

## The International Research Training Group "Droplet Interaction Technologies" (DROPIT): Selected Results

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### Abstract

The International Research Training Group (IRTG) "Droplet Interaction Technologies" (GRK 2160/1) was established in October 2016 to focus on detailed droplet processes. Droplet interaction technologies have a large number of applications in a variety of technological processes, such as spray cooling, fuel injection, coating technologies or the generation of encapsulated materials in the pharmaceutical industry.

A key feature of this large research project lies in the systematic study of the interdependencies between small-scale and large-scale dynamics through an integrated numerical, experimental and theoretical approach. The objective is to identify the mechanisms through which small-scale interactions at the interface can couple with and influence large scale features in the main flow.

DROPIT is a joint initiative of the University of Stuttgart in Germany, the University of Bergamo and the University of Trento in Italy. The project consists of 17 subprojects, which are structured into three main research areas (drop-gas interaction, drop-wall interaction, drop-liquid interaction). It involves researchers from a large number of different disciplines like Mathematics, Environmental Engineering, Aerospace and Mechanical Engineering, Informatics and Computer Sciences. The project further consists of an extensive qualification program which aims at fostering the education of young scientists and providing them the knowledge and skills to conduct independent research.

The paper gives an overview of the structure and the research activities within GRK 2160/1 as well as on the qualification program implemented. Selected scientific results, e.g. on multi-scale modelling of droplet dynamics in compressible flows, gas kinetic simulations of micro-drop-gas interactions, upscaling of coupled free-flow and porous-media flow processes, micro- and macro-drop impact dynamics with miscible fluids and novel optical techniques for micro-fluid dynamics are shown.

The main purpose of the paper is to familiarize colleagues with this extensive research effort in the area of droplet interaction technologies and to exchange ideas and promote future collaboration with others in this field.

**Keywords:** droplet dynamics, numerical methods, experiments, splashing, porous media

### Introduction

Droplet interaction technologies find application in a large number of technological and industrial processes. These include spray cooling in the food and chemical industry, spray drying absorption for waste and pollutant treatment in process engineering, droplet collisions for the generation of powders and encapsulated material in the food and pharmaceutical industry, drop evaporation and droplet-wall interaction in internal combustion and aeronautical engines as well as in coating technologies. In all these applications, small scale fluid dynamics may have a huge impact on the large scale flow pattern, leading to drag reduction, heat transfer enhancement or depression, phase transition kinetics (e.g. drop condensation or nucleate boiling), acoustic impedance and optical reflection. To date the consequences of the presence of different length scales on macroscopic properties and the associated amplification of surface transport has remained largely unexplored, being limited mainly to the formulation of empirical correlations based solely on macroscopic observations. The novelty and uniqueness of the GRK 2160/1 lies in the fact that here a systematic study is undertaken to investigate the interdependencies between small-scale and large-scale dynamics in the field of droplet interaction technologies. Due to the complexity of the problem, the analysis of such micro/macro interactions is not limited to one single aspect. Rather, an integrated approach is chosen that evolves along three parallel pathways, namely a numerical, experimental and theoretical approach [1]. More detailed information concerning the International Research Training Group GRK 2160/1 can be found online: [www.project.uni-stuttgart.de/dropit/](http://www.project.uni-stuttgart.de/dropit/).

### Structure of the International Research Training Group GRK2160/1

The International Research Training Group is structured into three main research areas (RA-A to RA-C), comprising 17 subprojects, listed below together with the responsible principle investigators:

### Research Area A: Drop-Gas Interaction

- SP-A1 Modelling of deformed, multi-component liquid drop evaporation (Cossali, Tonini, Weigand)
- SP-A2 Multi-scale modelling of the evaporation process (Munz, Rohde, Dumbser)
- SP-A3 Gas-kinetic simulation of micro droplet - gas interaction (Fasoulas, Lamanna, Bassi)
- SP-A4 Numerical methods for compressible multiphase flows with complex equations of state (Dumbser, Munz)
- SP-A5 Modelling of spray evaporation (Cossali, Tonini)
- SP-A6 Mathematical and numerical modelling of droplet dynamics in weakly compressible multi-component flows (Beck, Bassi)

### Research Area B: Drop-Wall Interaction

- SP-B1 Droplet collisions with solid superhydrophilic surfaces (Roth, Cossali)
- SP-B2 Drop impact/deposition onto micro-structured hydrophobic and superhydrophobic surfaces (Santini, Roth)
- SP-B3 Characterisation of porous media by X-ray micro computed tomography (Santini, Ertl)
- SP-B4 Compressible effects in droplet interactions with textured walls (Rohde, Bassi)
- SP-B5 Numerical computation for drop impact on textured surfaces (Weigand, Dumbser)
- SP-B6 Upscaling of coupled free-flow porous media flow processes (Helmig, Santini)

### Research Area C: Drop-Liquid Interaction

- SP-C1 Micro and macro drop impact dynamics with miscible liquids ((Lamanna, Roth, Tonini)
- SP-C2 Single and multiple drop impact into a deep pool (Santini, Cossali, Helmig)
- SP-C3 High-order numerical methods for multi-component incompressible flows in pools (Bassi, Munz)
- SP-C4 Visualisation of droplet-liquid interaction (Ertl, Santini)
- SP-C5 Development of novel optical technique for micro-fluid dynamics (Weigand, Lamanna, Cossali)

In **RA-A**, the research activities focus mainly on the optimization of evaporation models for sprays. The objective is to improve the accuracy of current evaporation models by including effects of small-scale processes on the global, drop-vaporisation rate. This entails non-equilibrium, thermodynamic effects at the drop interface (SP-A3), local curvature effects (SP-A1, SP-A5) and multi-component effects (SP-A1, SP-A6). In addition, subprojects (SP-A2, SP-A4, SP-A6) focus on the development of numerical models for droplet dynamics and evaporation by taking into account multi-scale and/or compressibility effects.

In **RA-B**, the research activities are mainly dedicated to the understanding and modelling of drop impact on solid structured surfaces. This includes textured surfaces (SP-B4, SP-B5), pre-treated surfaces with hydrophobic or hydrophilic coatings (SP-B1, SP-B2) or even porous structures (SP-B3, SP-B6). The objective is to gain detailed understanding on how micro- or nano-scale structures can affect macroscopic detectable quantities and transport processes.

In **RA-C**, the applications are focused on drop collisions (on film or into a pool) with miscible fluids. In SP-C1 and SP-C5, the main objective is to understand how miscibility-gaps and thin-films micro-dynamics influence the large-scale impact dynamics and resulting drop size distribution. Deep pool dynamics in single and multiple drop impact is investigated experimentally and numerically in SP-C2 and SP-C3, respectively. Visualisation methods in support to a better understanding of numerical and experimental results are developed in SP-C4.

### Qualification program

The increased interdependence of economies and technologies together with the need of reducing the ecological footprint of industrial processes requires excellently qualified researchers and engineers with an interdisciplinary background and international experience. Our qualification program is especially designed to meet these requirements. Interdisciplinary elements are strengthened to enhance the quality of the education. Here, a special emphasis is placed on basic knowledge in the natural sciences and in engineering as well as in mathematics, always applied to the topic at hand.

The experiences of former Research Training Groups are incorporated in the present study program. However, new elements are also added to attract excellent students as well as to take into consideration the growing importance of experiences abroad. Special emphasis is placed on the following elements:

- Individual study program comprising graduate-level lectures,
- A yearly joint doctoral meeting to discuss the scientific progress of the IRTG with the participation of members from the advisory board,
- Lecture series of the scientific members of the Research Training Group and guest researcher,
- Seminars of external scientists,
- Annual organization of an international workshop,
- A three-yearly international summer school, organized directly by the doctoral students to foster their self-

- management skill,
- An individually conceived stay abroad for six months is intended.

The home institutions of the scientific members of the Research Training Group are the University of Stuttgart, the University of Bergamo and the University of Trento. All doctoral students participating in the International Research Training Group (IRTG) GRK 2160/1 have to enroll in one of the available graduate academies: GRADUS (Stuttgart), ISA (Bergamo) or DICAM (Trento). Due to the regional separation, modern web-based communication techniques are routinely used. The research data of the projects are exchanged using servers.

## Results and discussion

In the following some selected results of some subprojects are shown, which have been obtained within the first years of the project.

### SP-A2 (Mueller, Munz, Dumbser): Multi-scale modelling of the evaporation process

The FLEXI code of the Institute of Aerodynamics and Gas Dynamics at the University of Stuttgart [2] is a high order discontinuous Galerkin code. The main purposes of the code are scale-resolving simulations in the context of the compressible Navier-Stokes equations, e.g. DNS or LES. In recent years, several novel features have been added, e.g. a shock-capturing scheme [3] based on finite-volume sub-cells and an extension to multi-phase flows [4]. The latter combines a ghost-fluid and a level-set method to allow sharp-interface simulations of compressible two-phase flows.

The main goal of this subproject is the development of a numerical method that allows for detailed investigations of droplet dynamics, in particular droplet evaporation, in the compressible regime and its implementation into the multi-phase FLEXI version. Several important aspects are currently under investigation including e.g. new evaporation models and the improvement of a tabulation scheme for real equations of state. Furthermore, results of the developed scheme will be compared with those of diffuse interface models as well as experimental data.

A major concern in multi-dimensional droplet simulations is the occurrence of spurious currents due to an inaccurate representation of the droplet surface and its curvature, which results in a violation of pressure equilibrium across the droplet surface. The numerical approach to track the interface by a level-set transport equation provides the interface location and its first and second order derivatives, which are needed to calculate the normal vector and the curvature of the interface, respectively. For a detailed description of the used methods, the reader is refer to Fechter et al. [4]. An improvement to the described algorithms has been developed that allows a reduction of the spurious currents at a reasonable expense. Typically, the Navier-Stokes equations and the level-set equation are solved on the same computational grid by the same numerical approach, which results in similar resolutions of both equation systems. While we retain the grid for simplicity and efficiency, we make use of the  $p$ -adaptivity of the discontinuous Galerkin scheme and solve the level-set equation with a higher polynomial degree.

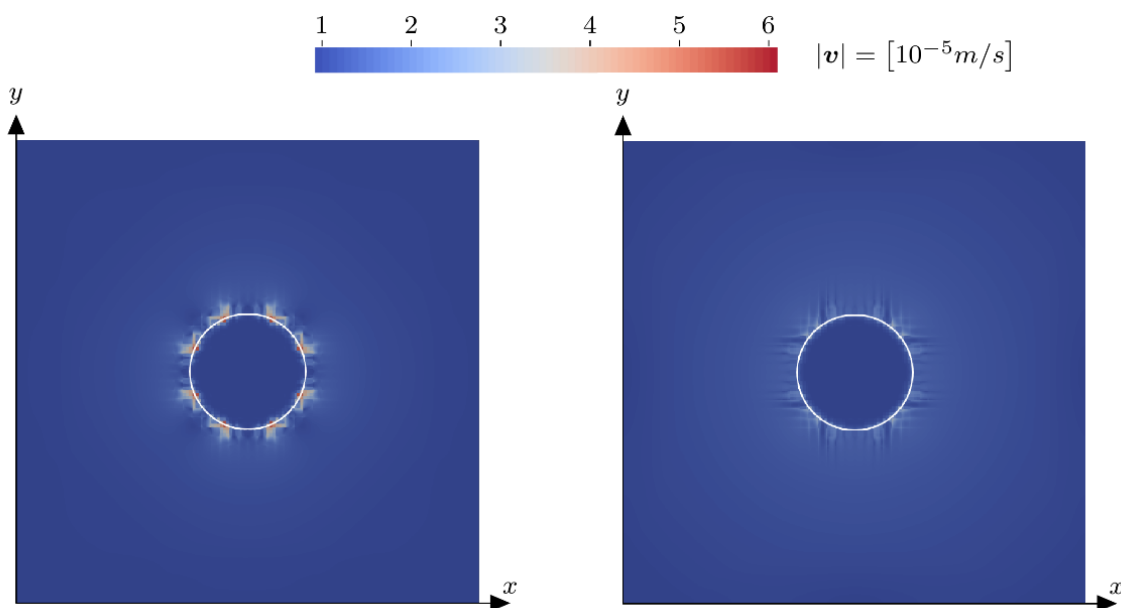


Figure 1. Spurious Currents with  $N_{\text{level-set}} = 2$

Figure 2. Spurious Currents with  $N_{\text{level-set}} = 3$

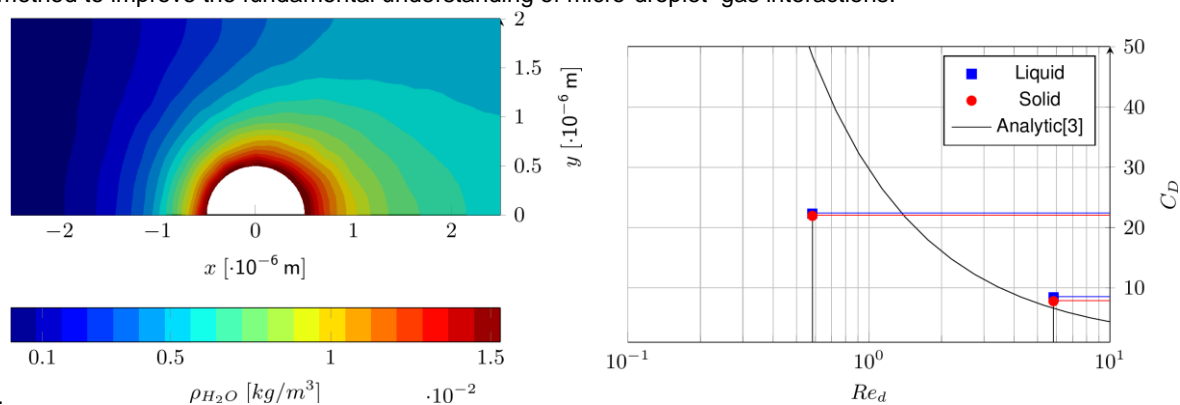
This allows us to choose different spatial resolutions for the geometry and the flow field and hence to optimize the simulation setup with respect to accuracy and costs. Here we simulate a droplet in pressure equilibrium on a 50x50 Cartesian grid and choose a polynomial degree of 2 for the spatial resolution of both the flow field and the level-set. In the second calculation, the polynomial degree of the level-set ( $N_{\text{level-set}}$ ) is increased to 3. Figure 1 demonstrates the occurrence of spurious currents, illustrated by showing the velocity magnitude around the droplet. Figure 2 shows the reduction in their amplitude for a higher polynomial degree of the level-set. In pressure equilibrium, the exact solution has zero velocity everywhere. Therefore, the second result is significantly better. The droplet position is indicated by the white line, the zero of the level-set function.

The next step is to combine this result with new evaporation models at the phase interface to simulate more complex two-phase flow patterns.

### SP-A3 (Reschke, Fasoulas): Gas-kinetic simulation of micro-droplet-gas Interaction

Most numerical approaches for gas-fluid interactions are based on continuum methods. A main disadvantage is the necessity of continuum assumptions, including local thermodynamic equilibrium and limitations to quasi-steady conditions. Within SP-A3, the interaction between gas flows and liquid micro-droplets are simulated using the Direct Simulation Monte Carlo (DSMC) method [5], which approximates the gas flow from a microscopic point of view allowing an investigation of non-equilibrium effects. Consequently, a comparison between DSMC and existing analytic or continuum-based results is of fundamental interest to analyse the effects of equilibrium assumptions and flow unsteadiness. With the DSMC, the gas flow is simulated by approximately solving the fundamental Boltzmann equation. Herein, the particle distribution function is statistically reconstructed with  $N$  representative discrete particles distributed in space. In contrast to Molecular Dynamics simulations, the deterministic description of each microscopic particle state and interaction is not of interest. Movement and collision are decoupled in every simulation time step and collisions are solved statistically using phenomenological models. Macroscopic values such as number density and heat fluxes are then calculated as moments from the resulting sampled particle distribution. In SP-A3, the open source tool PICLas [6] is used, a highly flexible tool for simulation of rarefied 3D plasma flows which is cooperatively developed by the Institute of Aerodynamics and Gas Dynamics (IAG) and the Institute of Space Systems (IRS) at the University of Stuttgart. In particular, different gas-surface interaction models are implemented to account for the occurring phenomena.

For the simulation of liquid boundaries, the Hertz-Knudsen equation has been implemented in a first step with which it is possible to calculate the number of evaporating particles per time step. The saturation pressure is defined by the Antoine equation for a given liquid temperature. Energies and velocities of particles evaporating from the liquid surface are sampled from a Maxwell distribution. For the simulation of the condensation process, colliding particles of the same species as the liquid are removed. The remaining gas particles are reflected applying diffuse scattering. Different test cases have been simulated, e.g. microscopic droplet evaporation effects for moving droplets. Figure 3 shows as an example the results for the drag coefficient in comparison to an analytic solution for low Reynolds numbers [7]. Significant differences occur in particular at higher Knudsen numbers of about 0.05 and above. The reasons might be continuum breakdown effects, which however have to be further investigated by additional simulations and validated by experiments. This relatively simple example illustrates the potential of the DSMC method to improve the fundamental understanding of micro-droplet-gas interactions.



**Figure 3.** Drag coefficient for an evaporating and a solid sphere simulated with PICLas compared to analytical values for respective Reynolds numbers. Parameters used for the simulation: 3D, Flow velocity 10 m/s, gas/droplet temperature 293 K, gas density 1.165 kg/m<sup>3</sup>, droplet diameter 1 / 10 μm, Knudsen number 0.05 / 0.005, total simulation time 10<sup>-6</sup> s, simulation time step 10<sup>-11</sup> s.

### SP-B6 (Ackermann, Helmig): Upscaling of coupled free-flow and porous-media-flow processes

The exchange of mass, momentum and energy across a drop-covered interface between a porous medium and an adjacent free-flow is essential for many technical applications and environmental scenarios. Modeling these

exchange processes requires a detailed understanding of the common interface and the interface processes depending on drop formation and growth. While the droplet-related interface processes happen at the micro-scale, the two flow regimes are usually governed by a macroscopic flow behavior.

In the following, we assume a single-phase gaseous free-flow and a two-phase liquid-gaseous flow in a porous medium. If the liquid phase in the porous medium reaches the common interface, it either evaporates directly into the free-flow or forms liquid drops on the porous surface. These drops have a direct impact on the exchange processes between the two flow regimes, among others by reducing the interface area available for transversal gas flux and by reducing the cross-section available to the free flow.

The aim of SP-B6 is to extend the upscaling technique by Baber et al. [8] to transfer the droplet-related micro-scale interface processes onto the macro-scale. The upscaled information can then be used by the macro-scale flow models to determine the drops' influence on the macroscopic flow behavior. Numerical models for the macro-scale flow regimes as well as a simple coupling concept, are already implemented in our in-house code DuMu<sup>x</sup> [9].

The interface is modelled as a lower-dimensional third domain between the free-flow and the porous medium model domains as shown in Figure 4. The lower-dimensional domain approximates the multi-scale behavior of drop formation, growth, and detachment. In the upscaling approach, the contributions of several pores are summed up to one drop. This allows computing the drop-free and drop-covered percentage of the interface. The coupling conditions for the exchange of mass, momentum and energy between the free-flow and the interface as well as between the interface and the porous medium are then weighted with these percentages to obtain a multi-scale approach. The drop formation and growth can be monitored, such that the current drop volume and its temporary evolution are the outcomes of our model. In addition, changes in the flow behavior caused by the interface drops will show in the macro-scale solutions towards complex drop dynamics such as spreading, merging and film flow.

The current model includes only the detachment of drops from the porous surface. The next step is to extend it towards complex drop dynamics such as spreading, merging and film flow.

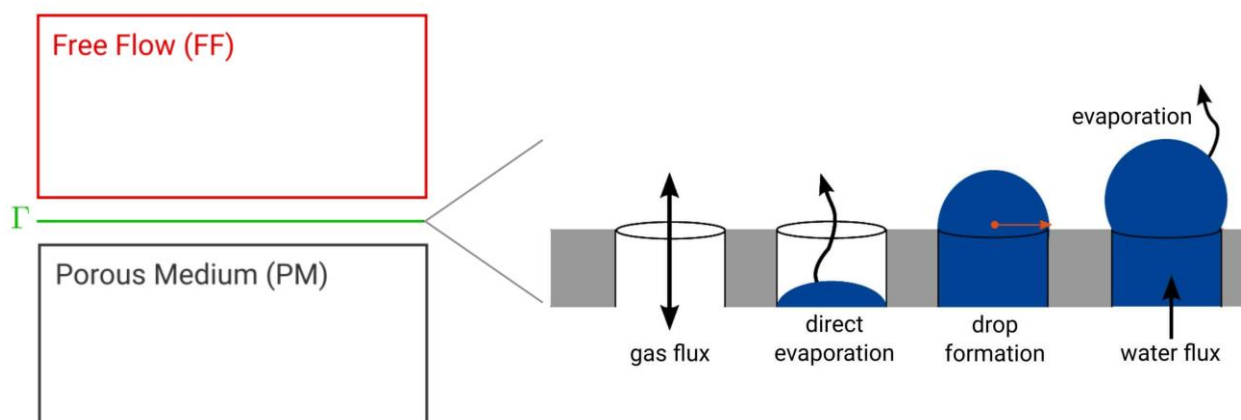


Figure 4. Lower-dimensional interface domain with drops

#### SP-C1 (Bernard, Lamanna, Roth, Tonini): Micro- and macro-drop impact dynamics with miscible liquids

This sub-project is aimed at understanding the outcomes related to liquid droplet impact on thin wall-films, by a unified approach coupling micro-scale flows within the wall-film with the corresponding macroscopic feature, i.e. the “crown” as represented in Figure 5(a). There is an ongoing intense cooperation with SP-C5 in order to develop novel observation techniques to capture the microscopic flow field within the wall-film. As a first step towards this goal, an extensive experimental database of macroscopic observations for a wide range of droplet and wall-film viscosities, wall-film thickness, and droplet impact velocity is built up. This database focuses on impacts with different liquids for droplet and wall-film (‘two-component’) in order to understand the role of droplet and wall-film liquids, and the effect of their miscibility gap. The experiments were conducted on a two-perspective high-speed shadowgraphy imaging system [10]. Preliminary investigations [11] on the limit between deposition and splashing outcomes provided a macroscopic understanding of the sensitivity to impact conditions (impact velocity, droplet diameter, liquid properties and dimensionless wall-film thickness  $\delta$ ). In the derived empirical correlation (Eq. 1) of the deposition/splashing limit, the fluid properties were taken as averages of the corresponding droplet and wall-film properties. This deposition/splashing limit led to a good repartition of the three crown-type outcomes: deposition, transition and splashing. Here, transition outcomes correspond to the formation of secondary droplets without ejection. Interestingly, the area near the limit where transition outcomes are observed behaves like a buffer zone, where all three crown-type outcomes statistically cohabit. Beyond this area, only deposition or splashing could be observed.

$$Oh_{ave} Re_{ave}^{1.29} = (4400 + 8900 \delta^{1.44})^{0.625} \quad (1)$$

In order to understand the deposition/splashing limit, it is necessary to determine the driving parameters of the fingering instabilities occurring during transition and splashing outcomes. This requires an investigation of crown expansion kinetics. A first study [12] focused on the scaling of maximum crown rim radius  $R_c$ . It is shown that the commonly used global maximum is not always representative of the expansion process. Indeed, the radius may keep increasing after the crown height recedes, as can be seen in Figure 5(b). The proper scale for rim radius expansion was found to be the radius at maximum crown height. The sensitivity of this length scale to the impact conditions was investigated and compared to predictions of the inviscid, one-component model of Roisman et al. [13]. This model was then empirically modified to take viscosity effects into account.

Rather than considering the time evolution of  $R_c$  and height  $H_c$  separately to characterise crown expansion, we now consider the time evolution of a unified parameter as the crown rim displacement from the impact location  $S_c$  (see Figure 5(a) for the geometric definition, and Figures 5(b), 5(c) for its temporal evolution). First, the energetic contribution to crown rim kinetic energy in both radial and axial directions is accounted for in  $S_c$ . Second, it is evident from Figures 5(b), 5(c) that the time evolution of  $S_c$  exhibits a maximum in both examples, in contrast to  $R_c$ . The time duration from the instant of impact to the time at which  $S_c$  reaches its maximum is then defined as the crown expansion stage. Interestingly, the time evolution of  $S_c$  during expansion can be fitted with a quadratic polynomial, plotted with dashed lines in Figures 5(b), 5(c), and exhibiting coefficients of determination greater than 0.99 in our entire database. This implies that the crown rim expansion could be modelled as a constant acceleration process as was suggested in a recent study on unsteady sheet fragmentation [14].

In summary, the work carried out in SP-C1 so far in cooperation with SP-C5, was to link the macroscopic features -impact outcomes- to relevant and quantifiable crown kinematic parameters in order to better comprehend the microscopic observations within the wall-film.

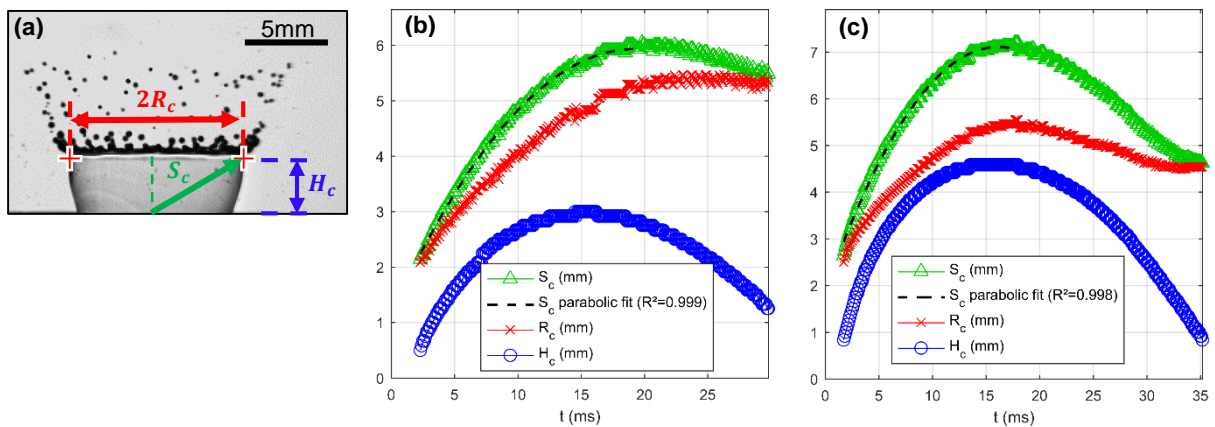


Figure 5. (a) Typical splashing case of a droplet impacting on a wall-film. The crown rim radius  $R_c$ , the rim height  $H_c$ , and the expansion parameter  $S_c$  are highlighted. (b), (c) Typical temporal evolutions of  $R_c$ ,  $H_c$ ,  $S_c$  and its parabolic fit till  $S_{c,max}$  for two types of crown rim radius expansion.

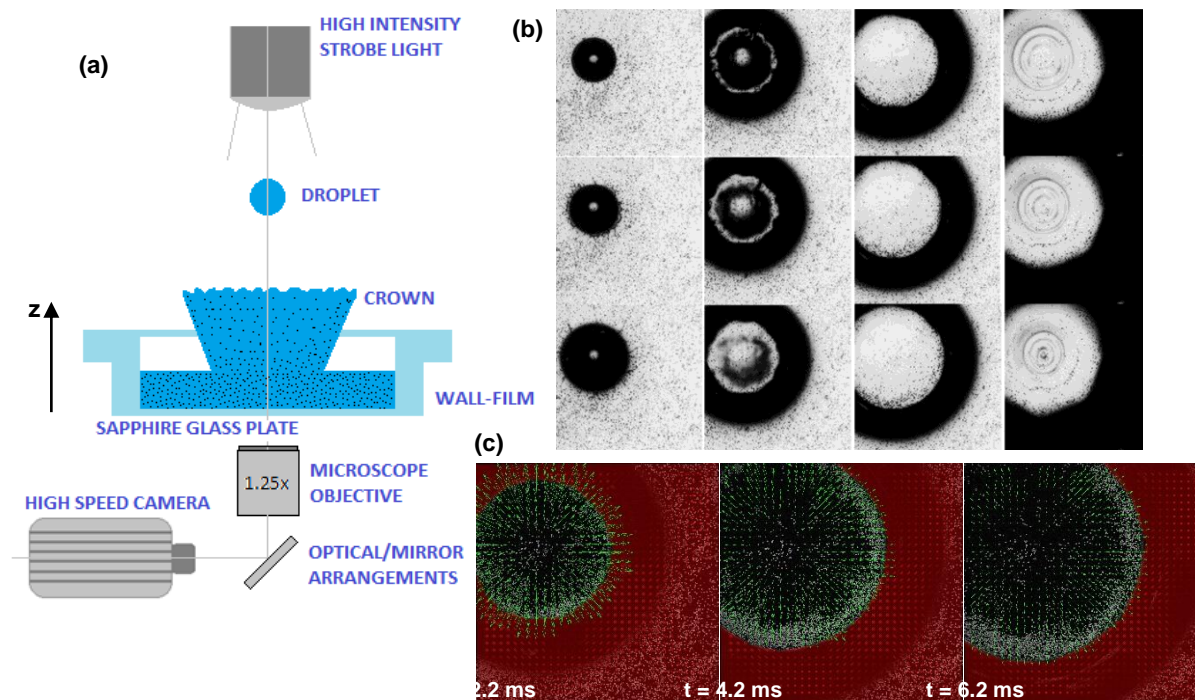
### SP-C5 (Vaikuntanathan, Weigand, Lamanna, Cossali): Development of novel optical technique for micro-fluid dynamics

The main goal of this subproject is to develop optical techniques for understanding the microscopic mechanisms leading to the macroscopic outcomes observed in SP-C1 and SP-C2 dealing with liquid droplet impact on thin wall-films and deep liquid pools, respectively. The current phase of this subproject is focused on understanding the velocity field within the wall-film responsible for the macro-scale outcomes of deposition, transition, and splashing as observed in SP-C1. For measuring the velocity field within the wall-film the experimental approach based on  $\mu$ -PIV is explored. There are several challenges in using the conventional  $\mu$ -PIV technique to the problem of droplet impact on wall-films. The traditional  $\mu$ -PIV technique, based on a double-pulsed low repetition rate laser and a high-resolution low frame rate camera, gives high temporal and spatial resolutions at a localized space-time coordinate in the flow field [15]. This is ideally suited for steady flows in micro-channels where it has been widely used [15]. The droplet impact phenomenon, on the other hand, is highly unsteady, characterised by spatio-temporal changes in the velocity field within the wall-film, as well as the wall-film thickness. Hence the traditional  $\mu$ -PIV cannot be employed here to get an overall picture of velocity field within the wall-film.

In order to overcome the limitation of traditional  $\mu$ -PIV technique, a high-speed  $\mu$ -PIV is employed. The entire set-up is schematically shown in Figure 6(a). A high-speed camera together with a high intensity and high repetition rate light source (strobe LED or laser) is used. A similar arrangement has been used for measuring velocity field inside droplets impacting on dry solid surfaces [16]. In the present case, the illumination is either in shadowgraphy mode (as in Figure 6(a)) or from the bottom of the pool. The wall-film is formed on top of a sapphire glass plate. Liquid droplet impact on this wall-film is imaged through the sapphire glass plate from bottom with the help of

microscope objectives giving overall magnifications from 12.5x to 400x. The image is projected onto the sensor of the high-speed camera giving spatial and temporal resolutions of 5  $\mu\text{m}$  (at 12.5x) and 200  $\mu\text{s}$  (at 5,000 fps), respectively. The wall-film is seeded with polystyrene tracer particles of diameter around 30  $\mu\text{m}$ .

Figure 6(b) shows typical high-speed microscopic shadowgraphy images of water droplet impacting on water wall-film. Figures 6(c) shows the corresponding velocity field calculated from selected images using PIVlab [17]. This gives an overall picture of the spatio-temporal evolution of velocity field within wall-film during the crown expansion stage. One of the limitations of the shadowgraphy approach is the inability to observe the velocity field within the wall-film near the neck region of crown base (dark region in Figure 6(b) and red masked region in Figure 6(c)). The ongoing experimental campaign uses a combination of shadowgraphy and bottom-lit illumination, and higher magnification with smaller tracer particles to measure z-resolved velocity field near the crown neck. Furthermore, to measure out-of-plane velocity component in this region, astigmatism  $\mu$ -PTV [18] will be explored.



**Figure 6.** (a) Schematic of the  $\mu$ -PIV experimental set-up, (b) typical high-speed  $\mu$ -PIV images from shadowgraphy (the droplet size is around 2.5 mm; time increases from top to bottom and left to right), and (c) typical z-averaged velocity field calculated from selected images similar to those shown in (b).

### Summary and Conclusions

This paper has shown the organisational structure, the qualification program and some selected results from selected subprojects within the International Research Training Group GRK 2160/1: “Droplet Interaction Technologies”, which has been established in October 2016. The work in the first funding period of this IRTG focuses on single drops and on the changes in the macroscopic flow properties due to the coupling between small scale effects with large scale effects on flow dynamics. Some selected results have been shown of SP-A2 on numerical investigations in compressible flows, on gas-kinetic simulations for micro-drop-gas interactions (SP-A3), on the upscaling of coupled free-flow and porous media flow processes (SP-B6). In SP-C1 some results are shown for droplet-film interactions for binary miscible fluids and SP-C5 introduced first results on novel measurement techniques for micro-fluid dynamics.

### Acknowledgements

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## Nomenclature

$H_c$	crown height [m]
$Kn$	Knudsen number [-]
$N$	number of discrete particles [-]
$M_{\text{level-set}}$	polynomial degree of level-set [-]
$Oh$	Ohnesorge number [-]
$R_c$	crown rim radius [m]
$Re$	Reynolds number [-]
$Sc$	crown rim displacement from impact location [m]
$t$	time [s]
$x, y, z$	coordinates [m]
$\delta$	dimensionless film height [-]
$\rho$	density [ $\text{kg m}^{-3}$ ]
$\Gamma$	interface location [-]

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