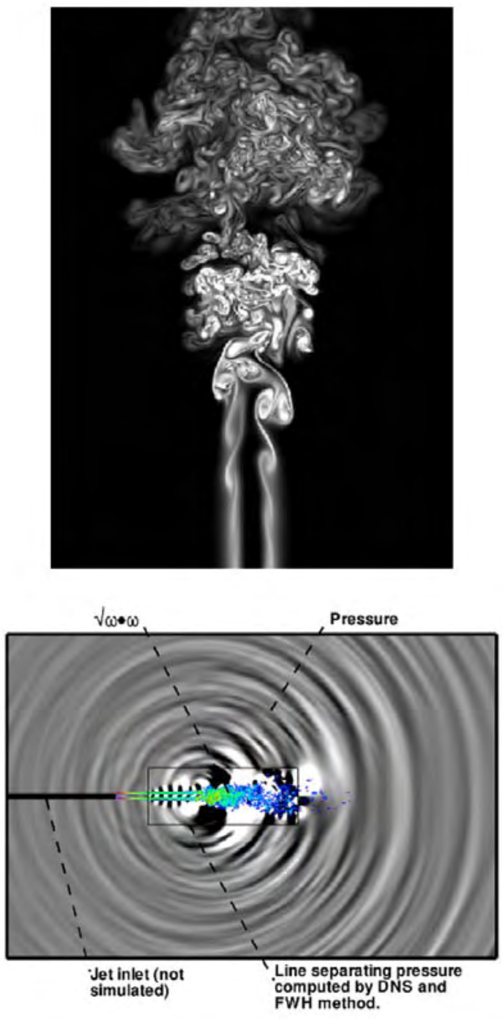

Figure 6: *Top: the vorticity magnitude in a round jet with* $Re = 5000$ *and* $M = 0.8$. *The computational grid consisted of 768x384x384 grid points. The calculations have been performed on 192 nodes of a IBM-SP6 supercomputer and took roughly two weeks computing time. Bottom: the acoustic near and far field.*

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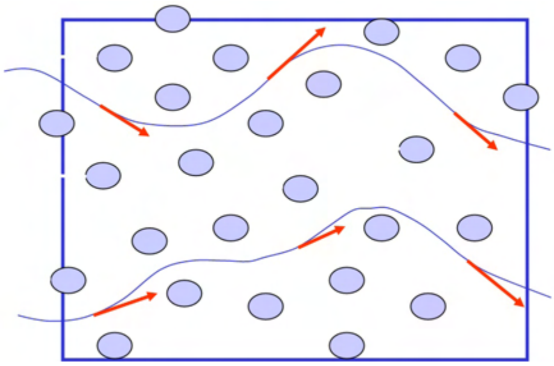
Best Practice Guidelines for Computational Fluid Dynamics of Dispersed Multi-Phase Flows

Editors

Martin Sommerfeld, Berend van Wachem
&
René Oliemans

The simultaneous presence of several different phases in external or internal flows such as gas, liquid and solid is found in daily life, environment and numerous industrial processes. These types of flows are termed multiphase flows, which may exist in different forms depending on the phase distribution. Examples are gas-liquid transportation, crude oil recovery, circulating fluidized beds, sediment transport in rivers, pollutant transport in the atmosphere, cloud formation, fuel injection in engines, bubble column reactors and spray driers for food processing, to name only a few. As a result of the interaction between the different phases such flows are rather complicated and very difficult to describe theoretically. For the design and optimisation of such multiphase systems a detailed understanding of the interfacial transport phenomena is essential. For single-phase flows Computational Fluid Dynamics (CFD) has already a long history and it is nowadays standard in the development of air-planes and cars using different commercially available CFD-tools.

Due to the complex physics involved in multiphase flow the application of CFD in this area is rather young. These guidelines give a survey of the different methods being used for the numerical calculation of turbulent dispersed multiphase flows. The Best Practice Guideline (BPG) on Computational Dispersed Multiphase Flows is a follow-up of the previous ERCOFTAC BPG for Industrial CFD and should be used in combination with it. The potential users are researchers and engineers involved in projects requiring CFD of (wall-bounded) turbulent dispersed multiphase flows with bubbles, drops or particles.



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www.ercoftac.org

Or from:

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