Selected Results of the Collaborative Research Center “Droplet Dynamics under Extreme Ambient Conditions - SFB-TRR 75”

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Abstract

A fundamental understanding of droplet dynamics is important for the prediction and optimization of technical systems involving drops and sprays. The Collaborative Research Center (CRC) SFB-TRR 75 was established in January 2010 to focus on the dynamics of basic drop processes, and in particular on processes involving extreme boundary conditions, for example near thermodynamic critical conditions, at very low temperatures, under strong electric fields or in situations involving extreme gradients in the boundary conditions. The goal is to gain a profound physical understanding of the essential processes, which is the basis for new analytical and numerical descriptions and for improved predictive capabilities. This joint initiative involves scientists at the University of Stuttgart, the TU Darmstadt, the TU Berlin, and the German Aerospace Center (DLR) in Lampoldshausen within 18 projects. The present contribution provides a brief overview of the structure of this CRC, of projects being carried out at the SFB-TRR 75 and some scientific highlights of selected projects. The main purpose of this article is to familiarize colleagues with this extensive and dedicated research effort in this area of drop dynamics and to motivate further collaboration with others in this field.

Keywords

Droplet dynamics, extreme boundary conditions, spray combustion, phase change.

Introduction

Many processes in nature and technology are influenced by droplet dynamics. These include ubiquitous phenomena and applications, such as rain clouds or fuel injection into combustion chambers, but also highly advanced devices such as rocket engines or spray based production processes in the pharmaceutical industry. While there are many scientific results available for droplet processes and complex systems, they are often restricted to moderate ambient conditions. However, many processes take place under extreme boundary conditions. This holds for the near-critical or supercritical conditions in modern combustion engines as well as for thunderstorm clouds with their high electric fields or supercooled droplets impinging on airplane wings, to name just a few examples. Much less research has been conducted in these areas, which is due to the high effort in theoretical and numerical modelling or the necessary complexity of experimental equipment. Therefore, detailed research in this area not only demands extensive development or improvement of experimental techniques and numerical models, but also very close interaction between numerical and experimental research. Thus, the consequent involvement of expertise from fields like thermodynamics, fluid mechanics, mathematics, computer sciences, electrical engineering and visualization is required. The SFB-TRR 75 combines the knowledge and experience of scientists from the above-mentioned subject areas.

Following the insight that complex droplet dynamic processes are determined by the interaction of fundamental processes, the CRC investigates since 2010 such processes. Selected results of the work in the SFB-TRR 75 can be found for example in [1-4]. In the current phase the CRC operates 18 subprojects in three research areas, which are listed below together with the individual involved project leaders:

Research Area A: Methods and Fundamentals

- TP-A1: Interactive visualization of droplet dynamic processes (T. Ertl, S. Boblest)
- TP-A2: Development of numerical methods for the simulation of compressible droplet dynamic processes under extreme conditions (C.-D. Munz)
- TP-A3: Analysis and num. of front and phase field models for droplet dynamics (C. Rohde)
- TP-A4: Molecular dynamics simulations of droplet evaporation in the non-linear response regime (F. Müller-Plathe)
- TP-A5: Simulation of the mechanical deformation and movement of droplets under the influence of high electric fields (E. Gjonaj, S. Schöps)
- TP-A7: Modelling and simulation of droplet collisions at changed ambient pressures, high velocity- and concentration gradients and for immiscible fluids (D. Bothe, K. Schulte)

Research Area B: Free Droplets

- TP-B1: Investigation of the behaviour of supercooled droplets concerning evaporation, condensation and freezing at different boundary conditions (B. Weigand)
- TP-B2: Experimental investigation of droplet evaporation under extreme conditions using temporally highly resolved laser diagnostic methods (G. Lamanna, A. Dreizler)
- TP-B3: Modelling and simulation of droplet evaporation in different gas environments under supercritical conditions (A. Sadiki)
- TP-B4: Experimental investigation of transient injection phenomena in rocket combusters at vacuum conditions with flash evaporation (M. Oschwald)
- TP-B5: Modelling and simulation of the flash evaporation of cryogenic liquids (A. Kronenburg)
- TP-B6: Droplets subjected to temperature- and velocity gradients using atomistic simulations (J. Vrabec)

Research Area C: Droplets with Wall-Interactions

- TP-C1: Numerical simulation of the transport processes during drop impingement onto heated walls with special consideration of the evaporating three-phase contact line (T. Gambaryan-Roisman, P. Stephan)
- TP-C2: Highly resolved measurements of heat transfer during drop impingement onto a heated wall with particularly consideration of evaporation at the three phase contact line (P. Stephan, T. Gambaryan-Roisman)
- TP-C3: Impact of supercooled droplets onto cold surfaces (S. Jakirlic, C. Tropea)
- TP-C4: Interaction of a single drop with a heated wall at high ambient pressures (I. Roisman, C. Tropea)
- TP-C5: Mechanical and electrical phenomena of droplets under the influence of high electric fields (V. Hinrichsen)

- TP-Z Administration of the SFB-TRR 75 (B. Weigand)

In Research Area A numerical and analytical methods are developed which are prerequisites for conducting the work in the other research areas. In addition, methods for visualization are developed and applied to various other subprojects. All projects in Research Area A contribute fundamental results to Research Area B and Research Area C. In Research Area B free droplets are investigated. Here, investigations involve freezing droplets in clouds, droplets behaviour near the critical point as well as flash evaporation. In Research Area C droplet-wall

interactions are investigated. This includes drop impingement on heated walls, droplet-wall-interactions of supercooled drops as well as droplet behaviour in high electric fields.
The administration of the CRC is embedded in TP-Z. Within this project an extensive guest scientist program is organized which involves a large number of international renowned experts. Further information can be found on the web-page: www.sfbtrr75.de.

Results and Discussion

In the following some selected results of the CRC are presented and discussed.

Binary Collisions of Immiscible Fluids

(TP-A7, TP-B1: V. Kunberger, J. Potyka, K. Schulte, B. Weigand, Institute of Aerospace Thermodynamics, University of Stuttgart and TP-C4: B. Schmidt, I. Roisman, Institute for Fluid Mechanics and Aerodynamics, TU Darmstadt in cooperation with D. Baumgartner and C. Planchette from Graz University of Technology)

Binary collisions of immiscible fluids with different fluid combinations were investigated experimentally with a focus on the collision morphology and the influence of wettability. Three different fluid pairs were selected. The total wetting behaviour was observed using the silicone oil M5 and an aqueous glycerol solution. The partial wetting case was studied with bromonaphtalene and an aqueous glycerol solution. The third fluid combination was hexadecane and an aqueous glycerol solution. The experiments were conducted with an acoustic levitator. The other fluids were dropped from a needle and to distinguish them from the glycerol solution, they were coloured with blue dye. Both droplets were similar in size of about 2 mm. The collision was observed with two high speed cameras. All of the studied collisions were in the separation regime which was expected due to the relative velocities investigated. For the partially wetting fluids de-wetting was observed in several cases, leading to an almost complete separation of the fluids after the collision, which is shown in Figure 1.

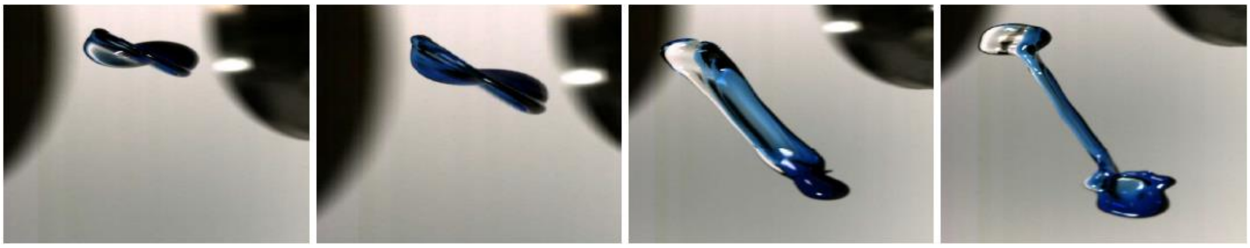

Figure 1. Collision of partially wetting fluids (bromonapht. and 73.5% aqueous glycerol solution) with de-wetting.

Figure 2. Collision of partially wetting fluids (hexadecane and 73.5% aqueous glycerol solution).

In the images of the colour camera, it was observed that after spreading over the glycerol solution, the bromonaphtalene receded, leaving a small isle of liquid on top of the glycerol and the remaining fluid mass moved downwards due to its momentum. De-wetting was neither been observed for the fully wetting case nor for hexadecane. It was also possible to measure different characteristic parameters during the collision: The encapsulation time, the rim velocity and the relative velocity of the droplets. The difference between the rim velocity and velocity derived from the encapsulation time is that during the encapsulation time only a thin film of the fluid moved across the surface, whereas most of the fluid mass moved along the impacted droplet with the rim. It was possible to estimate the order of magnitude of the velocities. It was found that always $U_{\mathrm{rim}} < U_{\mathrm{rel}} < U_{\mathrm{encap}}$ for the experimental series conducted. There was no significant difference in the characteristic velocities for fully and partially wetting fluids. As the use of a coloured camera proved to be very useful for the observation of the collision morphology of immiscible fluids, a new campaign with a refined setup is currently under preparation.

Investigations of Multi-Component Fluoroketone Jet Injections at High-Pressure Conditions: Simulations in a Eulerian-Eulerian context

(TP-B3: D. Kuetemeier, A. Sadiki, Energy and Power Plant Technology, TU Darmstadt)

There is a great interest in trans- and supercritical atomization processes in high pressure and temperature applications, e.g. rocket engines, high pressure piston engines and chemical production. Therefore, a detailed understanding of trans- and supercritical processes is essential to improve such applications. Most of those applications have an injection process in common: Sub- or supercritical fluids are injected and atomized, while mixing processes occur in order to optimize combustion efficiency or chemical reaction rates. A Eulerian-Eulerian approach is utilized to establish a framework which is capable to produce accurate predictions of thermodynamical processes surrounding and crossing the critical point of single species simulations as well as of mixed species systems in particular. In mixtures at extreme thermodynamic conditions one can observe shifting of the critical point of the mixture in comparison to the single species. Therefore, it is essential to be able to retrieve all possible states of sub-, trans- and supercritical mixtures, regardless of their (pseudo-) gaseous or (pseudo-) liquid state. In order to establish such a numerical tool which is both computationally efficient and economically acceptable, a Large Eddy Simulation (LES) framework which includes the WALE subgrid-scale model and well-adapted multi-component species diffusion and mixing models is used to study fluoroketone jet injection configurations at high-pressure conditions. All LES simulations are conducted with the open-source solver OpenFOAM utilizing an in-house low Mach solver which includes real gas properties by means of the Peng-Robinson equation of state to deal with high pressure conditions. The configuration under study features supercritical fluoroketone injected through an elliptic orifice into a supercritical

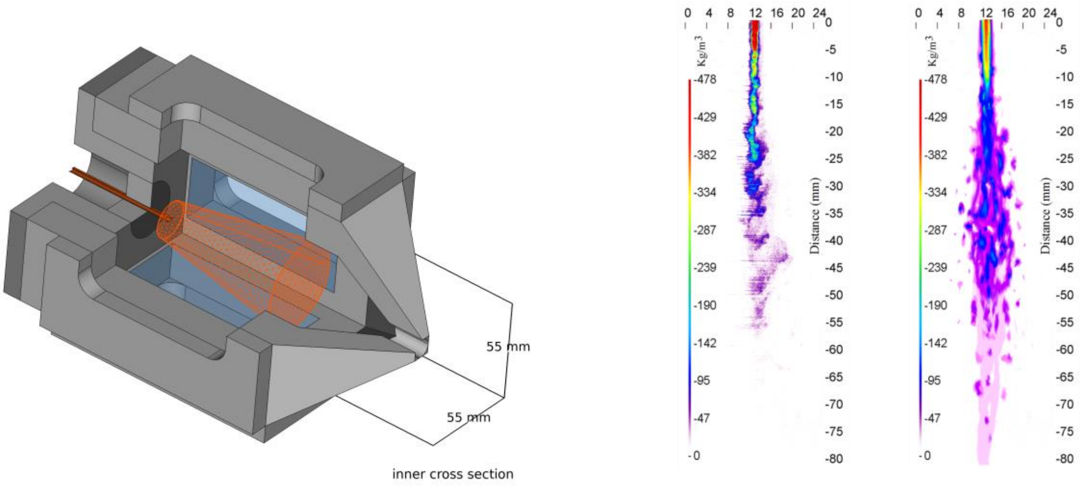

Figure 3. Left: Computational domain embedded in a drawing which corresponds to the experimental setup used in [5, 6]; Right: Comparison of experimental [5] and preliminary simulation results of the density field.

helium environment as experimentally investigated in [5, 6]. Exemplary, a preliminary qualitative result representing the density field is shown in Figure 3 in comparison with available experimental data [5]. Thereby, the jet penetration is well predicted while a deviation is observed in the jet spreading rate.

Modelling and Simulation of the Flash Evaporation of Cryogenic Liquids

(TP-B5: J.W. Gärtner, A. Kronenburg, Institute for Combustion Technology, University of Stuttgart)

The development of new upper orbit thrusters aims at replacing hypergolic propellants such as hydrazine by more environmentally friendly fuels such as hydrogen or conventional hydrocarbons. Combustion of the latter typically implies the injection of cryogenic propellants into a near vacuum that leads to a superheated state of the liquid and a rapid and strong evaporation. This process is called flash evaporation. Due to the evaporating liquid the flow exits the injector with a higher pressure than the ambient conditions which leads to a shock system downstream. A compressible two-phase solver has been developed in OpenFOAM [7, 8] to simulate the flashing process from liquid injection to nucleation, bubble growth, breakup and coalescence. This solver uses the volume of fluid approach to distinguish between the two phases and the homogeneous relaxation model to calculate the evaporation rate. It is then applied to a jet of flashing cryogenic nitrogen case that is investigated experimentally in TP-B4. Some flow "anomalies" have been observed in shadowgraph movies where dark regions appear to be stationary in the flow or even floating slightly upstream (Rees et al. [9]). The simulations show that a recirculation zone forms after the Mach disk due to the interaction of regions of high speed at the side of the jet and of low speed after the shock front. While the shadowgraph images cannot proof the existence of such a recirculation zone the combination of numerical results and experimental data provide strong indication for such a phenomenon. In Fig. 4 the velocity profile of flashing liquid nitrogen with a superheat ratio of $\mathrm{R_p} = p_{Sat}(T_{inj}) / p_C = 48.1$ is compared to the shadowgraph image of the experiment. It can clearly be seen that the position of the recirculation zone matches with the dark region found in the experiment. In conclusion, the combination of numerical and experimental work demonstrates the existence of a shock in fully flashing flows with a high superheat ratio $\mathrm{R_p}$ and their effect on the flow further downstream.

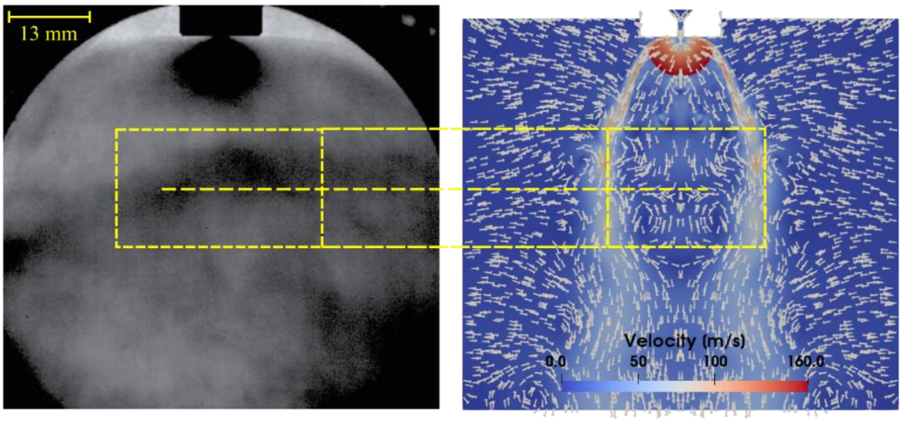

Figure 4. Shadowgraph image compared to simulations of the velocity magnitude and the velocity vectors. The position of the recirculation zone seen in the simulation is marked through the yellow box.

Interaction of a Single Drop with a Heated Wall at High Ambient Pressures

(TP-C4: J.B. Schmidt, I.V. Roisman, C. Tropea, Institute for Fluid Mechanics and Aerodynamics, TU Darmstadt)

Spray cooling is a promising high performance cooling technology achieving high heat transfer rates. Existing correlations to describe spray cooling are mostly empirical, since most sprays are complex and characterized by a wide distribution in drop diameters and drop velocities. Therefore, it is necessary to reduce the complexity of sprays to develop physics-based models of spray cooling, achieved by studying single drop impacts.

The isothermal drop impact is determined by impact parameters, fluid properties, surface parameters and ambient conditions. The non-isothermal drop impact is additionally affected by thermal influences, such as boiling and/or Marangoni effects. Drop impacts onto a surface with a low superheat lead to drop deposition and slow evaporation of the drop. In cooperation with TP-C1 the heat flux of two parallel impacting droplets has been described in [10]. Above saturation temperature, nucleate boiling can be observed. The heat flux in the nucleate boiling regime is described in [11] and shown in Fig. 5 by the resulting residence time $t_{deposit}$. With increasing substrate temperature, the drop starts to rebound, while sticking to the surface, causing a phenomena called drop dancing [12]. From the surface temperature T_{σ} on, vapor bubbles are leading to vapour clusters and the drop rebounds, caused by thermosuperrepellency [13]. The residence time of the drops is in the order of the natural oscillation time of drops t_{σ}. The short residence time allows to model not only the heat flux of a single drop impact but also the heat flux of a spray impact by superpositioning single drop events, as described in [14]. With high impact velocities, local contact between the drop and the surface can be observed even at high surface temperatures, as described for the thermal atomization regime [12]. The thermal atomization is characterized by a strong nucleation with a fine secondary spray [15]. The measurement of the local heat flux during drop impact in different impact regimes with a high spacial and temporal resolution is shown in [16]. A comprehensive review of the single drop impact and spray cooling can be found in [17].

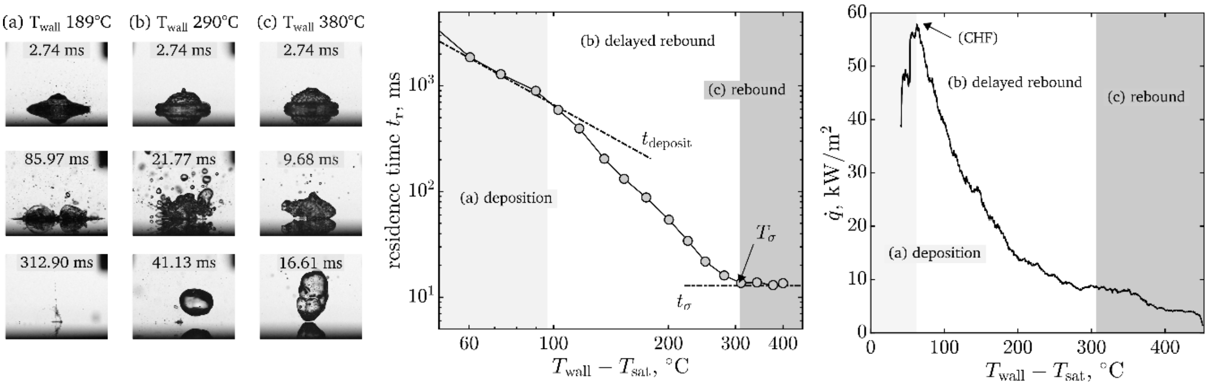

Figure 5. Side view observations of single drop impacts in the impact regimes drop deposition, delayed rebound and drop rebound. The plot in the middle shows the corresponding residence times with the corresponding models in the drop deposition regime $t_{deposit}$ and the drop rebound regime t_{sigma}. The right plot shows a boiling curve of an impacting drop chain with similar impact parameters. The onset of nucleate boiling correlates well with the critical heat flux (CHF), while the thermosuperrepellency correlates well with a constant heat flux.

The current focus of the project is the heat flux of a drop chain impacting onto a hot surface. In Fig. 5 an exemplary boiling curve is shown together with the three drop impact regimes drop rebound, delayed drop rebound and drop deposition. This study will help to develop still missing elements of a reliable spray cooling model, based on the description of the hydrodynamic and thermodynamic processes in the drop and in the spray.

Ice Nucleation under the Influence of High Electric Fields

(TP-C5, J.W. Löwe, V. Hinrichsen, High-Voltage Laboratories, TU Darmstadt)

Power distribution and transmission systems are operated at different environmental conditions. Especially, in cold regions the efficiency and reliability of the system might be highly affected by ice accretion at overhead line conductors or high-voltage insulators. Whether the presence of an electric field promotes or inhibits the formation/accretion of ice is investigated in the scope of TP-C5. Therefore, ice nucleation in supercooled water droplets is examined under well-defined boundary conditions with respect to the temperature of the droplets and the applied electric field strength. Several different types of electric fields, namely constant, alternating and transient electric field are used to determine the impact of electric fields on ice nucleation. In addition, the strength, frequency and time constants of the electric field are varied to reveal the relevant physical mechanisms and to contribute to the ongoing and contrary discussion if electric fields can influence ice nucleation or not. While constant electric fields are identified to have a minor influence on ice nucleation [18], the effect of alternating electric fields on ice nucleation is significantly larger [19]. The electric field promotes ice nucleation and causes the droplets to freeze at higher temperatures compared to the reference case without an electric field. Exemplary results for the impact of an alternating electric field are shown in Fig. 6. The liquid fraction N_l/N_0, where N_l is the number of liquid droplets at a temperature ϑ and N_0 the number of initially liquid droplets, depending on the droplet temperature ϑ_d is shown for various electric field strengths. Especially, high electric field strengths significantly promote ice nucleation. Besides the electric field strength, the frequency of the electric field is identified to also affect ice nucleation. Generally, the impact of the electric field on ice nucleation is more of singular nature rather than stochastic. Each droplet is associated with a characteristic electric field strength necessary to impact ice nucleation (similar to the already known influence of temperature), which is shown by the increasing number of droplets affect by the electric field for increasing electric field strength, see Fig. 6. Consequently, ice nucleation might be significantly affected by high electric fields. The impact depends on several influencing factors like the electric field strength, frequency and type of the electric field, which are investigated in the scope of TP-C5 under well-defined conditions.

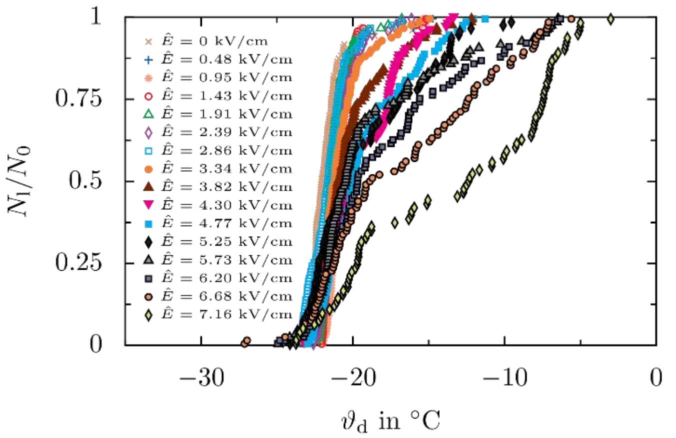

Figure 6. Ratio of liquid droplets N_l and initially liquid droplets N_0 (“droplet survival curves”) depending on the droplet temperature ϑ_d, for varying electric field strengths $\hat{E}$ and a constant frequency of $f = 50$ Hz. Reprinted figure with permission from [19], Copyright 2021 by the American Physical Society.

Conclusions

The paper has shown the structure of and the work carried out in the Collaborative Research Center SBF-TRR 75: “Droplet Dynamics under Extreme Boundary Conditions”. The work in the current funding period of this CRC focuses on groups of several drops and on the behaviour and application of sprays under extreme ambient conditions.

Acknowledgments

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Nomenclature

E	electric field strength [V m^{-1}]
f	frequency [Hz]
N_0, N_1	initial liquid drops, liquid drops [-]
$t_{deposit}$	residence time of a drop [s]
t_σ	time of natural drop oscillation acceleration [s]
T_σ	onset temperature of thermosuperrepellency [°C]
R_p	superheat ratio
U_rim, U_rel, U_encap	velocities (rim; relative; based on encapsul. time) [ms^{-1}]

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