Fuel Injector Research for Sustainable Transport

FP7-265848-FIRST

Final Publishable Summary Report

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Co-ordinator:	**Rolls-Royce PLC**

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1. Executive Summary

The principle objectives of the FIRST (Fuel Injector Research for Sustainable Transport – FP7 265848) project were to develop our understanding and predictive modelling capabilities of the atomisation and soot production processes relating to aviation engine combustors. With the improved understanding of the physics and the upgrades to industrial modelling tools gained in FIRST the design tools of aviation engine combustors are now improved enabling a future reduction in aviation emissions. In this way the FIRST project has helped to increase the competitiveness of European aviation industries. The project was structured into four research work packages with more details given in the following paragraphs.

In Work Package 2 fundamental work was performed to improve sub-modelling techniques to describe the atomisation process and soot formation. For spray the project developed methods, such as, Volume of Fluids, Level Set, Conservative Level Set and Smooth Particle Hydrodynamics. Some models are computationally expensive and work was performed to implement and develop Adaptive Mesh Refinement techniques to resolve only the most critical areas of the interface between air and liquid. Also, the parallelisation of some of the codes was developed so that computations could be run simultaneously on many computer cores greatly reducing overall calculation times. Within this work package the development of soot sub-models was performed with attention focussed on the modelling of the soot precursor molecules. Different modelling strategies have been developed and shown improved predictive capabilities and our knowledge of the thermodynamic and chemical kinetics of soot formation has been advanced.

The activities in Work Package 3 provided the experimental data used to validate the improved numerical models and increase our understanding of the physics of atomisation and soot producing flows. Experimental data was collected from test rigs of simple fundamental geometries, idealised injector configurations and actual aviation engine injectors. The geometries included planar liquid sheets in shear flows, jets in shear flows, simplified swirling flow injector geometries and various aviation injectors as used by the project's industrial partners. A multitude of experimental techniques were developed and applied within this project and these provided information on liquid droplet sizes, particle size distributions, liquid breakup lengths, liquid flapping frequencies and the relation to aerodynamic velocities. Experiments with ideal and industrial injectors also provided data on soot formation, the relation to combustion species such as OH, fuel location and temperature fields providing exceptional information for the development of numerical models.

Development of spray and soot models in ideal geometries was the focus of Work Package 4. RANS and LES codes were updated with the new models validated in Work Package 2 and used to predict experimental data obtained in Work Package 3. The full modelling techniques were used to assess the spray characteristics and their effect on soot production in more representative configurations. RANS and LES simulations of ideal injector geometries using finite rate chemistry, a sectional approach for PAH formation and a two-equation soot model have been applied to the experimental soot database described above with some success. This result is very encouraging considering that in the past soot modelling has been very inaccurate.

Work Package 5 exploited the developed codes and experimental data to improve the industrial partner's design tools for modelling spray and soot production. Improvements in the design tools have been validated against injector and combustor geometries for helicopter and aircraft combustor applications. Traditionally, empirical calculations have been used to provide spray boundary conditions and the work in the FIRST project has greatly improved this weak area. The various methods mentioned above for the primary break up, secondary break up, spray transport and particle clustering have been validated on real world combustors. The improvements in knowledge of the spray boundary conditions has meant that the efficacy of the new soot modelling techniques have also been explored in combustor environments and applied with more confidence.

2. Project context and main objectives

The main objectives of the FIRST project were to deliver a fuel spray atomisation prediction capability, which could represent the unsteadiness of the atomisation process for gas turbine injectors, and to deliver an improved soot/particulate modelling methodology for combustion CFD. These objectives broken down into a little more detail below:

The project aimed at delivering essential experimental data measured using advanced, high speed diagnostics across a range of geometries representing different methods of atomisation (filming or jet), and a range of operating conditions (low to high pressure). This was important to clarify the dominant physical processes in the fuel spray and to validate the numerical models developed. Similarly, the measurements of soot would be critical to the understanding of the soot processes as well as validating the numerical models. All experimental techniques developed in FIRST in support of both sprays and soot would be available for application to the research and development of future injection systems and combustors.

Improvements to the numerical modelling of sprays would provide a capability that would use the fuel injector geometry in combination with the fuel and air flow conditions to predict the fuel injector’s spray properties with an emphasis on the spatial and temporal unsteadiness. These properties would include the droplet size distribution, the air and fuel placement in either mean or fluctuating quantities. These spray quantities could then be transferred into multi-physics CFD calculations of the combustor geometry for the prediction of combustion functional performance and exhaust emissions. The numerical simulation methods would be split into two research avenues. Firstly, highly accurate direct numerical simulations would be used to further the understanding of the atomisation process and to provide information for the modelling techniques for more practicable lower resolution models. Secondly, to deal with realistic configurations, two-fluid models and phenomenological models would be developed based on the information provided from the high resolution modelling and validated against the experimental work.

The soot tasks in FIRST would aim at delivering a more accurate methodology for predicting the soot emissions in combustion systems. This would be in the form of sub-model code to be embedded in CFD tools and a methodology or practice for its implementation and use. Before the project, industrial calculations of combustors did not include complex chemistry. In FIRST, gas phase chemistry would be limited to reactions with Polycyclic Aromatic Hydrocarbons (PAHs) and soot would be treated as additional species with relevant, validated oxidation reactions. After development and validation of CPU intensive academic soot modelling tools, the resulting modules would be incorporated into industrial codes in reduced form for exploitation. The resultant soot predictions would essentially be enhanced by the more accurate fuel spray boundary conditions.

The project was divided in six Work-Packages as can be seen in Figure 1. The research ran from December 2010 to November 2014.

The consortium was constituted of twenty participants from the United Kingdom, France, Germany and Italy.

Rolls-Royce PLC (Coordinator)
A2 Photonic Sensors
GE AVIO
CERFACS (Centre Européen de Recherche et de Formantion Avancée en Calcul Scientifique)
CNRS (Centre National de la Recherche Scientifique), CORIA and LEGI labs
DLR German Aerospace Centre
EnginSoft
Imperial College of Science, Technology and Medicine

UPMC (Université Pierre et Marie Curie)
KIT (Karlsruher Institut fuer Technologie)
Loughborough University
MTU Aero Engines AG
ONERA (Office National d'Etudes et de Recherches Aerospatiales)
Rolls-Royce Deutschland
Snecma
Turomeca
Universita degli studi di Bergamo
Universita degli studi di Firenze
ARTTIC
Scitek consultants

3. Scientific and Technological results/foreground

A summary of the scientific and technological results is provided below.

3.1 WP2

This Work package is devoted to the development and test of simulation methods to tackle the physical and chemical processes from:

- the primary and secondary atomisation of the liquid,
- the spray behaviour (formation, transport, evaporation)
- to the soot formation

The primary atomization of liquid fuel in airblast injector systems is one of the most difficult phenomena to predict. In the framework of this work package, an effort was undertaken to improve **Direct Numerical Interface** methods in order to be able to simulate accurately what is going on in academic configurations representative of industrial ones. Different types of methods were used in this work-package: Volume of fluid (UPMC), coupled Volume of fluid – level-set (CORIA, ONERA), conservative level-set (CORIA), Smooth Particle Hydrodynamics (KIT), multifluid diffuse interface method (ONERA).

Numerical simulations are known for becoming unstable for atomization processes with large density ratios coupled with large shear. CORIA thus developed a new consistent mass and momentum flux computation using Rudman type technique in ARCHER code (coupled Level Set / VOF / Ghost fluid methods). The original method was using two grids and the project partners set-up a more efficient algorithm, in order to carry out all the calculations on a single grid. An adaptive mesh refinement algorithm for incompressible two phase flows with the interface capturing method was also developed. Specific effort was devoted to the parallelization of this new code, and emphasis was put on load balancing which remained a great challenge when grid refinement was used. Several tests cases were run in order to validate the code before large computations on air assisted atomization were performed. In Figure 2, an example of round liquid jet atomization is shown with adaptive mesh refinement.

During the FIRST project, significant improvements have been added to the DyJeAt code developed at ONERA. A new parallel adaptive mesh refinement based on paramesh library was developed to get a more accurate interface capture at a lower computational cost. It was mainly based on block refinement, where block stands for at least a hundred computational grid cells. Mass conservation through a coupled level-set /Volume of fluid/Ghost fluid was also taken into account. Finally, as the ultimate goal of such direct interface simulation is to give the droplets diameters distribution at the end of the atomization process, an original Eulerian-Lagrangian coupling strategy has been developed strongly linked with the AMR (Adaptive Mesh Refinement). As the atomization rate increases downstream, more and more small droplets are produced, this will lead to refinement everywhere in the computational domain and the benefit of AMR is lost. In order to avoid this drawback, based on relevant criteria of droplet under-resolution, the latter are transformed either in spherical volumic droplet or in point droplet particle and in both cases transported in a Lagrangian way. An example of Eulerian-Lagrangian AMR simulation corresponding to ONERA planar sheared liquid sheet is shown in Figure 3.

UPMC has extensively worked on the testing and improvement of Gerris, a free Volume-of-Fluid code with octree. Several bugs have been corrected but serious problems remain that prevent performing certain types of simulations. In order to circumvent these difficulties, UPMC has started the development of two new free codes, ParisSimulator and Basilisk. An example of simulation with also Eulerian-Lagrangian coupling corresponding to the LEGI experiment (thick sheared liquid film) is plotted in Figure 4.

CORIA has developed and applied numerical methods for primary atomization to realistic injectors (code YALES2). The aim was twofold: i) to validate the numerical strategy in terms of accuracy and robustness, ii) to identify the bottlenecks and the potential improvements. The simulations of the triple injector, the ONERA liquid sheet with swirl and of the Turbomeca injector highlighted the need for high mesh resolution at the air/liquid interface, which may only be obtained through manual or automatic local mesh adaptation. In Figure 5, is shown the simulation of sheared liquid film in turbomeca injector configuration.

KIT developed a Smoothed Particle Hydrodynamics (SPH) method with the goal to predict primary breakup of liquid fuels in industrial air blast atomizers. The motivation for using this new approach is mainly due to the shortcomings of commonly used numerical methods for multiphase simulation when it comes to the treatment of air assisted atomizers. The most important features of the code are robust inlet and outlet boundary conditions, as well as arbitrary periodic boundaries. Regarding the physical modeling of multi-phase flows, a new surface tension model was implemented which allows the handling of realistic fluids (air, fuel). In the course of the project 2D and 3D simulations have been conducted. Basic test cases have been computed to validate the physics and the numerics of the code. To assess the capabilities of the method regarding primary atomization, an experimental setup from the KIAI project has been used as reference. The results obtained by corresponding 2D and 3D simulations show that SPH is capable to correctly reproduce the experimental observations qualitatively as can be seen in Figure 6. Shear driven liquid film transport, accumulation and flapping effects, the formation of liquid sheets and droplets match the experimental findings. To be able to quantitatively compare statistical results, such as mean droplet diameters or break up frequencies, more detailed and comprehensive simulations are necessary.

ONERA has been also working on an industrial/engineering oriented approach which would allow multi-phase flow simulations to inject the droplet by taking into account the largest scales of the primary atomization unsteady process. This approach is designed to be integrated in existing LES combustion solvers, where fuel is represented by a dispersed phase. A more detailed resolution of droplets generation is obtained by performing a time-resolved simulation of the liquid sheets (or jet) atomization by a multi-fluid solver, and then by employing an atomization model to detail the local droplets generation. The multi-fluid solver allows the capture of the main features of primary atomization, in particular the longitudinal large scale oscillation and the formation of the largest liquid structures. This information feeds a sub-grid droplet generation model which acts as an advanced spray injector, able to interact with the chamber multi-phase flow and furnishing accurate inlet condition for the dispersed phase solver. This approach is meant, in the long run, to replace the current statistical simplified and steady-state injection models. In Figure 7, two results are shown on primary atomization simulations based on large scale approach, the first one corresponds to the ONERA experiment on planar liquid sheet, the second one to the TURBOMECA injector. It should be emphasized that this is the first time such a calculation has been successfully performed. Indeed, with the same tool, one can simulate the complete primary atomization phenomenon in an industrial configuration.

Concerning the subscale models for the spray formation, IMPERIAL developed several models of progressive complexity and realism and implemented them in the openFOAM solver. Namely a new Lagrangian-Eulerian solver was developed in the openFOAM environment, as the one offered was not capable of modelling transient and coupled simulations. Figure 8 shows slices through the sudden expansion test case, some distance downstream of the step with the flow structures present in the flow. Correlating the surrounding flow structures with sudden changes in the curvature of the particle trajectories provided insight into those structures responsible for sudden and large changes in particle trajectory directions. Summarizing, openFOAM's capabilities where evaluated through a series of academic configurations of progressive complexity with the subsequent development of custom solvers for use in generating detailed LES datasets of Eulerian-Lagrangian simulations of a particle laden axisymmetric sudden expansion to be used for the evaluation of the phenomenological model using in

During the FIRST Project UNIBG developed a numerical methodology to predict the flow inside the nozzle and at nozzle exit proximity in a swirling pressure injector for aero-engine applications under isothermal non reacting environment, whose geometric and operating conditions have been provided by AVIO. A combination of single and two-phase flow Eulerian models implemented in in-house and commercial CFD codes has been used to predict the flow in the selected injector (see Figure 9(a)) with the scope to provide the necessary input conditions for successive atomisation modelling. The models have been applied to take-off test case scenarios. Figure 9 b) presents a sample of the two phase flow development within the injector and at nozzle exit proximity as predicted by 3D VOF simulations. The results evidenced that, among the selected parameters, the lamella thickness and the injection flow rate are the most sensitive ones to the evaluation of the d_{30} mean diameter. A novel formulation of the primary atomisation model developed for swirling flows, has been proposed, accounting for turbulence and aerodynamic effects on the liquid primary break-up. Figure 10 reports the probability density functions for two flow rates, calculated according to the maximum entropy formalism model, and using as inputs the values of d_{30} and d_{max}. The results confirm the remarkable effect of fuel injection operating conditions on the spray drop sizes, while the deviations of the predictions linked to the numerical accuracy in predicting the flow development within the selected injector are less evident, provided that detailed two-phase flow CFD simulations on sufficiently high refined grids are used to acquire the necessary boundary conditions for the atomisation modelling.

Concerning soot modelling, new sophisticated models have been developed and tested and applied to industrial combustor configurations.

At DLR, sectional soot precursor model with reversible surface chemistry was developed and implemented in THETA. The new model includes stable PAH (polycyclic aromatic hydrocarbon) molecules and reactive PAH radicals. The PAH radicals allow a more accurate and reversible modelling of PAH surface chemistry. The prediction of soot particle size distributions close to the sooting limit and the sensitivity of predicted size distributions with respect to the equivalence ratio are significantly improved. The onset of soot formation is delayed due to reversible effects, yielding better soot predictions in a series of laminar premixed flames. Furthermore, the model accurately describes instability of PAHs at high temperatures. Furthermore, the soot model was successfully coupled to the LES turbulence modelling approach and applied to a well-characterized turbulent sooting jet flame. Significant improvements were obtained compared to earlier RANS simulations. Accurate resolution of the instantaneous flame structure was identified to be crucial for soot predictions in turbulent combustion. Then, a detailed chemical kinetic mechanism, developed earlier, for n-heptane/toluene combustion and PAH formation was extended with cross reactions for n-heptane and toluene derivatives. The model was validated against literature data on flame speed for toluene/air and n-heptane/air mixtures, shock tube auto-ignition for n-heptane/toluene mixture, PAH concentration profiles and soot volume fractions measured in n-heptane and toluene laminar premixed flames and in n-heptane/toluene/O2/Ar flame. The agreement between measurements and simulations is sufficiently good for all measured data.

There is a need to link the properties of a particular fuel to its sooting tendency. To this effect, IMPERIAL conducted ab initio methods at the G4, G4MP2 and G3B3 level and these were used to determine thermodynamic properties of PAHs involved in soot nucleation and oxidation sequences. Test cases for laminar premixed flames, laminar diffusion flames and PSR/JSR geometries have been computed and an evaluation of updated PAH formation and oxidation mechanisms performed. The formation and oxidation of aromatics is also crucial in the context of links to surrogate fuels used in design calculations. In the current work, the recommended aromatic n-propyl benzene (nPB) component, resulting from the preceding EU funded CFD4C programme, has been further studied through accurate ab initio calculations. Results have been obtained for six side-chain hydrogen abstraction reactions at the “gold standard” CCSD(T)/jun-cc-pVTZ//M06-2X/6-311++G(3df,3dp) level. The current chemistry closures include the JetSurf 2.0 mechanism coupled with the work on nPB as well as substantial updates to the aromatics chemistry. Reaction rates based on G4 level thermodynamics, calculated using Rice–Ramsperger–Kassel–Marcus/master equation theory (RRKM/ME), have also been implemented for the cyclopentadienyl chemistry. The work has resulted in multiple updates of the underlying thermodynamic and chemical kinetic data used to describe soot nucleation and oxidation. The resulting chemical mechanism has been used to improve predictions of particle size distributions (PSDs) and overall soot levels in premixed as well diffusion flame environments through the further development of a sectional approach including the detailed PAH and soot inception chemistry. The ability of the devised model to reproduce PAH concentrations up to pyrene, used to define the smallest soot section via a presumed dimerization, has also been assessed using comparisons with laminar flame data. Finally, the prospect of simplifications of the detailed soot nucleation sequences has been assessed and the revised chemical kinetic mechanism delivered to industrial project partners.

3.2 WP3

The aim of this work-package was to develop and apply state-of-the-art experimental techniques for atomization and soot measurements. It therefore covers the physical processes investigated in FIRST.

For atomization, three different types of configurations were investigated:

- Fundamental configurations which provide a new insight in the physical process of primary atomization and allow developing new measuring techniques for very precise phenomena;
- Simplified injector configurations which allow developing simple empirical correlations applicable to various types of real injectors;
- Industrial injector configurations which give a final population of fuel droplets according to different operating conditions and initial parameters.

For soot measurements, several modern measurement techniques were tested and applied. The intent of the database created was to validate the soot formation and transport models developed in other work packages.

To understand better the physics of atomization, ONERA used a simplified geometry of a planar liquid sheet generator surrounded by two airflows. This design allows the setup to be representative of a real injection conditions in terms of liquid and gas velocities. This setup was adapted to perform various kinds of measurements, air velocities, boundary layers characteristics, frequencies, breakup length, drop sizing to be able to obtain as much information as possible on the atomisation process. Various configurations have been tested by changing air flow (thickness, velocity profile, ambient pressure) and liquid thickness. Mainly, the results show a relationship between breakup length and liquid flow rate (Figure 11). The influence of airflow configuration on oscillation frequency was also highlighted by the use of wall shear stress (Figure 12)

At CNRS-LEGI, besides the production of a large data base covering a wide range of flow conditions as well as more than ten different injector geometries, significant advances have been achieved on the understanding of atomisation mechanisms. In particular, quantitative agreements between stability theory and experiments have been obtained for the first time on the axial and transverse interfacial instabilities leading to the stripping of drops off the liquid film. Also, and over a wide range of conditions, the mean size of the drops due to stripping was shown to remain controlled by internal injector design, with a typical diameter evolving from a few (at high gas velocities representative of take-off) up to 20 (at low gas velocity representative of cruise regime) times the gas vorticity thickness at injection. The large scale instability was also thoroughly investigated, with new data on flow structure, flapping frequency, size distributions, fluxes and mean drop size evolution with control parameters: the drops formed by the large-scale instability happen to be typically ten times larger than those due to stripping. Moreover, hidden parameters acting on these interfacial instabilities were also unveiled that open the way to new atomisation control strategies. These improvements in the understanding of the physics of atomisation provide useful guidelines for optimal injector design. The data-bases are also helpful either to test direct numerical simulations or to feed numerical codes.

This work package framework was also the opportunity to develop new measuring techniques. A2 Photonic Sensors (A2PS) improved an optical fiber measurement technique for spray characterization, in order to answer the need to understand and qualify nozzles and injectors in aeronautical and turbomachinery domains. A2PS has improved its spray analysis sensor by primarily optimizing its sensing element: new optical probes with a “sensing length” four times smaller (from 60µm at the beginning of the project to 15µm now) were successfully manufactured. The reduction of the size of the sensing part led to an increased sensitivity to very small droplet, down to 10 µm. In addition, the data analysis algorithm used to analyze the data was also improved, validated on real spray data and implemented in a user-friendly software application. Several validations were performed, comparing this optical fiber solution to other well-known instruments and techniques. A comparison with a PDA system showed very good results agreement and also highlighted advantages of the optical probe system: experimental time saving thanks to its user-friendliness and ease-of-use, as well as a better capability to work with a wide span of droplet sizes. Another comparative experiment with a flowmeter highlighted the capability of the probes to reliably measure the flux and flow rate on a fine flow (Figure 13). The sum of the scientific achievements obtained on the optical probe technique led to the development of a fully functional measurement system, perfectly adapted to unidirectional sprays with droplet sizes as small as 10 µm and velocities up to 60 m/s. It also enabled the precise measurement of flow rate and flux even with a very high number of droplets per volume (very dense spray).

In this work package, simplified injectors experiments were carried out by ONERA and Imperial College. The effect of swirl on the atomisation of an annular liquid sheet was determined and data-sets were built in order to test numerical simulation developed in other tasks. At ONERA, a simplified configuration closer to the real flow pattern of an aeronautical swirl injector was used (Figure 14& Figure 15).

Measurements started with visualisations to qualify the influence of the swirl on liquid sheet. A larger expansion and a shorter breakup distance were visible (Figure 16)

An image analysis allowed quantifying the sheet breakup length (Figure 17). High speed visualizations have been used to determine flapping frequency of the sheet. The swirl increases the frequency. Comparison with planar sheet configuration was also conducted, the frequency being lower.

Drop size characterization was undertaken with a Malvern system at 80 mm from nozzle exit to take into account secondary breakup. The swirl presence diminishes the final droplet size (Figure 18).

Prior to FIRST, Interferometric Laser Imaging for Droplet Sizing (ILIDS, see Figure 19) for the simultaneous measurement of droplet size and velocity had only been performed on automotive fuel injectors. While the Optical Connectivity (OC) technique for determining the break-up length had never been applied to pre-filming atomizers. Imperial College (IC) was the first to apply the ILIDS and OC techniques on a prefilming airblast atomiser, typically found in aero-engine combustion systems and pioneered the concurrent application of both techniques. Instrumentation and data processing algorithms were developed for the simultaneous collection of measurements and their interpretation. The spray characteristics of two prefilming atomizers (designed at IC and ONERA) were reported. Experiments were performed for different air and water flow test conditions.

ILIDS measurements were reported for different axial and radial positions away from the nozzle exit and axis respectively (Figure 20). The increase in Sauter Mean Diameter (SMD) of droplets towards the spray edge for both atomizers was explained on the basis of larger centrifugal force acting on the bigger size droplets due to the swirling flow. The average droplet velocity plots in case of the model atomizer showed the presence of an induced vortical flow structure causing flow reversal near nozzle axis, which arose due to the swirling motion of the air. Away from the nozzle axis, the droplet velocity was downward and increased till the droplets lost momentum near the edge of the spray. Apart from the basic velocity statistics, the spatial droplet-droplet velocity correlations (R_{dd}) and Radial Distribution Functions (RDF) are presented for different droplet size classes. Measurements of R_{dd} quantified the strength of the intra-phase coupling of the droplet flow field in both the axial and radial directions. The RDF for the different droplet size classes indicated that the larger droplets (45-60 µm) showed greater tendency to form instantaneous droplet clusters in the sprays. The average cluster dimension decreased towards the spray edge. The break-up length of the liquid sheet was measured by the LIF technique, and the measurements were reported for different Reynolds number of water flow for the same air flow rate. Finally, the statistics including the fluctuations of droplet concentration and its correlation with the droplet velocity, which are vital for understanding the droplet cluster formation, were measured.

At KIT**,** an experimental approach of the **p**lanar **l**aser **i**nduced **f**luorescent (PLIF) method as shown in Figure 22 was adopted to investigate the onset of primary breakup (surface stripping) on the prefilmer. A model injector similar to the real prefilming airblast nozzle with an access for the PLIF technique was designed. The main challenge of the model injector design was the ability to generate a very homogeneous liquid film without the assist of air flow as shown in Figure 21 b. A new method for the evaluation of the film thickness was developed which considers the total reflection effect (Figure 22 b) at the air-liquid interface. The investigation of the film behaviour was performed at atmospheric and elevated pressure (4 bar) at varied momentum fluxes of liquid and air flow and at a different air flow orientation (swirl and non-swirl air flow). Due to inaccessibility of ligaments inside the prefilmer using the PLIF approach, investigation of the surface stripping was performed by considering the average film thickness. Surface stripping occurred at a particular flow condition where a rapid decrease in the average film thickness was observed. Comparisons of the interaction of the two phases were performed at different mean air velocities, momentum flux ratios (MR) of liquid and air flow (Figure 23 a) and We-number. The results revealed that the mean air velocity (Figure 23 b) and the density of air (Figure 24 b) are the main parameters that influence the occurrence of primary breakup. The results also showed that primary breakup occurred at a specific We-number regardless of the boundary and operating conditions. However, momentum flux ratio could not predict the surface stripping for different liquid flow rates (Figure 23 a).The investigation of air flow orientation (Figure 24 a) revealed that at the same boundary conditions, film breakup with swirled air starts at lower air pressure drops than for the non-swirl configuration. However, the film breakup with swirl configuration takes place over a broader range of air pressure drops. This work indicated that surface stripping occurred within the prefilmer at a specific boundary and operating conditions, which affects the droplet dispersion downstream the injector, i.e. inside the following combustor and therefore the heat release distribution in the combustor.

This work package was also the opportunity for KIT to study droplet size distributions by varying different parameters that influence the spray characteristics, hence, the Sauter Mean Diameters (SMD) of a double swirled prefilming airblast injection system (IS). The varied parameters were the geometry of the IS with a linear downscaling factor of 2 and flow boundary conditions. The SMDs of the entire spray were determined by combining the results of two different measurement methods; particle dynamics analysis (PDA) and a patternator that measures the radial mass flux distribution. The main reason for combining different measurement techniques was to include the non-spherical droplets, which were not detected by the PDA measurement system, by the determination of the mass flux distribution. Pictures of the two measurement techniques are shown in Figure 26. The experiments mainly focused on the determination of global SMD and investigating the effect of the geometry and air flow conditions on the atomization and spray using swirled prefilming airblast ISs. The effect of geometry was investigated by linear downscaling of the prototype IS. It was shown that geometrical scaling of swirling flows affects the centrifugal force, which influences the droplet dispersion and hence the radial liquid mass flux distribution as shown in Figure 26b. At the same flow and thermodynamic conditions the SMD of the downscaled IS was increased. At constant We-number the influence of air velocity (pressure drop) was much bigger than the influence of scaling (exit diameter). At the same We-Number higher SMD distributions near the axis for the scaled nozzle were detected due to the higher pressure drop which striped (surface striping) part of the liquid from the prefilmer inside the IS as shown in Figure 27a. However, the relative mass fraction showed that these SMD distributions possess a negligible mass fraction (Figure 27b), and a very few number of droplets that created marginal effect on the global SMD. Additionally, two different measurement methods to determine the mass distributions of the spray were examined and the global SMD was calculated (Figure 28). The result showed that with a combined technique of patternator and PDA the global SMD does not change significantly for different relative axial distances: this lead to the conclusion that the combined technique is a more realistic approach.

During the FIRST project, many experiments were also carried out on realistic injector geometries.

Within an air-blast atomiser the momentum of the air is used to break up the liquid fuel into a spray prior to combustion. An experimental investigation should thus incorporate the key geometric features which produce this flowfield. At Loughborough University, this programme was divided into two phases with the aim of assessing the importance of the representative aerodynamic flow field on the fuel break up: Phase 1 focused on characterising the aerodynamic flow field being presented to the pre-filming surface using a model of a generic LDI injector, at 3:1 scale to enable instrumentation access; Phase 2 used 1:1 scale hardware upon which the Phase 1 geometry was based. Thus both geometries provided an aerodynamic flowfield thought representative of modern industrial geometries currently being considered for future low emission aero engines. The Phase 1 geometry (Figure 30) incorporated two concentric swirl vane passages designed to provide a highly turbulent, swirling, representative aerodynamic flowfield. Within passage A was a pre-filming surface onto which fuel could be introduced and measurements were made both with and without fuel. Radial profiles of velocity, pressure and flow angle indicate the basic flow field characteristics which include the presence of swirl and the fluid movement caused by the pre-filming passage geometry (Figure 31). Flowfield contours indicate a velocity field containing wakes from the upstream swirl vanes which become stretched as they progress downstream and undergo some radial movement towards the pre-filming surface (Figure 32). The presence of such features will lead to circumferential non-uniformity in the fuel break up. The total pressure loss incurred by the flow is up to a quarter of the injector pressure drop which will affect the momentum of the air and hence its ability to break up the liquid film. This data defines the flow field that is presented to the pre-filming region of the injector, and provides both inlet boundary conditions and validation data for CFD predictions. Phase 2 included the development of a unique technique that can provide both temporal and spatial information on the fuel film and its thickness as it develops along the pre-filming surface (Figure 33). The mean fuel distribution on the pre-filmer is influenced by aerodynamic flowfield features and fuel gallery feed (Figure 34). Acoustic excitation of the atomising air stream demonstrated the time-resolved response of both the liquid film and the droplet flowfield (Figure 35). In the far-field spray the spray characteristics (Figure 36) spatially correlate with the upstream aerodynamic flow field (Phase 1) and/or developments associated with the liquid film. These features affect local stoichiometry and atomisation and are likely to be of increasing importance with the need to (i) develop low emission injectors and (ii) develop numerical methods that can capture the injector performance.

In addition to this work, the sprays from lean and rich burn fuel injectors were measured by SCITEK using PDA to provide validation results and boundary conditions for Rolls-Royce CFD predictions of aero engine combustors (Figure 36, Figure 37 & Figure 38). Upgrades to atmospheric test rigs at Rolls-Royce provided for measurements from injectors in a simplified plenum or engine sector geometry. Testing at pressures up to 5 bar and over 500 K was performed in an alternative rig with injectors surrounded by a quartz tube allowing laser access downstream of the injector. To date, uncertainty remains over the most appropriate method for scaling engine conditions to test rig capabilities and after initial assessment it was decided to scale on either momentum ratio or kinetic energy ratio whilst holding injector pressure drop constant. Measurements of the sprays from different alternative fuel blends was also made and compared to the baseline results to determine what issues may arise with a change to renewable fuel types. Calibration of the PDA system by SCITEK identified a data validation issue previously missed by the equipment manufacturer and this was rectified. Detailed maps of fuel droplet sizes and velocities were measured at a range of different conditions for the two types of fuel injector within the various test rig configurations and this information was passed to the relevant modelling tasks in the FIRST project. The experimental information was used for the validation of new spray models and provided the boundary conditions for new soot model calculations. It was seen that the downstream arrangement of the test rig can significantly affect the spray results near the fuel injector and the closest combustor representation should be used on test rigs providing results used for CFD modelling of engine combustors. Wide spray cone angles and large volumes of fuel spray made testing at some conditions extremely challenging, such that measurements at conditions relating to higher engine power were not achievable. Comparison of spray results at atmospheric and, elevated pressure and temperature showed differences in particle sizes which may be attributed to evaporation and increased secondary atomisation. As such, great care needs to be used when scaling rig results to engine simulations. Comparison to different alternative fuels also showed differences in particle sizes and velocities, which is attributed to differences in the macro properties of the liquids. The figures supplied show boundary conditions obtained from the rich burn injector, contour plots of spray characteristics downstream of the lean burn injector and the comparison of the alternative fuel blends.

Lastly, this work package provided analysis and data-sets on soot formation inside a burner. A first task was devoted to setting up a high-quality data set describing sooting turbulent pressurized flames, suited for validation of combustion models including soot chemistry. Relative to the European project SiA, an optimized model combustor was developed even better suiting needs from simulation (Figure 39). A large suite of different optical and laser-based diagnostics was applied to this burner, operated at increased pressure, resulting in the desired comprehensive data set. This includes soot concentration maps, a fine grid of CARS temperatures and statistics, OH distributions and velocity fields. In addition some instantaneous correlations were measured such as OH/soot and PAH/soot to show feasibility. Few flames were characterized in full detail, for others, trends are available with a lesser degree of details. The richness of data available for the reference operation condition is shown in Figure 40. Trend studies included the effect of pressure, equivalence ratio and air split between the two swirled combustion air in-flows. In addition to that, the very sensitive influence of secondary air injection past the primary combustion zone was studied. The trends can easily be tracked based on time averaged quantities while increased insight becomes available when analysing instantaneous data, thus making use of the high temporal and spatial resolution of laser diagnostics. In addition, DLR applied some of the diagnostics simultaneously to deduce correlations and to demonstrate the feasibility of the procedure. The data set provides an excellent test case for soot model validation, the comprehensive set of quantities being important to check different sub-models of CFD codes, i.e. cold flow, turbulent mixing, gas phase kinetics, and soot chemistry.

Two staged LDI injectors were also supplied by RRD and integrated into the high pressure single sector test section BOSS. The injectors were tested at different load conditions, with pilot-only operation, using several planar optical test methods (LII (Laser-Induced Incandescence), Planar Mie scattering, OH chemiluminescence with Abel inversion and PIV measurements of velocity field, using an enhanced dual-sensor setup developed specifically for highly luminous environments). In addition, smoke numbers were measured at the combustor exit using an optical smoke meter. Correlations between the different measured quantities were established, and their parametric dependencies investigated. This study achieved a qualitative understanding of soot formation mechanisms in the specific scenario of a lean burn system, and generated a complete data set in a format suitable as reference case for CFD validation. The spatial distribution of soot volume fractions was investigated at idle and part load conditions in a pilot-only operation by optical diagnostic methods, with emphasis on soot formation for different equivalence ratios and two injectors with different swirl conditions, correlating soot formation regions with flow field structures and shapes of reaction zones. The change of the flow pattern from isothermal to reacting flow was demonstrated in a first step. In this study, it appeared that from the large difference between isothermal and pilot only operation, due to the sharp spatial gradients of the soot concentration distribution, it was absolutely necessary to measure the flow field at the correct fuel placement to understand the convective effects influencing soot production and oxidation. Fuel placement being coupled to luminosity, the ability to measure PIV in highly sooting flames was a breakthrough in the ability to understand the influence of design features on soot formation. In agreement with previous studies, it was found that soot is formed predominantly in the upstream directed part of the S-shaped pilot flow near the interface to the outer main flow (example Figure 41). However, it was shown that the exact shapes of the spatial distributions, as well as the amount of soot formed, depend strongly on equivalence ratio and on details of the flow field, which result from geometric features of the injector. The trends were explained qualitatively using data on soot formation kinetics in combination with flow field-dependent residence times.

3.3 WP4

In WP4, numerical methods were tested and validated for both topics, the soot formation and the atomisation process. The validation of the atomisation models covered the **computation of the dense spray** inside the injector as well as the **secondary atomisation**. Additionally to Physics based models, phenomenological models were developed and tested in regards to **spray boundary conditions** and modelling of **droplet cluster** formation. The **soot formation** modelling developed in the FIRST project was tested inside analytical test cases as well as complex combustion systems.

For the calculation of the **dense spray** and the atomisation process downstream of liquid fuel injection, a phenomenological model has been developed in the context of Large Eddy Simulation of aeronautical combustion chambers. The numerical tool used is the Large Eddy Simulation solver AVBP, co-developed by CERFACS and IFPEN, a massively parallel unstructured code that explicitly solves the reactive Navier-Stokes equations in compressible form. AVBP is used by many laboratories in Europe as well as industrials such as SAFRAN.

More precisely, spray/wall interactions, liquid filming and primary breakup process for airblast atomizers have been focused on in this work (see turquoise boxes in Figure 42). For spray/wall interactions, correlations from the literature have been used. The originality and novelty of this work is the development of a model for both the thin liquid film generated at the walls and the breakup process at the atomizing edge. The thin liquid film model is derived by simplification of the Navier-Stokes equations and described by a Lagrangian approach. The atomisation model is characterised by a drop size distribution, whose coefficients are calibrated from the KIT-ITS prefilming experiment sketched in b.

Figure 43a.

First, the phenomenological model has been evaluated in the KIT-ITS prefilming experiment. Several Large Eddy Simulations have been performed using the computational domain shown in Figure 44, varying the gas velocity and the liquid fuel. The numerical results show a reasonable agreement with the measurements in terms of liquid film height, and a good agreement in terms of velocity profile and droplet distribution downstream the prefilmer edge, as shown in Figure 45.

Second, the phenomenological model has been evaluated in the Large Eddy Simulation of an evaporating non-reacting SAFRAN Turbomeca helicopter combustion chamber operated at atmospheric pressure. As there is no droplet distribution measurements available close to the injector in a real combustion chamber and the KIT-ITS group has shown that phenomena occuring in real injector configurations are very similar to those observed in the academic prefilming experiment, the phenomenological model calibrated on the KIT-ITS experiment has been directly used in the TURBOMECA combustion chamber (Figure 46a.). The comparison with the experimental droplet distribution measured in the volume D probed by a particle sizer downstream the airblast atomizer (cf blue rectangle in Figure 46a.) is displayed in Figure 46b., showing good agreement.

The phenomenological model proposed in this work has been successfully applied in a real aeronautical configuration by TURBOMECA engineers in Task 5.1.3.2 to evaluate the impact of the atomisation process on the spray flame structure.

The **secondary atomisation** modelling was tested and validated with a detailed investigation of the secondary break-up phenomena in an industrial geometry developed by GE Avio. In order to test the accuracy and reliability of the numerical models, the commercial code Ansys® CFX has been compared with the open source code OpenFOAM in different operating conditions. A first evaluation of three different secondary atomization models (Schmehl, TAB and MCAB) has been investigated in Ansys® CFX starting from the injection characteristics of the droplets (primary break-up) supplied by UNIBG and developed in T2.2.5 and 2.2.6. An evaluation of the spray characteristics (penetration, angle) and droplets' distributions have been used to identify the differences between the models with the conclusion that the behaviour is very similar in the global characteristics, while some differences are visible in the local distribution. Then, one fixed operating condition has been used for the comparison between Ansys® CFX and OpenFOAM, where the same algorithms used in CFX have been implemented and exploited by UNIFI. The trend is similar in the normal penetration and spray angle for the simpler approach (one-way coupling) while some differences are visible in the axial penetration and droplets' distribution when a two-way approach is used in the two codes. The lack of experimental data does not permit an understanding of the accuracy of the models used.

Additionally, a phenomenological model in regards to **spray boundary conditions** was developed. Although many research groups are currently working on advanced numerical methods to account for complex liquid injection phenomena, there is still today a need for physics-based and phenomenological liquid injection models. The purpose of phenomenological models is to provide reliable spray injection conditions for CFD codes at an acceptable CPU cost. These phenomenological models are solution of inverse problems based on spray measurements. This task aims to apply the whole chain to a SNECMA injection system, from the establishment of the experimental database to the development of a phenomenological injection model and finally the calculations with both RANS and LES approaches of the SNECMA combustion chamber using the liquid injection model.

First, ONERA has done detailed spray characterisations by Particle Doppler Anemometry downstream from the SNECMA injection system for several different operating points (idle, approach and derivatives). These characterisations have been performed at the edge of the state of the art, i.e. a few millimetres downstream from the injection plane, but a few tens of millimetres from the fuel injection points. Then using these measurements, ONERA has proposed a response surface methodology to specify the spray characteristics at the real fuel injection location, using an optimisation method based on surrogate modelling. This multi-objective problem is solved by genetic algorithms and provides the set of optimal solutions. The surrogate model is built thanks to Kriging method from an initial design of experiments enriched by the points that maximize the uncertainty of the model in order to improve its accuracy. The boundary conditions proposed minimize the distance between computed and measured distributions of droplet size and velocity in the measurement section.

Finally, the suitability of the derived spray boundary condition has been evaluated in RANS and LES calculations, using CEDRE (ONERA) and N3S (SNECMA), and AVBP (CERFACS) respectively. The numerical results have been compared between each other and with numerical results in the measurement section. Moreover, comparisons have been made with the standard procedure at SNECMA to prescribe spray boundary conditions. The comparisons show good agreement with the available spray measurements downstream from the injection plane.

Overall, the task shows the capacity of such a phenomenological model based on measurements downstream the injection system can reproduce the correct physics without simulating the early complex processes of primary and secondary breakup.

The stimulus for the **droplet cluster modelling** work is the inability of the currently available RANS modelling tools to predict certain phenomena, experimentally observed, within the dispersed phase. Namely, particle/droplet preferential concentration and droplet trajectories in recirculation zones and regions of flow separation. The consequences of these limitations are that the instantaneous non-uniformity/homogeneity of droplet concentration spatial distributions observed experimentally at high Reynolds number flows cannot be observed in the corresponding modelling efforts. The Imperial College developed fully coupled incompressible Eulerian-Lagrangian solvers for use within the OpenFOAM modeling package. In addition a phenomenological model for particle dispersion that uses Kinematic Simulations (KS) was developed to model the smaller scales of the dispersed flow in a RANS framework. The model was tested on an axi-symmetric sudden expansion test case for two distinct particle class sizes and several mass loadings. Results were compared to LES calculations performed and to RANS simulations employing the commonly used dispersion model as well against experimental data.

The limitation of current RANS Lagrangian tracking dispersion models may be traced back to the fact that the 'computed' instantaneous flow eddies in Monte-Carlo models are only prescribed from the local values of the turbulent kinetic energy and the local dissipation rate of the flow field from which a fluctuating component of velocity is assigned to the particle. There is no physical flow structure information contained within these 'constructed' eddies. The developed model uses the standard (u)RANS technique for modelling the bulk of the flow field but then employs KS within each ‘computationally constructed’ eddy in order to introduce a more realistic flow structure for the smaller scales of the flow, which are not computed in a typical RANS calculation. Performance of the developed model is improved over the existing models and, for certain regions of the flow, predictions are very similar to the LES results but is still limited by the RANS framework it was designed for. The developed model is not restricted to the aero-combustor sector but is equally suited for use in a wide range of fields from biological modelling to environmental flows.

As an additional atomisation task, a systematic cross-comparison between selected test cases was performed, capturing latest experimental results as well as results of newly developed numerical tools. Simulations in 2D and 3D of a sheared plane liquid sheet with the DyJeAt code developed at ONERA have been performed, keeping the momentum flux ratio M constant when room pressure is varied. The simulations give qualitatively good agreement with ONERA experiments concerning large-scale instability frequency and break-up length evolution with air flow velocity. Furthermore, the morphology of the primary atomization of the simulation is the same as the experimental one. However, a discrepancy is found concerning the values of the flapping frequency. Simulations overestimate systematically by a factor of 2 over the experimental ones. For the moment no clear argument was found to explain this difference. Also, 3D simulations of the sheared round liquid jet experiment of CNRS-LEGI have been performed using the ARCHER code of CNRS-CORIA. A strong influence of the shape of air inlet profile and specifically of the boundary layer was found. Furthermore, increase of resolution and domain size is mandatory to give at least qualitatively the main spatial liquid jet evolution.

Additionally to all this work related to the atomisation process, the modelling of the **soot formation** was tested and validated in WP 4 as well. At the DLR Stuttgart, unsteady Reynolds averaged Navier-Stokes simulations (URANS) and large eddy simulations (LES) of a well characterized aero-engine model combustor with finite-rate chemistry (FRC) were conducted. The simulations gave insight into the complex formation and destruction processes of soot at technically relevant conditions. It was shown, that a recently developed PAH (polycyclic aromatic hydrocarbons) and soot model is able to predict soot under complex combustion conditions at elevated pressure. Finite-rate chemistry is employed for the gas phase, a sectional approach for PAHs and a two-equation model for soot. Thus feedback effects such as the consumption of gaseous soot precursors by growth of soot and PAHs are inherently captured accurately.

In agreement with the experiment a precessing vortex core (PVC) was observed in the ethylene fuelled combustor. This requires that the computational grid covers swirlers and fuel supply. The PVC intensifies mixing of fuel, primary air and hot burnt gas from the inner recirculation zone, thereby supporting flame stabilization and subsequently influencing soot. It was shown by comparison of URANS and LES results that, although, URANS accurately predicts the time averaged reactive flow field in terms of velocity and temperature and also resolves coherent structures such as PVCs, it has limitations when a fine resolution of the instantaneous flame structure is important, as for the prediction of soot. Significantly better soot predictions were thus achieved by LES.

At ONERA, the influence of the fuel spray atomisation on the soot formation in the pilot zone of a multipoint staged injector was investigated. For this goal, ONERA had to achieve the numerical simulation of the DLR burner using different soot models and to compare the numerical results with the experimental measurements obtained by DLR in the framework of the subtask 3.4.1. The DLR burner works with gaseous fuel (ethylene). Different optical diagnostics have been applied to this burner. In particular LII measurements provided very useful information for the validation of the numerical strategy for the soot prediction. From the comparison between calculation and experiment it was deduced that the use of the soot model of Leung combined with a Flame Tabulated Chemistry (FTC) was a convenient approach to calculate the soot formation in a gas turbine combustor. Indeed, in a LES calculation it was possible to correctly reproduce the shape of the soot volume fraction field as well as the magnitude of this volume fraction using this approach. Other approaches such as those using the simple Magnussen soot model or the more complex SIA soot model (Lagrangian model) turned out to be less appropriate.

In the second part ONERA had to achieve, with the approach for soot selected in the first part, the calculation of the TLC burner working with kerosene and to investigate the influence of the size of the injected kerosene droplets on the soot formation. Three different sets of data for the droplets size were tested. As expected the largest droplets (20 µm in diameter) give rise to the largest amount of soot downstream of the pilot injector: The relatively slow evaporation of these droplets leads to a low quality of mixing at low scale resulting in a higher rate of soot formation. However more soot is obtained with the very small droplets (5 µm in diameter) than with droplets of intermediate size (10 µm in diameter). The explanation to this behaviour is that the early evaporation of the very small droplets results in the creation of pockets of limited extent with a high concentration of gaseous fuel which are burning in the shape of diffusion flame. It must be noted that, whatever the droplets size, the soot particles are strongly oxidized before the outlet section of the burner so that almost no soot is emitted by the TLC combustor under the conditions of the calculation (take off conditions).

Overall, the Work Package 4 did a broad validation and testing of different numerical methods with respect to atomisation phenomena and soot formation. It can be shown that the models developed in the framework of FIRST are helpful to capture the physics of both phenomena. The validation with technically relevant geometries, however, showed also the limitation of the different models and the importance of further work in both research fields.

3.4 WP5

In a gas turbine combustion system for application in aviation, the liquid spray distribution has a large impact on the aero-thermal performance such as operability, efficiency and emissions (NOx, CO and Soot). However, currently there are no generic and computational affordable methods available to predict the spray break-up process. In addition these methods of predicting spray preparation are largely empiric and are normally valid for a certain fuel spray nozzle design. Within WP5 the spray break-up models developed in WP2 based on phenomenological and advanced physics models were used by the industrial partners: RR, RRD, SN, MTU and AVIO, for industrial combustors. Results were also compared to experimental data which was obtained in WP3. Furthermore, current available soot models are not sufficiently accurate to support the design of new environmentally friendly combustors. The soot models were developed in WP2 by IMPERIAL and DLR-VT. Within WP5 they are exploited by RRD and RRUK. The soot model was applied to industrial aero-engine combustors and results compared to engine soot data.

The following section highlights the main results achieved in the framework of the FIRST project for WP5. The aim of majority of the tasks in this project was to develop spray and soot models which enhance the modelling capability of industrial configuration within reasonable computational effort. All computational cases where calculated at operating regimes of relevance to real application.

1.) Task 5.1.1 (RRUK, IC) – spray dispersion model was developed to improve turbulent dispersion in steady state CFD using simple turbulence models
2.) Task 5.1.2 (SN) –liquid film model was validated using experimental results from a flat lip pre-filmer test at LEGI
3.) Task 5.1.3 (TM) – in collaboration with CERFACS a high fidelity CFD of the combustion chamber of a helicopter engine was carried out. The results showed good comparison with measurements
4.) Task 5.1.4 (MTU) –the open source CFD code OPENFOAM was used to simulate a pre-filming air-blast atomizer. Experimental results from EBI Karlsruhe was used to validate the CFD results
5.) Task 5.1.5 (UNFI, GE AVIO) – a new liquid film model was developed in the framework of the open source code OPENFOAM

6.) Task 5.1.6 (UNIBG, GE AVIO, EST) – liquid flow in a pressure swirl atomizer was simulated at varying operating conditions by UNIBG. These results were used by EST to generate a artificial neural network based spray model
7.) Task 5.1.7 (RRUK) – detailed simulation of liquid and air phase in alean burn fuel injector was carried out using high fidelity approach like volume of fluid
8.) Task 5.1.8 (TM) - in collaboration with CORIA a high fidelity CFD of the combustion chamber of a helicopter engine was carried out. The results showed good comparison with measurements
9.) Task 5.2.1 (RRD, RRUK) – a new soot model was implemented into the RR in house CFD code PRECISE
10.) Task 5.2.2 (RRD, RRUK) – the new soot model was applied to lab scale gas flame, single sector experiment from DLR-VT and industrial test cases. Results were compared with traditional models. The new model was found to be computationally expensive. The importance of modelling mixing ,i.e., using higher fidelity turbulence models like LES was found

In task 5.1.1 a new Lagrangian dispersion model developed by Imperial College was implemented and tested by RRUK. This aimed to overcome the fundamental deficit of modelling turbulent particle dispersion in steady state CFD with simple turbulent modelling. Lagrangian tracking of droplet is widely used in combustion CFD simulations to model spray. Spray modelling can have a dramatic impact on the accuracy of predictions of relevant aero-thermal parameters (e.g. emissions, temperature traverse, metal temperature, flame stability, etc). However, spray modelling is extremely challenging due to the very wide range of length-scales to be catered for as well as the turbulent nature of the flow typically found in gas turbine combustors. While significant attention is usually paid to spray boundary conditions defined after primary break up is complete, the final air to fuel ratio distribution prediction is also strongly dependent on the ability to capture the turbulent interaction between the two phases. In the present task, a new turbulent dispersion model developed by Imperial College London within FIRST has been implemented by RRUK into the in-house code PRECISE and tested on two different combustor geometries to assess its impact on traverse prediction. Such model, based on a Kinematic Simulation (KS) concept, is inherently more suitable to model droplet clustering effects. The KS model was compared against well-established Gosman-Ioannides turbulent dispersion model and shown to behave qualitatively similarly. However, the KS model was demonstrated to predict higher levels of dispersion. The impact on prediction of temperature traverse of the KS model was shown to be significant for both combustor designs considered. Further work will need to be done to assess its impact on traverse for other combustor design styles traverse predictions as well as on emissions. As a result of the FIRST programme, a framework has been put in place to model spray turbulent dispersion more accurately.

In task 5.1.2 Snecma has validated its RANS film model against the experimental database generated by LEGI. The experimental configuration is a planar injection system with pre-filming. The validation concerns the mean characteristics of the film and also the distribution and characteristics (size, velocity) of the droplets available downstream of the pre-filmer lip.

During the FIRST project, in task 5.1.3, TurboMeca performed Lagrangian simulations for a helicopter combustion chamber at realistic operating conditions using the CFD code AVBP. This work was done in close collaboration with CERFACS. Pre-processing tools were developed to be able to convert 1D inputs (flow rates, temperature, pressure, hole angles, etc.) into 3D boundary conditions for large-eddy simulations. In particular, TM used the liquid film and atomization model from CERFACS (T4.1.3) in simulations and compared exhaust gases predictions with experimental data for two modeling approaches for the liquid boundary conditions. It was found that droplets distributions and evaporation are very different in the two approaches and it was shown that this effect influences the flame structures. An overall excellent agreement was found between available experimental data at the combustion chamber exit and the LES predictions, particularly the agreement was excellent for the simulation including CERFACS liquid boundary models (Figure 47). Finally from a high-performance computing point of view, this study demonstrated the capability of AVBP to be a viable industrial high-fidelity LES code, enabling restitution times largely compatible with conception timelines.

The objective of task 5.1.4 was the numerical investigation of the model injector of subtask 3.2.3.1 defined and experimentally investigated by the Engler-Bunte-Institut (EBI) at University of Karlsruhe. The non-commercial CFD code OpenFOAM was used with the *Volume of Fluid* approach (VOF) combined with LES-turbulence modelling. Figure 48 shows a scheme of the model injector and the numerical model. The experimental test rig allowed testing over a wide range of operation. By variation of the liquid and the gas velocities, an Air-to-Fuel ratio (AFR) of 0.5 up to 3.2 and a momentum ratio (M) of 0.9 up to 36 were achieved. A detailed validation of the numerical model was performed. Focused on one operation point, the temporarily averaged liquid film thickness was compared to the experimental results. Comparing the global average film thickness of the liquid film for this variation with the numerical results reveals overall a good agreement. The comparison showed a good agreement for 3-dimensional as well as simplified 2-dimensional models. Figure 49 shows this comparison for the operation point M=3.1. After this validation of the numerical approach with the available experimental data, the numerical results were used to create a better insight into the phenomena causing interaction of the liquid and the gaseous phase. The analysis of the numerical results in regards to the boundary conditions showed that the liquid-gas interface behaviour can be characterized by three regimes. Low gaseous velocities lead to a very flat interface without interaction of the two fluids. The interacting forces are in equilibrium and the interface shows no deformation. By increasing the air velocity, the aerodynamic forces cause a deformation and a wavy interface occurs. The interaction is comparable to a Kelvin-Helmholtz instability. Additionally, this transition includes weak onset of primary atomization which could be analysed numerically via a liquid mass balance. Increasing the air velocity further and exceeding a critical momentum ratio, the aerodynamic forces destroy the integrity of the interface. Surface stripping occurs and the formation of ligaments and droplets takes place already inside the injector. Figure 50 illustrates the regimes and shows the temporarily averaged film thicknesses for different operation points of the three different regimes. Analysing the liquid mass transfer into the gaseous phase reveals the significant part of liquid atomized for the third regime.

In task 5.1.5 GE Avio and UNIFI analysed the different phenomena of the injection system in ULN combustors. Contributions coming from University of Bergamo (WP2) and EnginSoft (T 5.1.6) have been exploited in this task. University of Firenze developed a multi-coupled Eulerian-Lagrangian solver in the framework of the open source code OpenFoam for reacting sprays including liquid film evolution and successive primary break-up of the film. The model is based on the thin film approximation solving film conservation equations (film thickness, momentum and energy) with the Eulerian approach on a 2D mesh extruded normally from the wall. Coupling with the gas phase is achieved on the film/gas interface maintaining equal interface velocity and shear stress on both sides. Coupling with the Lagrangian tracking includes implementation of a splashing model (for droplets hitting the wet surface) and of injection models to account for the primary break-up. These injection models are based on available correlations which are solved with updated film and gas properties at each computational iteration. This provides the required feedback from the film solver. Among the others, some of the implemented models are based on newly developed correlations developed in KIAI EU program by KIT for planar pre-filming air-blast atomizers. GE Avio provided the partners with the geometry of an injection system designed in the European Project NEWAC. GE Avio also provided a number of working conditions in which the characteristics of droplets had to be calculated. Results obtained by the models developed by the Universities (regarding spray boundary conditions) will be assessed and implemented in the in-house code so to improve the GE Avio capabilities in the analysis of reactive flows and the design capabilities of injection systems for low NOx combustors.

The emission indexes calculated with the boundary conditions from advanced models matched well with the experiments. It demonstrates that in modern combustors, based on lean combustion and equipped with pre-mixing duct, a good evaluation of the boundary conditions for the liquid phase is crucial because it has a big impact on the evaporation and mixing between fuel and air and it permits to get a better evaluation of the pollutant emissions and in general on the combustor performance. As a conclusion, it is highly recommended to use the validated multi-phase flow models to evaluate the statistics of droplets for the boundary conditions instead of using empirical correlations. These models can give information calculated in the same working conditions of the actual combustor, on the other hand the empirical correlations are strictly valid at the conditions of the experimental tests on which are based.

The target of task 5.1.6 was to define the liquid drop characteristics generated from the break-up of the liquid lamella exiting a ULN swirling injector, according to the geometric and operating conditions provided by GE AVIO in the Task T3.2.3.2. The internal flow and the liquid structure exiting the nozzle have been investigated by UNIBG in a typical pressure swirl atomizer for aero-engine applications under an isothermal non reacting environment, using a combination of single and two-phase flow Eulerian models implemented in-house and commercial CFD codes. A numerical methodology has been developed to provide the necessary input conditions for successive atomisation modelling. Furthermore, a novel formulation of the primary atomisation model has been developed by UNIBG for hollow cone swirling jets, explicitly accounting for turbulence and aerodynamic effects on the liquid break-up. The model determines the dominant mechanism responsible for liquid jet break-up and the mean, maximum and drop size distribution of the newly formed spray. The results were used by EST to form an artificial neural network based spray model. Traditionally the boundary conditions for the spray characterization were based on empirical formulation and literature formulas and the activity performed in this task wants to introduce a novel approach in order to identify such a boundaries. The work is based on the development of an expert system for the atomization scenario: starting from the Design of Experiments methodology, few baseline operating conditions have been chosen in order to investigate the primary and secondary break-up processes using Ansys® CFX and to define the relation between input parameters (pressure and temperature of the chamber, nozzle flow rate, etc.) with the characteristics of the spray (penetration, droplet distribution); then, response surface methodology (RSM) developed with modeFRONTIER® has been used for the evaluation of the spray behaviour in any physical scenario. These surfaces can now be used from GE Avio for the accurate study of the injection system and for the development of future injectors and combustors. No additional CFD computations are required for the spray evaluation because from the response surface is possible to identify the droplets characteristics in order to simulate the combustion process inside the chamber. The accuracy of this method depends on the initial number of configuration used in the DoE, but can be considered more consistent with the physics compared to the empirical correlations used until now.

In task 5.1.7 the simulation of primary break-up and comparison with experimental data was done. Two-phase CFD simulations of the generic prefilmer used by ITS Karlsruhe in the KIAI programme have been performed using an Eulerian approach, the Large Eddy Simulation Volume of Fluid (VoF) method. Comparison of the LES VoF results with the ITS Karlsruhe experimental measurements of droplet Sauter Mean Diameter (SMD) showed good agreement. A limitation of the VoF method is that, typically, very fine computational grids must be used in order to resolve the measured droplet sizes accurately. The limitation of available computational resources often means that such fine grids are not affordable, but reasonably good results can still be obtained with grids that are relatively coarse, as shown by the results in this task. The results of the LES VoF simulations have been compared with LIF and PDA measurements performed by Loughborough University within FIRST on the same lean burn fuel injector geometry. Comparison of the LES VoF predicted fuel film distribution and film thickness with the Loughborough University LIF measurements show good agreement. Again, limited computational resources meant that sufficient resolution in the computational grid in order to resolve the measured droplet sizes downstream of the prefilmer was not affordable, although a comparison of the LES VoF predicted fuel spray distribution was in good qualitative agreement with the Loughborough University PDA measurements. A similar approach has been used to simulate the primary break up of a typical rich burn injector. The LES-VoF was run on a small computational domain where the bulk of the primary break up is expected to take place. While the resolution was not enough to predict droplet size distribution, the simulation provides useful insight into the primary break up and the corresponding AFR distribution.

In task 5.1.8, TM obtained, in close collaboration with CORIA, results on two-phase flow simulations on helicopter combustion chamber injectors at realistic operating conditions using the CFD code YALES2. The study extended the initial results required in the DoW by also obtaining results on another air-blast configuration. In this task, TM used a level-set (LS) approach to track the liquid/gaseous interface, coupled with a Ghost-Fluid approach (GFA). For both configurations, purely gaseous simulations were performed and discussed. Gaseous simulations were compared, when available, with experimental data to validate the numerical setup and domain descriptions (Figure 51). Then two-phase flows were performed with various mesh refinement levels. It was shown that the YALES2 solver is able to calculate very large meshes (up to more than a billion elements), and that the treatment of the results is directly feasible in an industrial context. Yet, the work performed highlighted the limitations of the methodology. It was shown that despite strong geometrical simplifications and several iterations on the meshing strategy, the level-set approach combined with homogeneous mesh refinement is not yet adapted to industrial configuration specificities. It was indeed shown that the chosen approach was not yet viable in an industrial context in terms of computational resources. For the finest grids simulations atomization started to appear, and several small droplets were generated (Figure 52). Yet, a small quantity of under-resolved droplets was quickly lost. This effect was found linked to the inherent treatment of the level-set function and to the lack of resolution of the employed meshes. Further work will focus on development of the coupling numeric between momentum fluxes and the level-set function, as well as local mesh refinement. This further work will be supported by a PhD thesis funded by Safran, that started at CORIA in 2014.

Prior to the FIRST project, a two equation soot model has been used within the Rolls-Royce in-house combustion CFD code PRECISE-UNS. The reliability and predicting capability of this model has been shown to be limited. The applied reaction mechanism for flamelet type combustion models like the Flamelet Generated Manifold method, are based on reaction mechanism developed within the 6th FW EU project CFD4C. The objective of task 5.2.1 was to implement a comprehensive soot model based on detailed chemistry into PRECISE-UNS. DLR-VT has developed a sectional soot model, which is based on detailed chemistry and includes all the required physics of soot production and oxidation processes. A sectional (bin) model is used for the PAHs: the PAHs are grouped into 3 bin classes. The model the soot and PAH chemistry are described by chemistry reactions, which are read from a reaction mechanism. For the soot model two options are available; the soot can be modelled using a two equation model (mass fraction and number density), or by a bin model for soot. This detailed soot model has been implemented PRECISE-UNS (it has to be noted that most of the work has been done in a related project between DLR-VT and Rolls-Royce Deutschland). A solution method had to be developed to solve the detailed chemistry model within the PRECISE-UNS. PRECISE-UNS solves all equations sequentially and implicitly. However, since the detailed chemistry is stiff, the chemistry has to be solved for all species in a coupled way. Since solving all species equations coupled would result in a huge system of equations to be solved, the chemistry is first integrated over a representative timescale. From the integrated values source terms are extracted which are applied in the convection diffusion equations of the species. The detailed soot model has been validated against a range of academic test cases, ranging from laminar flames to sooting turbulent flames. Within the FIRST project the model has been applied to two aero engine combustors (see section 5.2.2.). Furthermore, a detailed chemistry model including the PAH chemistry has been obtained from Imperial College. The model can be used to with the Flamelet Generated Manifold model, in which soot reaction rates are derived from detailed species and tabulated in a look-up table.

In task 5.2.2 the newly developed soot model of DLR-VT first was been applied to a laminar 2-D Bunsen methane/air flame, the temperature result, compared to simulation of van Oijen is provided in Figure 53. Next the chemistry and soot model has been applied to a small Rolls-Royce engine combustor (RRD) and a large Rolls-Royce engine (RRUK) combustor. The temperature field as presented in Figure 54 compares well with that predicted by other chemistry models, the soot result, also presented in the figure, shows that the soot is completely oxidised at the exit of the combustor. Similar results are obtained for the large combustor, as shown in Figure 55. From the results is concluded that the soot model is correctly implemented, and works as expected. However, some more work has to be done on the oxidation chemistry. Furthermore, the chemistry model is numerically very expensive and some work will be needed to reduce the computational effort. Also, CFD computations have been performed on a Rolls-Royce lean burn injector, for which optical measurements are performed by DLR-AT within the BOSS rig (Big Optical Single Sector) within task 3.3.1. These CFD computations have been performed using the two equation soot model from Imperial College (Leung, 2002) coupled with the Flame Generated Manifold combustion model. The CFD results have been compared with the measured velocity and soot results and the results of the soot are presented in Figure 56. From these soot results it can be seen that the shape of the soot is predicted reasonably well. However, the soot oxidation in the CFD seems to be higher as in the experiments. The trend of soot mass fraction against the AFR is predicted correctly by the soot model. Additionally CFD computations have been performed on the DLR-VT gas turbine model combustor, for which a detailed and comprehensive measurement data set has been generated by DLR-VT within this project in Task 3.4. For this combustor the existing soot model from Imperial College and the newly developed model from DLR-VT have been applied using RANS and LES computations. The CFD results are compared with the experimental data. The velocity and temperature fields are better predicted by LES, although the RANS results agree quite well. For the soot results the differences between RANS and LES are larger, the shape of the soot concentration is much better predicted by LES, whereas, the absolute concentration is better matched by RANS (for the existing two-equation soot model from Imperial College). The experimental and averaged LES soot results are presented in Figure 57.

3.5 Figures

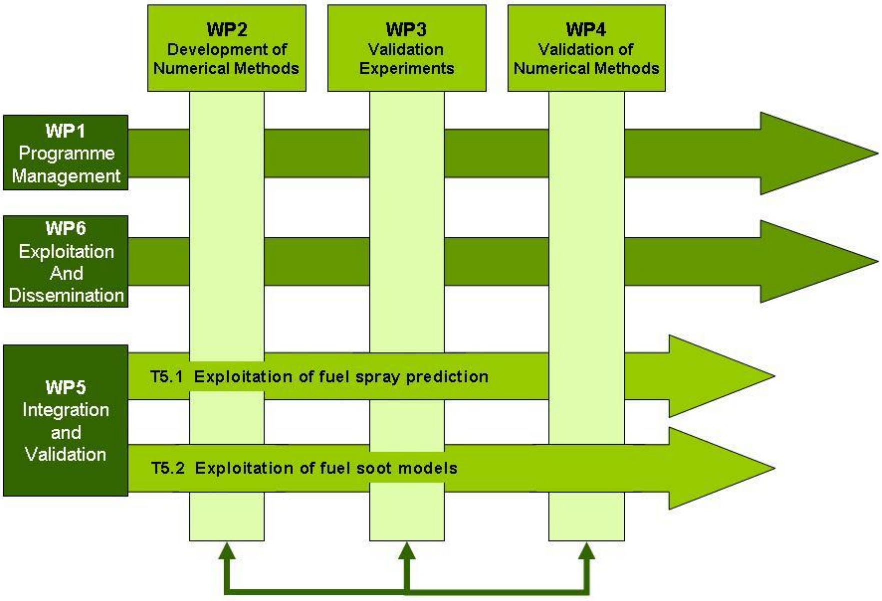


Figure 1: FIRST Project Work Plan Structure

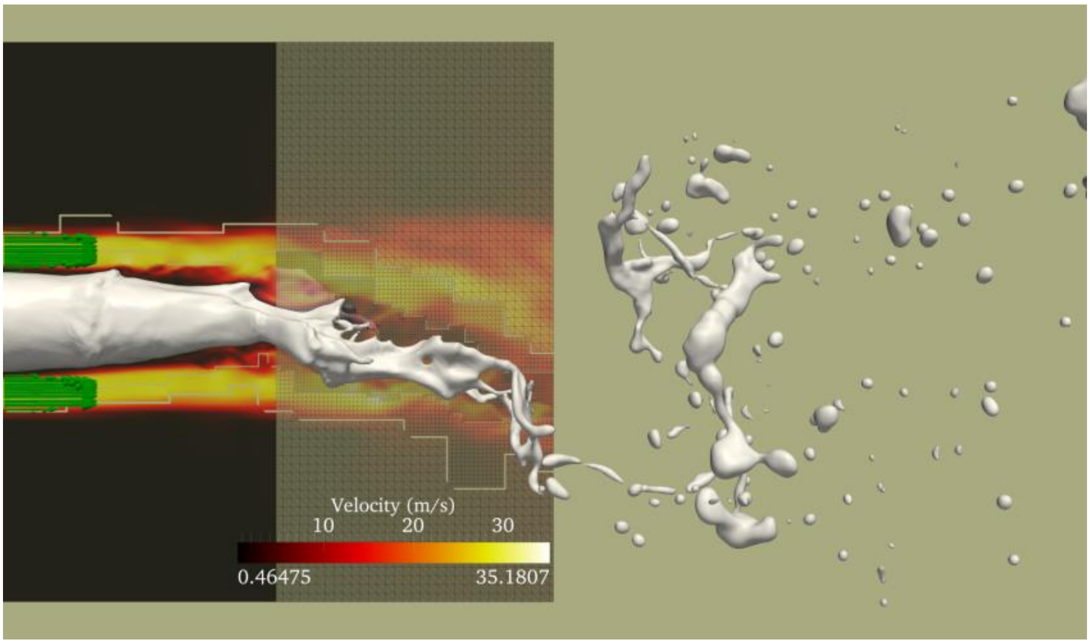


Figure 2: Sheared liquid jet simulation (experimental case T3.1)

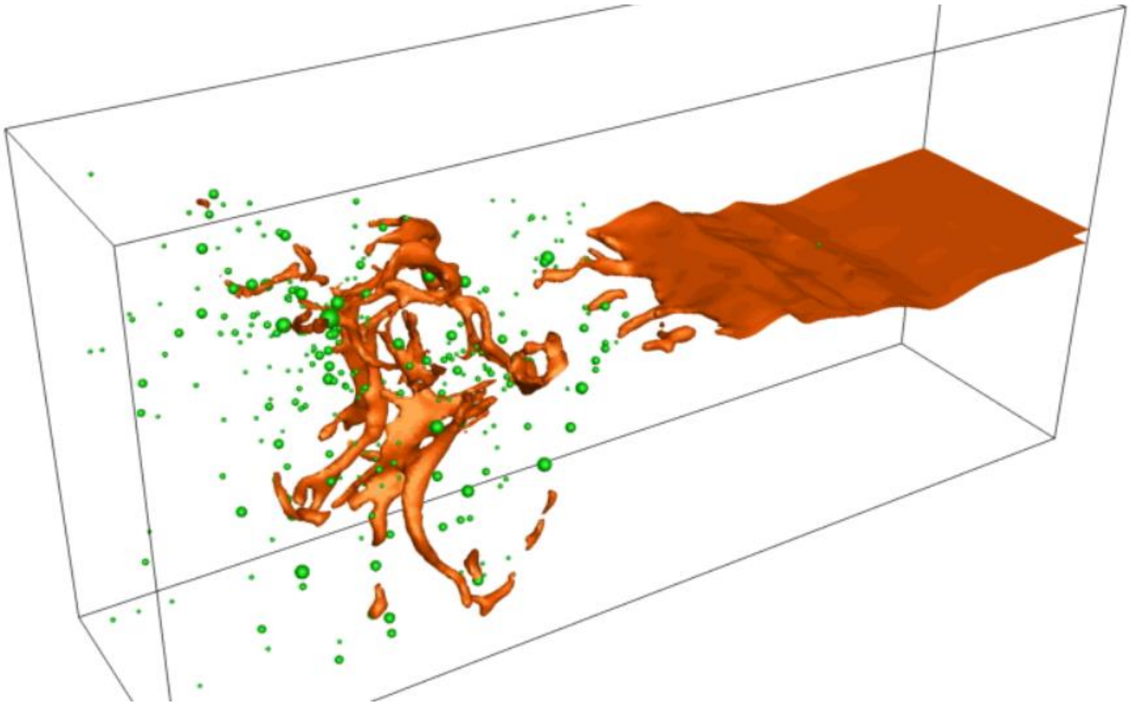


Figure 3: Example of Eulerian-Lagrangian coupling for the case of the sheared planar liquid sheet

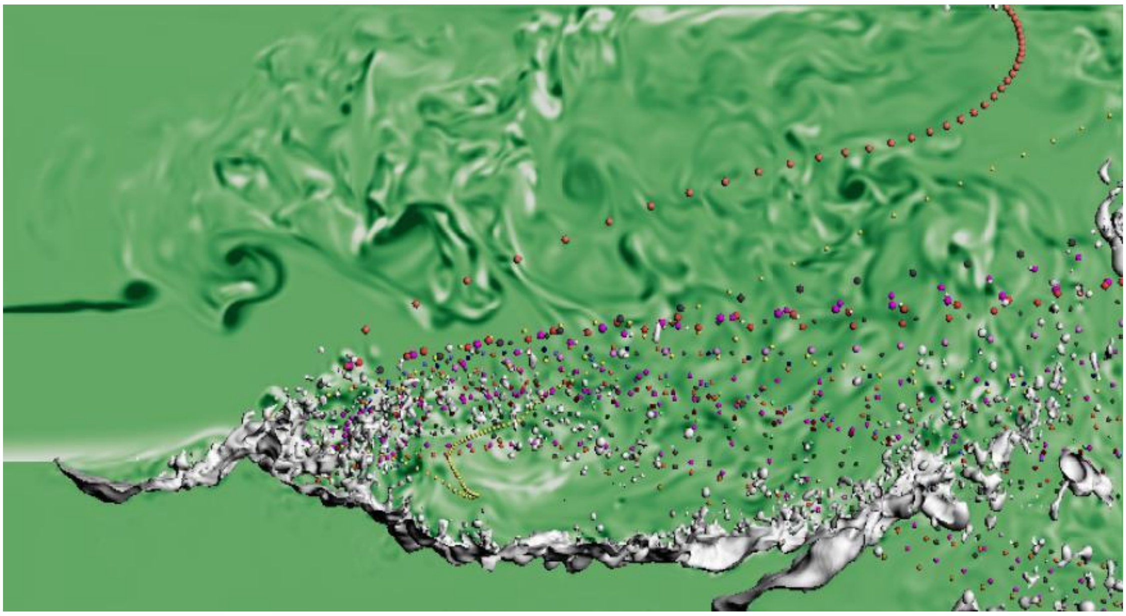


Figure 4: An atomisation simulation with the PARIS code. The colored spheres are example Lagrangian particle trajectories. Vorticity on the back plane is shown in shades of green.

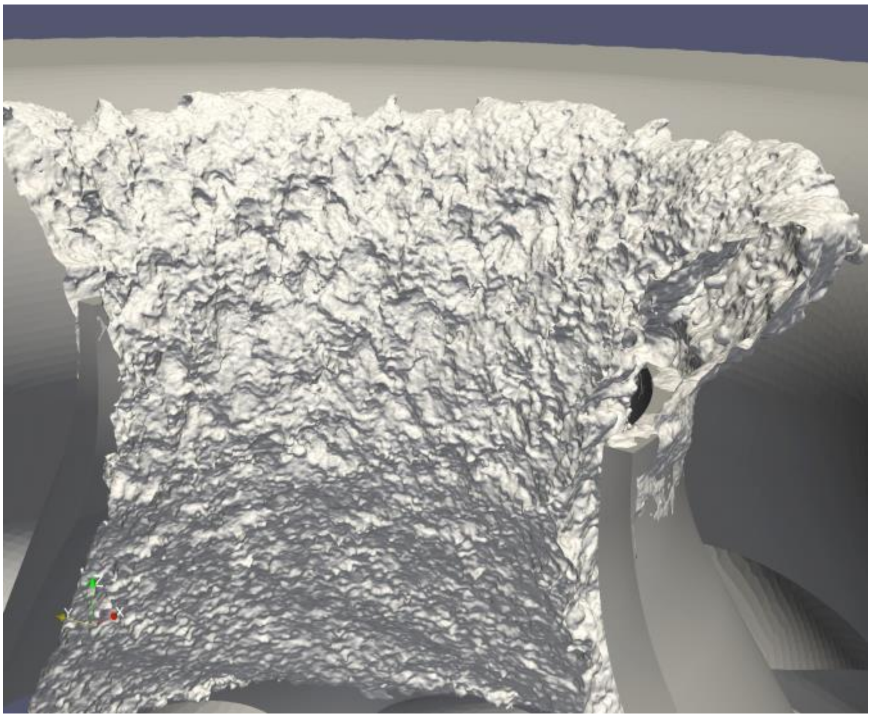


Figure 5: Simulation of the liquid film in the TURBOMECA injector

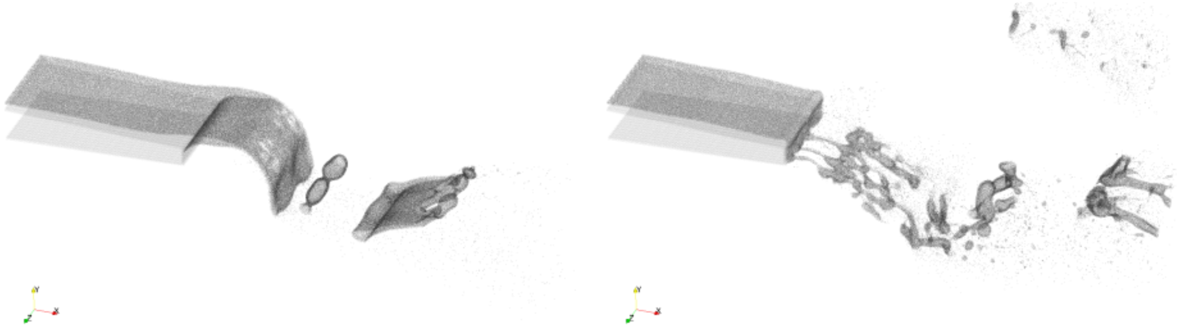


Figure 6: two snapshots of planar liquid film atomization – KIT experiment configuration

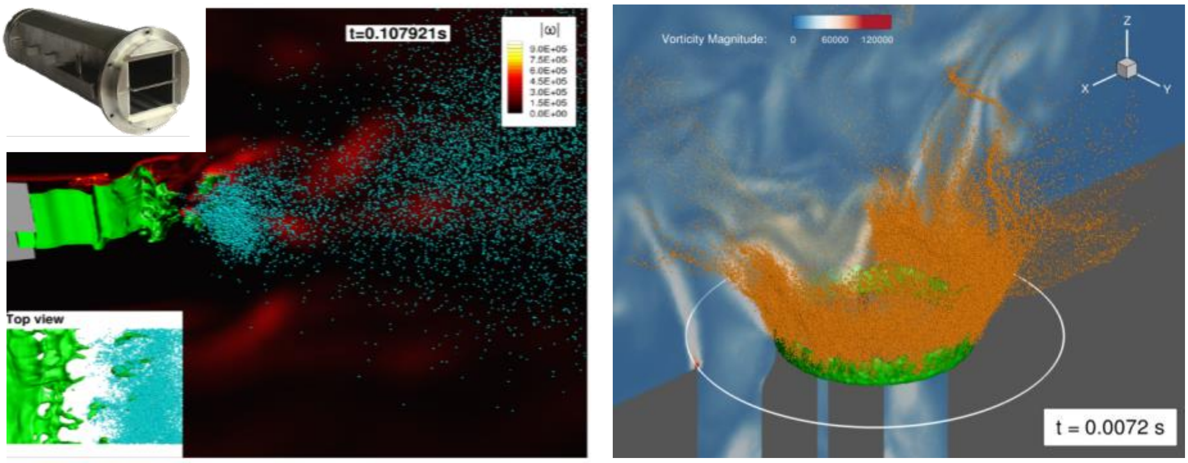


Figure 7: Multi-scale Eulerian-Lagrangian simulation of assisted atomization. Left: Planar liquid sheet. Right: Annular double swirled injector.

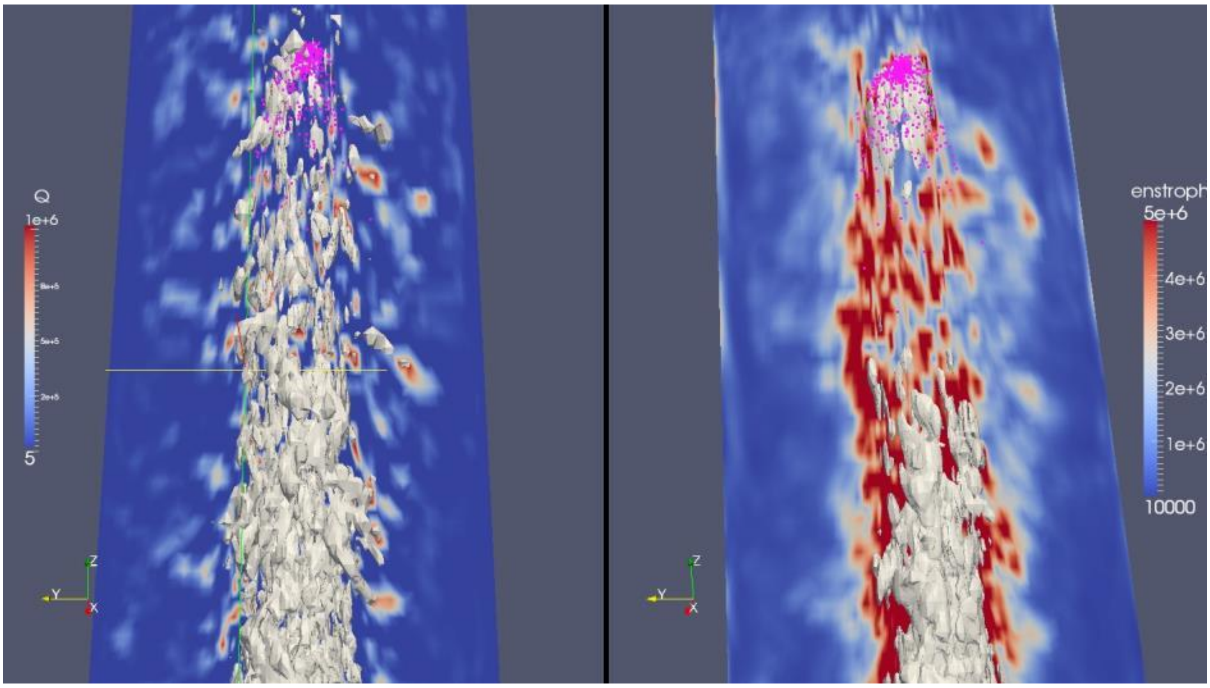
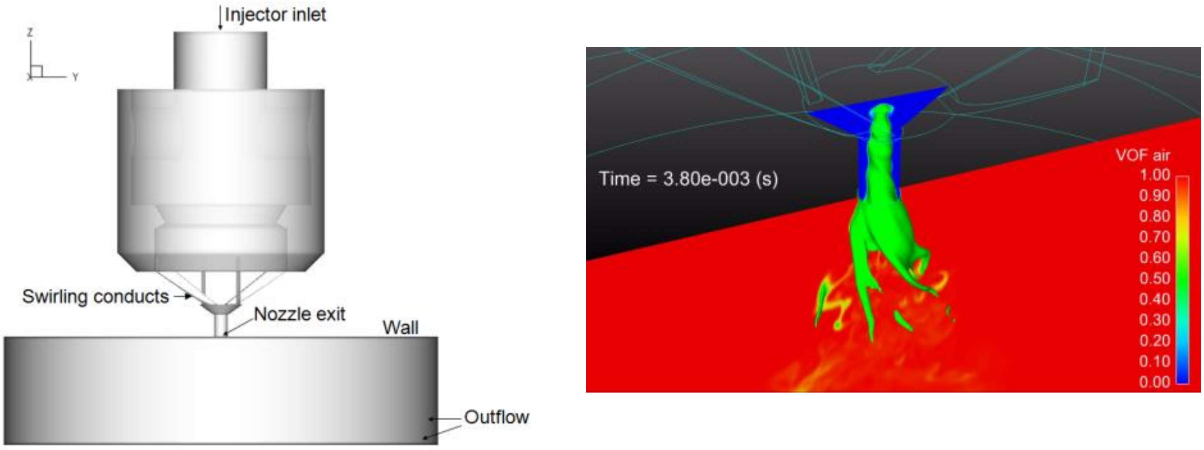


Figure 8 Sample sections though the LES domain showing clouds of particles (purple coloured spheres) with contours and slices of Q, the second invariant of the velocity gradient tensor on the left and similarly for enstrophy on the right.



a) **b)**

Figure 9: (a) Computational geometry for 3-D internal nozzle flow simulations. (b)) Sample of two-phase flow development below the swirling passages, as predicted by 3D VOF simulation

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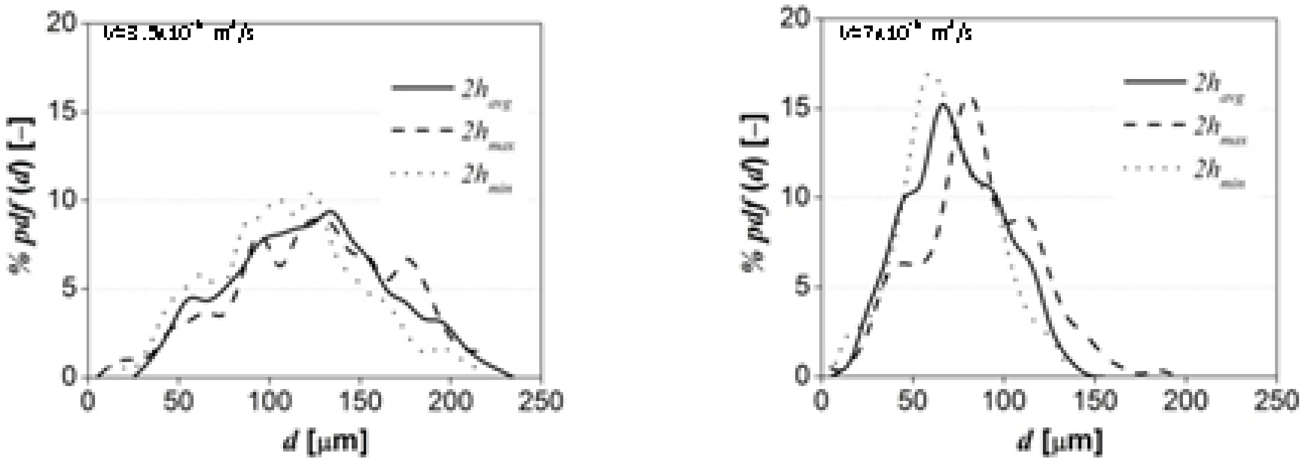


Figure 10: Probability density function distribution of drop diameter after primary break-up, function of the average, min and maximum values of the lamella thickness as predicted by 3D VOF simulations.

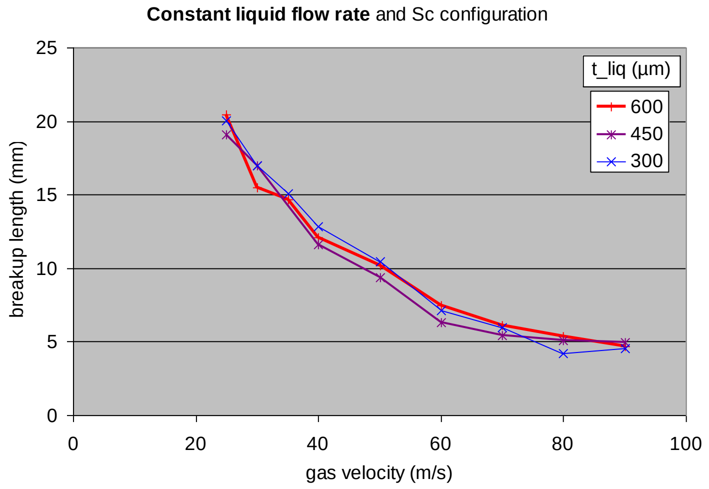


Figure 11: Breakup length according to air velocity for different liquid sheet thickness for the same liquid flow rate

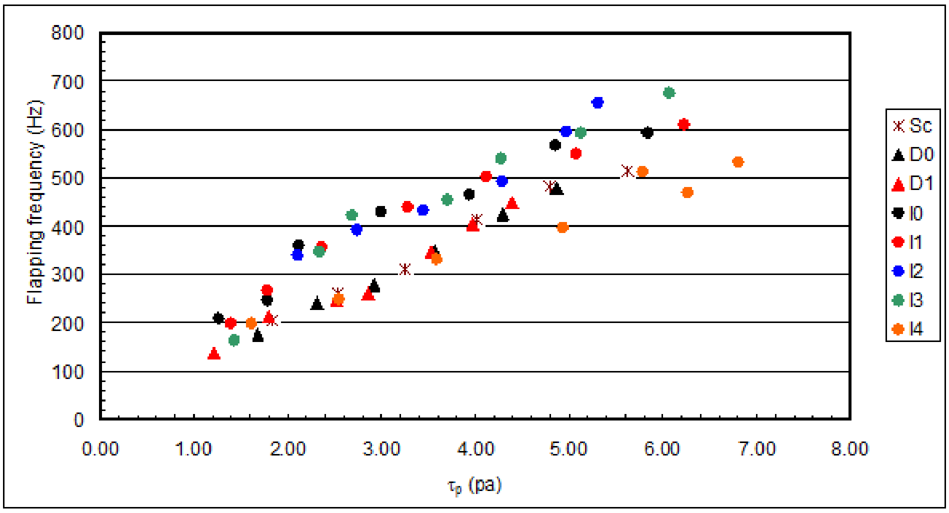


Figure 12: Flapping frequency evolution with wall shear stress (Liq: 300 µm – 2.2 m/s)

FLOW RATE	Q Flowmeter (l/h)	Q Probe (l/h)	*Deviation (%)*
With edge extrapolation	19.5	20.5	*4.99%*
Without edge extrapolation	19.5	17.8	*-8.78%*

Figure 13: Flow rate comparisons

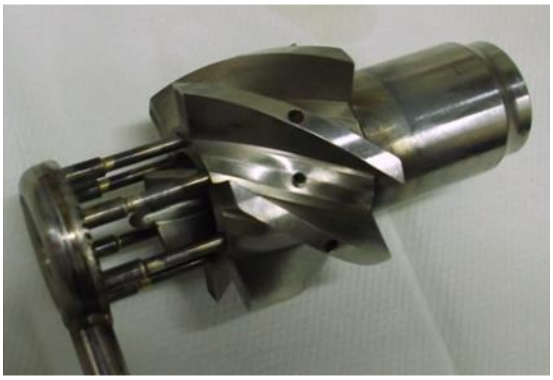
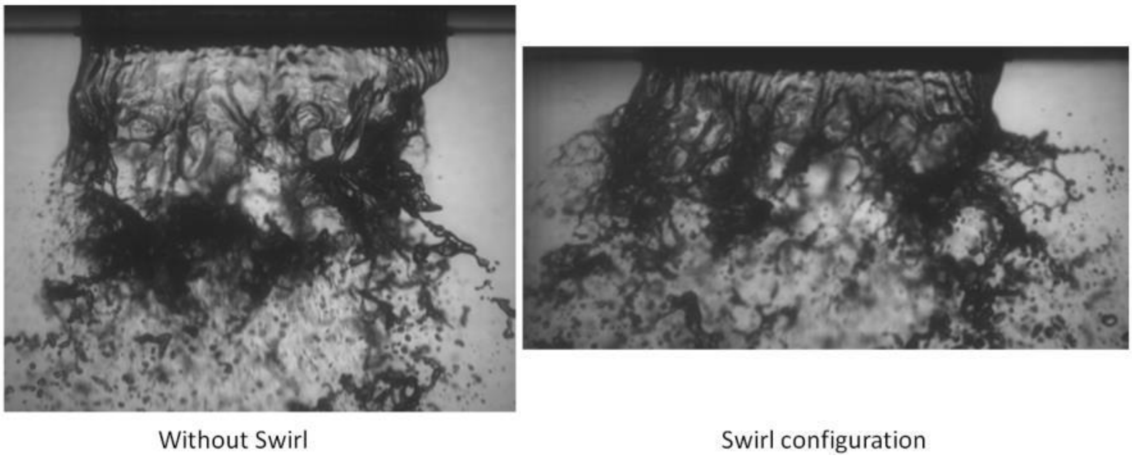


Figure 14: ONERA injector geometry: External swirl

Figure 15: ONERA injector geometry: Injector outlet



Without Swirl

Swirl configuration

Figure 16: Annular sheet atomisation (Air 30 m/s – Liq 2 m/s)

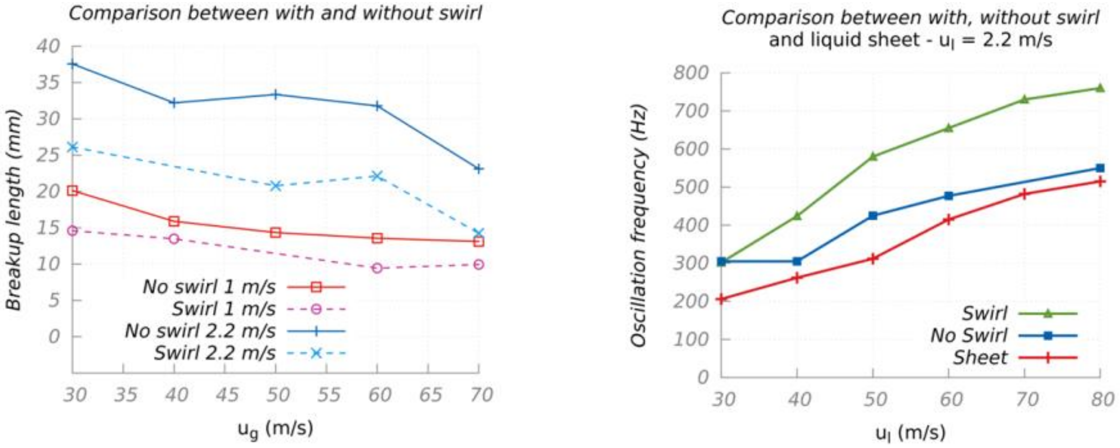


Figure 17: Breakup length and Oscillation frequency evolution.

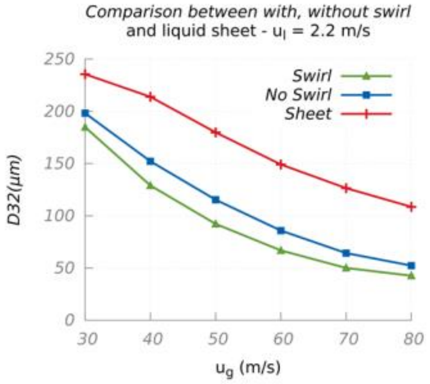


Figure 18: Droplet size evolution.

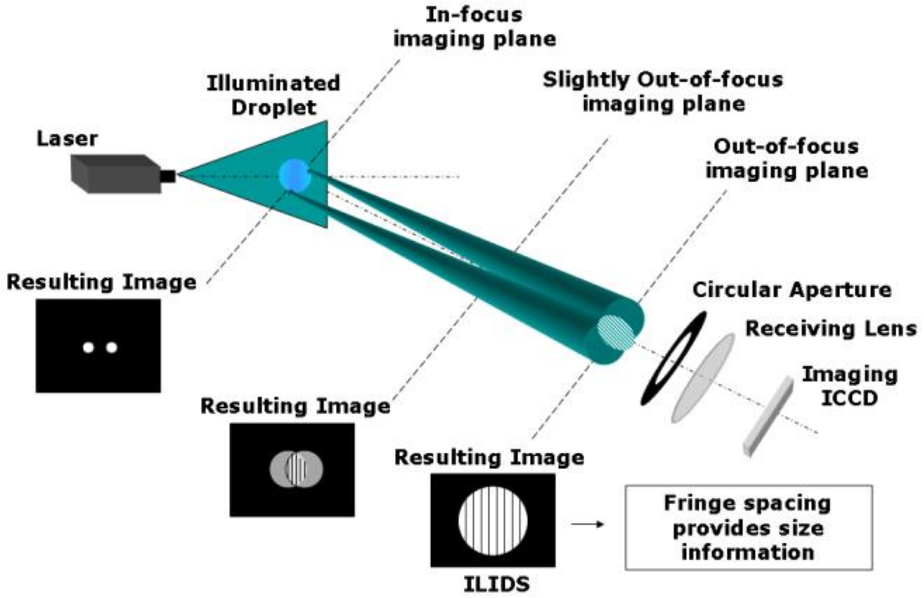


Figure 19: Schematic of the ILIDS technique

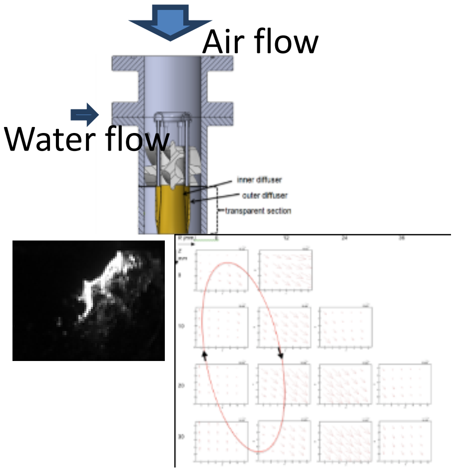


Figure 20: Schematic of the prefiliming atomizer with sample image of the OC image on the left and the measured droplet velocities on the right

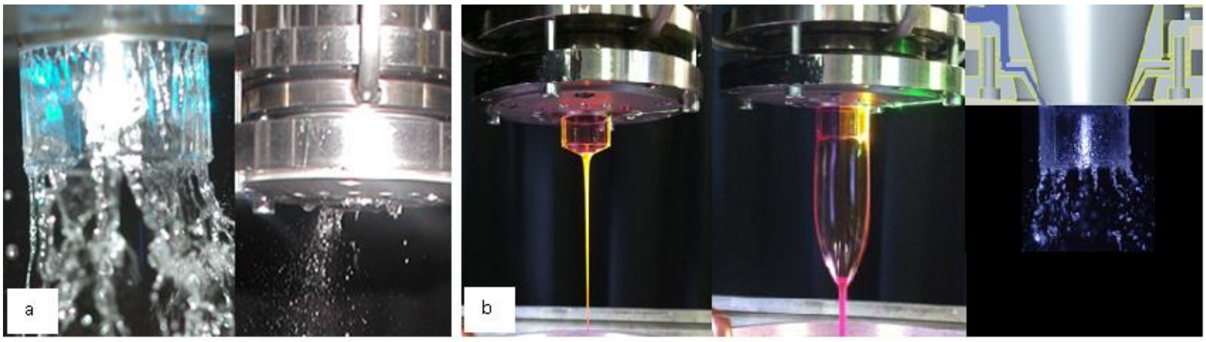


Figure 21: Homogeneity of liquid without air and with air (a) first design configuration, (b) final design configuration.

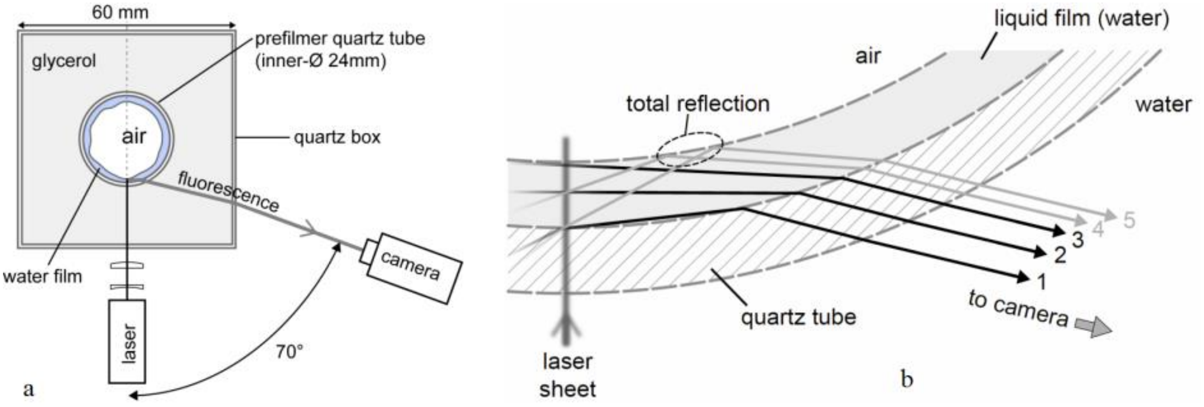


Figure 22: (a) Optical setup and (b) blow-up of the lower part of the circular tube in (a). The traces 1 to 5 correspond to the line-of-sights of different pixels of the camera perpendicular to the flow direction which 'reads' the film twice (effect of total reflection on the prefilmer).

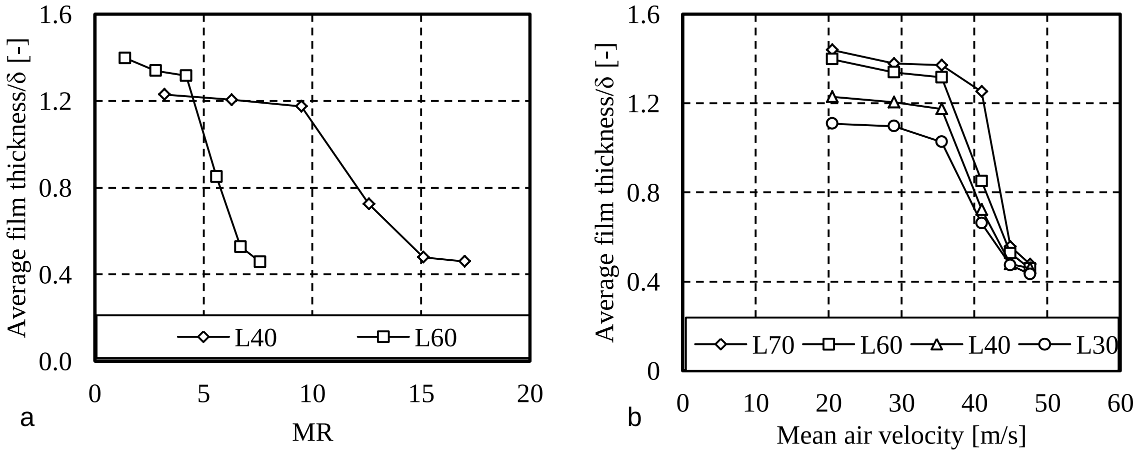


Figure 23: Film breakup observation for non-swirl flow:(a) by MR at constant liquid flow rates with increasing air pressure drop;(b) by changing the mean air velocity (air pressure drop) for different liquid flow rates at which breakup happens regardless of the liquid flow rate.

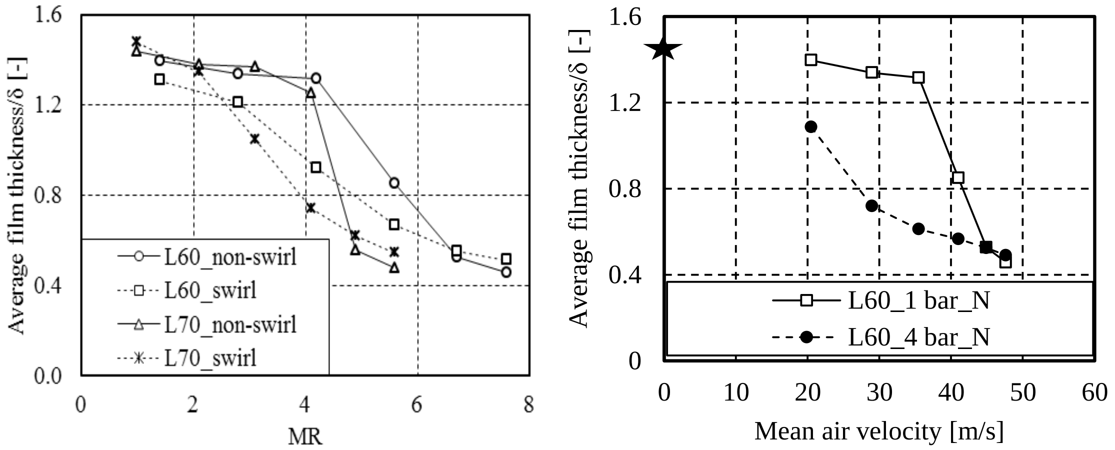


Figure 24: (a) Effects of swirl and non-swirl air flows at constant liquid flow rates (L60=60 kg/h) and the same air pressure drop for both liquid flow rates and both configurations at atmospheric pressure; and (b) comparison of operating conditions at the same liquid and mean air velocities (pressure drop).

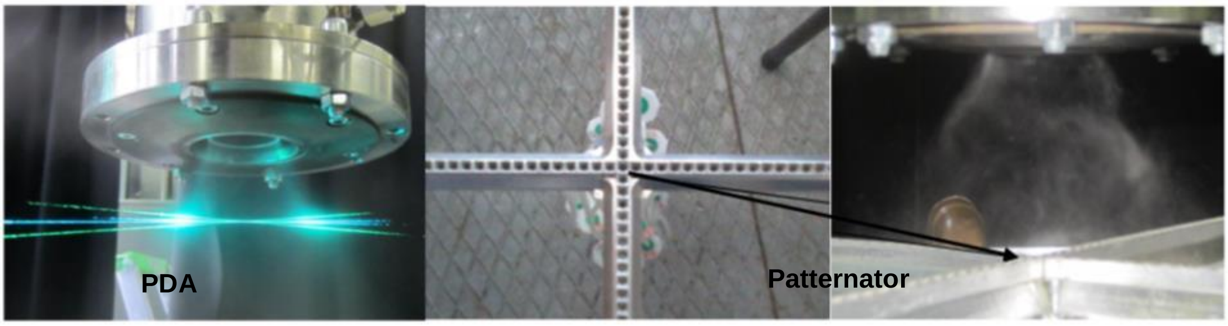


Figure 25: Picture of the PDA and patternator.

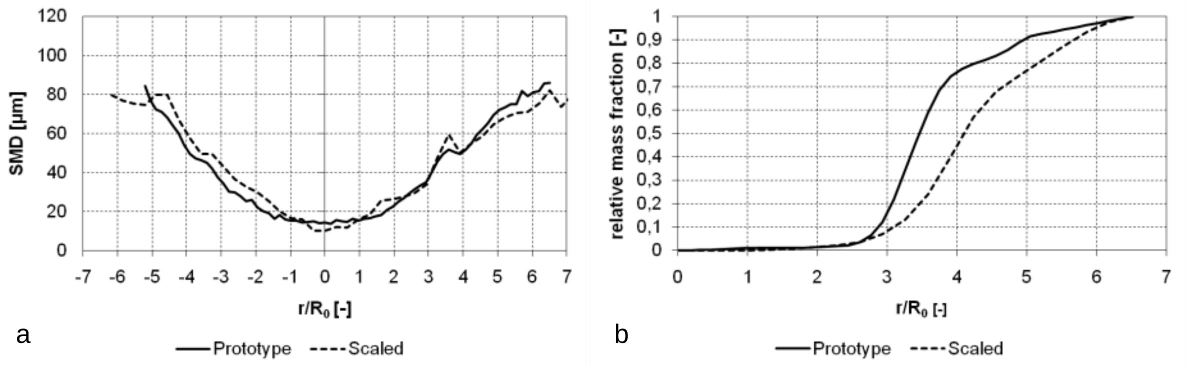


Figure 26: (a) Effect of scaling on the spray distribution at the same boundary conditions for the prototype and scaled IS; (b) comparison of relative mass fraction for (a).

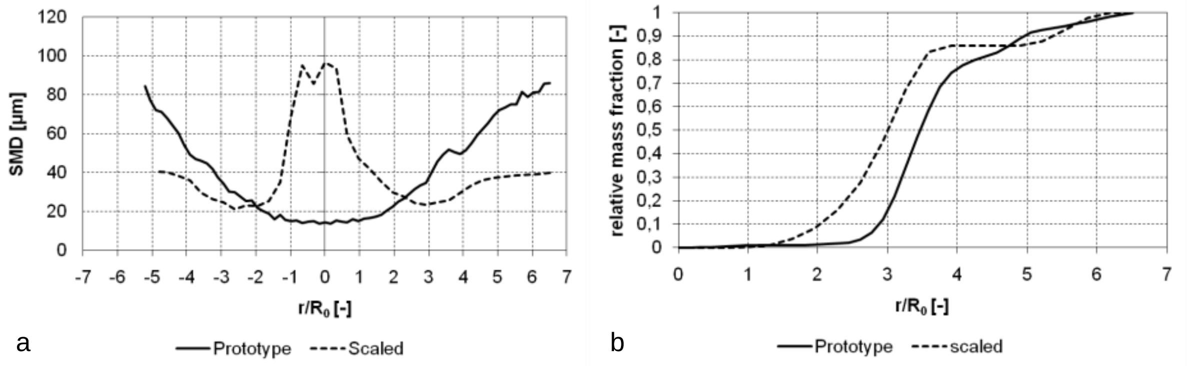


Figure 27: (a) Comparison of the two injectors at the same We-number (prototype nozzle at 3.5 % and scaled nozzle at 6.9 % pressure drops), (b) Comparison of relative mass fraction for (a).

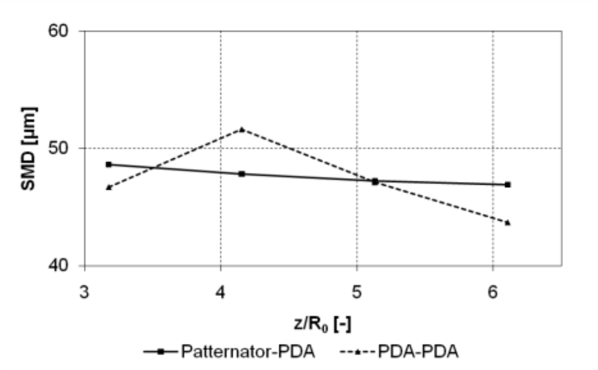


Figure 28: Comparison of the two combined measurement mechanisms (patternator-PDA and PDA-PDA) at different relative axial distance from the injector exit.

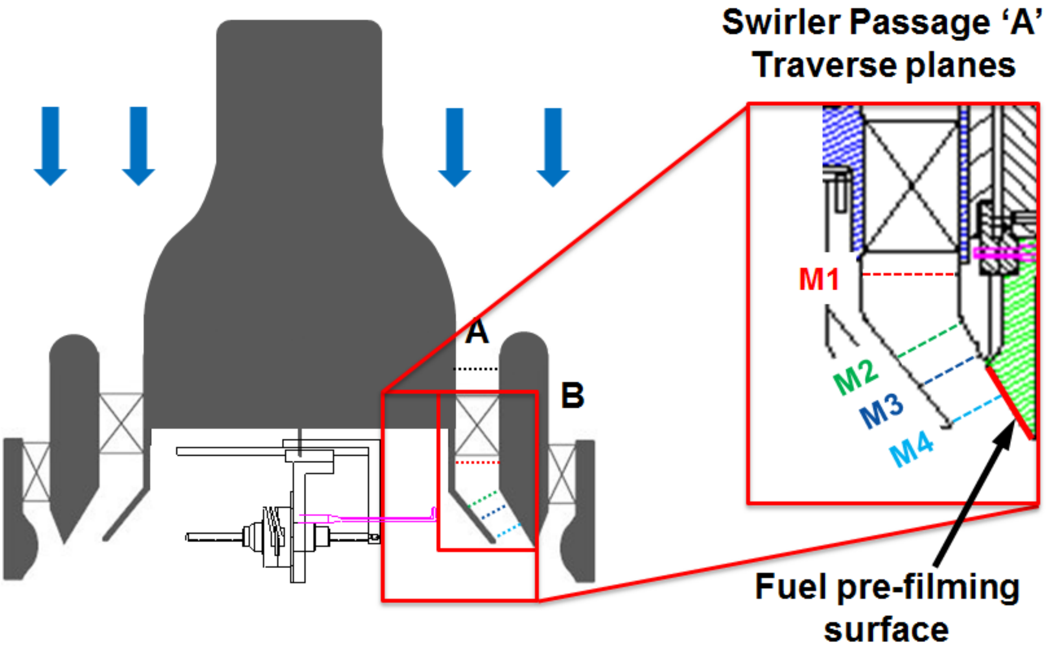


Figure 29: Phase 1 fuel injector geometry

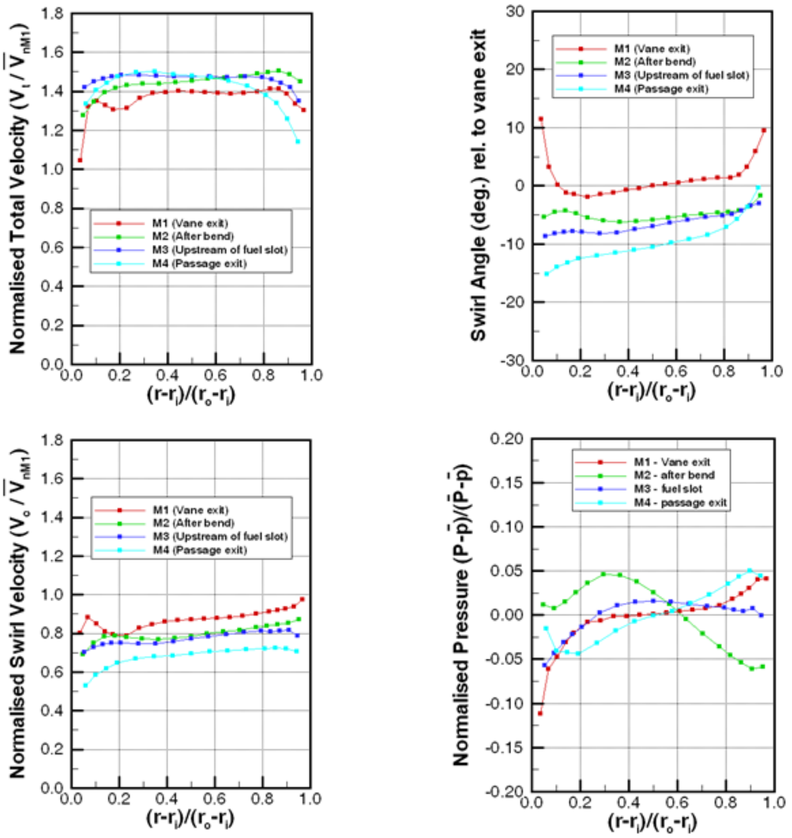


Figure 30: Radial profiles measured within passage 'A'

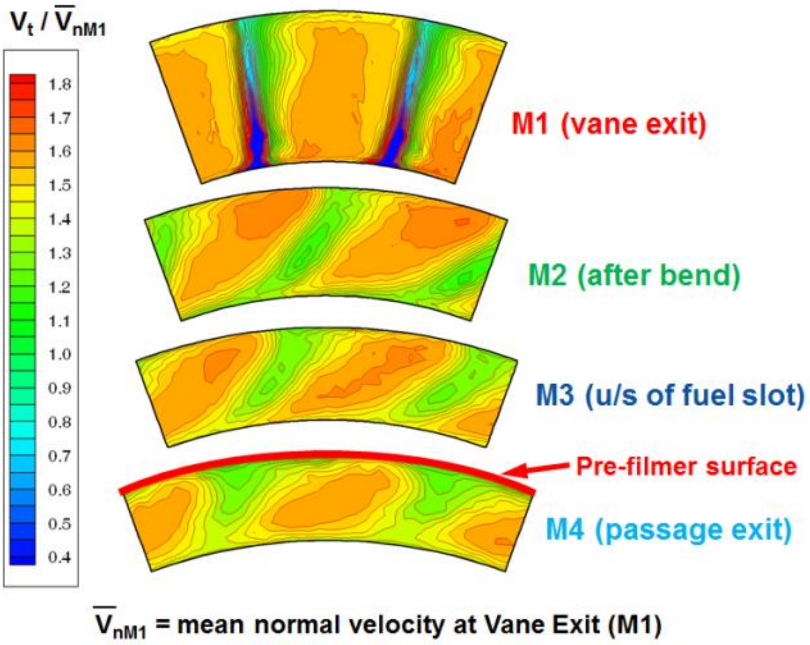


Figure 31: Contours of mean total velocity

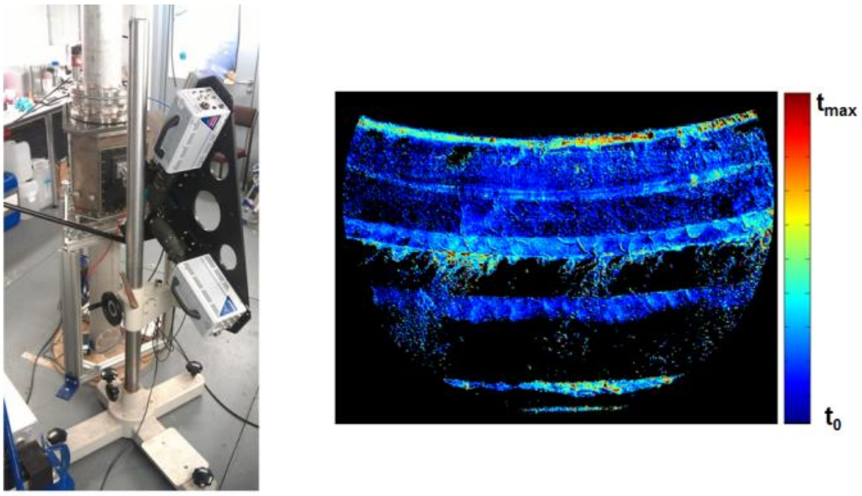


Figure 32: Film thickness measurement technique (instantaneous frame)

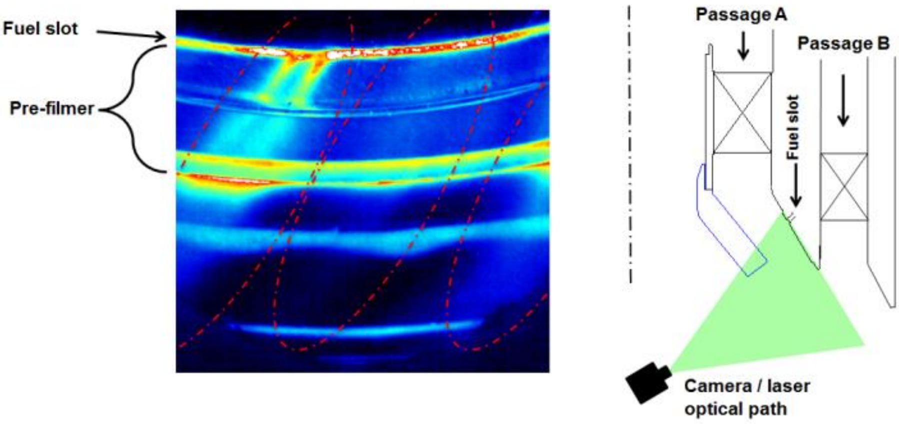


Figure 33: Mean fuel distribution indicated by LIF image

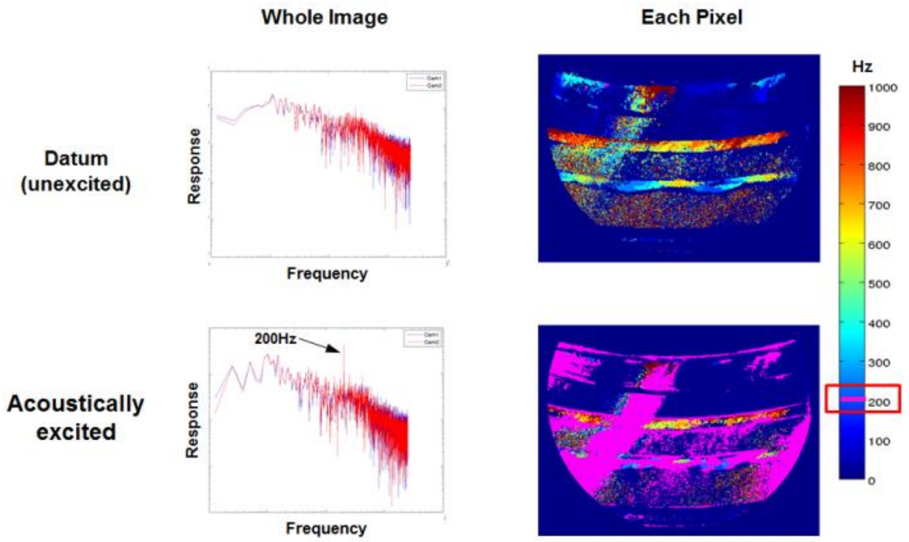
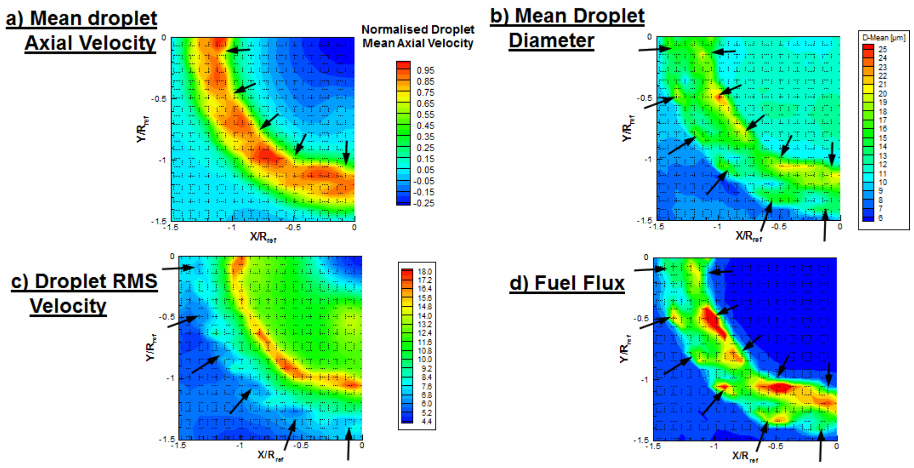


Figure 34: a) Whole image correlation b) Frequency of maximum energy

Response of fuel phase to aero-acoustic excitation



a) Mean droplet Axial Velocity

b) Mean Droplet Diameter

c) Droplet RMS Velocity

d) Fuel Flux

Figure 35: PDA measurements showing far-field spray characteristics

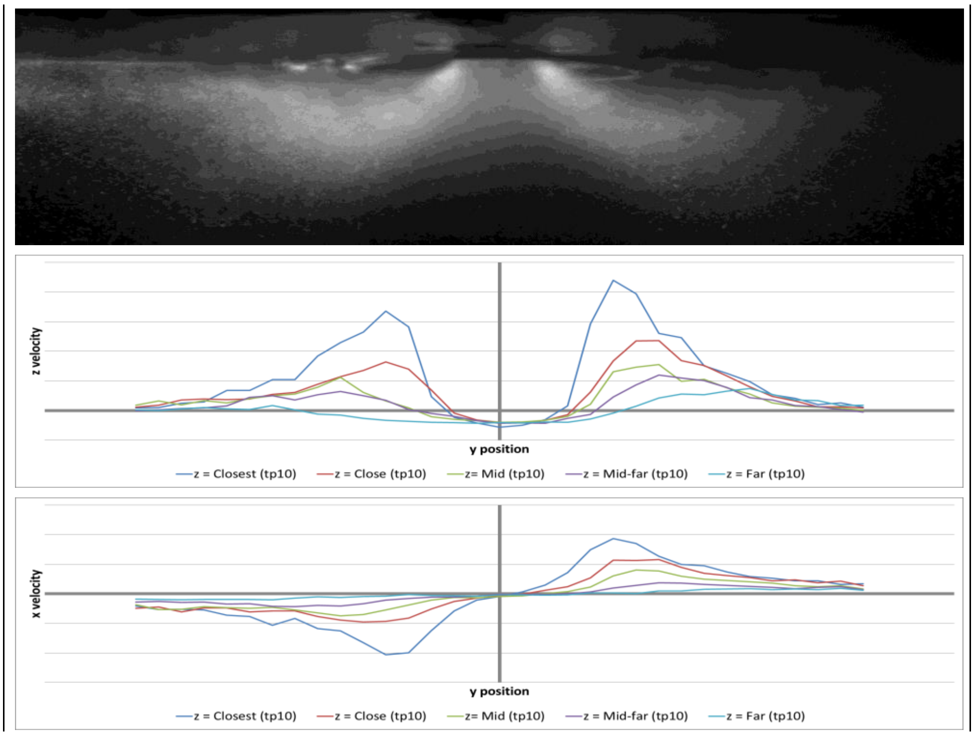
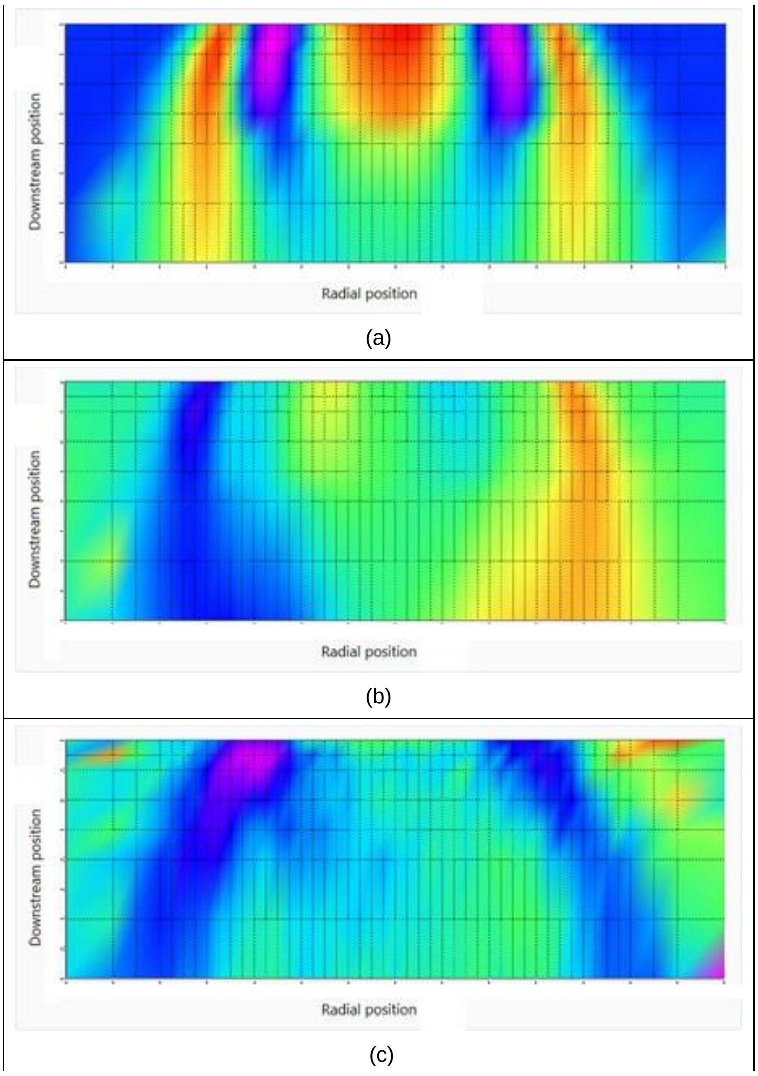


Figure 36: Rich burn injector in a simple air box configuration with boundary condition profiles used for CFD modelling



(a)

(b)

(c)

Figure 37: Contour plots of spray results downstream of a lean burn injector. (a) Particle axial velocity, (b) swirl velocity & (c) Sauter mean diameter.

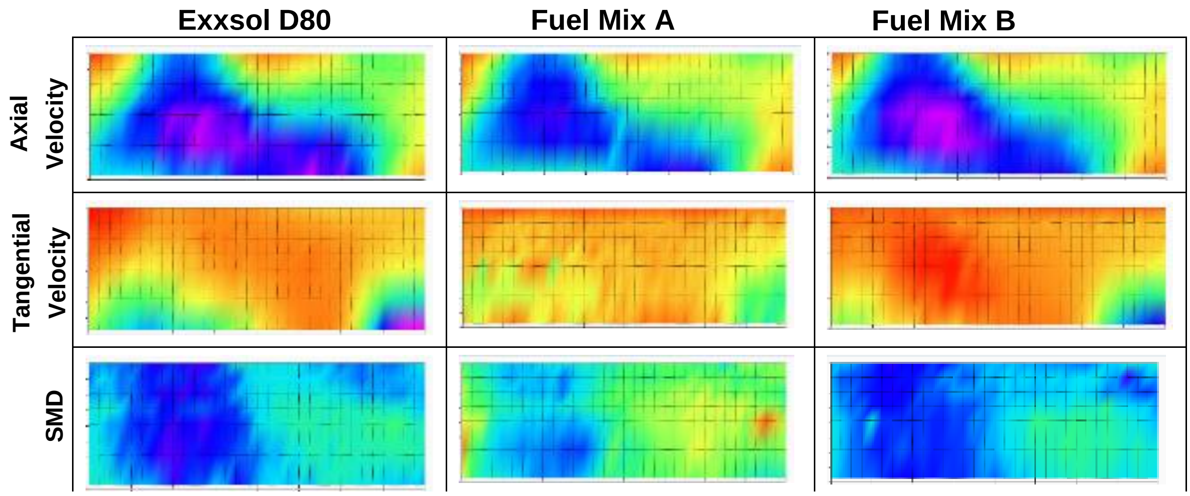


Figure 38: Comparison of alternative fuel blends using (Exxol D80), (Fuel Mix A = 18.2% Shellsol AB; 36.3% Jet A1; 45.5% Shell GTL) and (Fuel Mix B = 25% Jet A1; Shell 75% GTL).

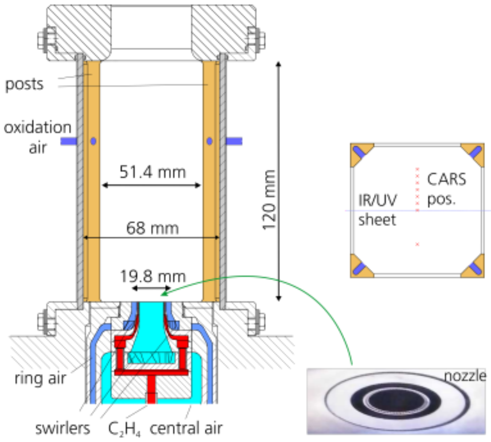
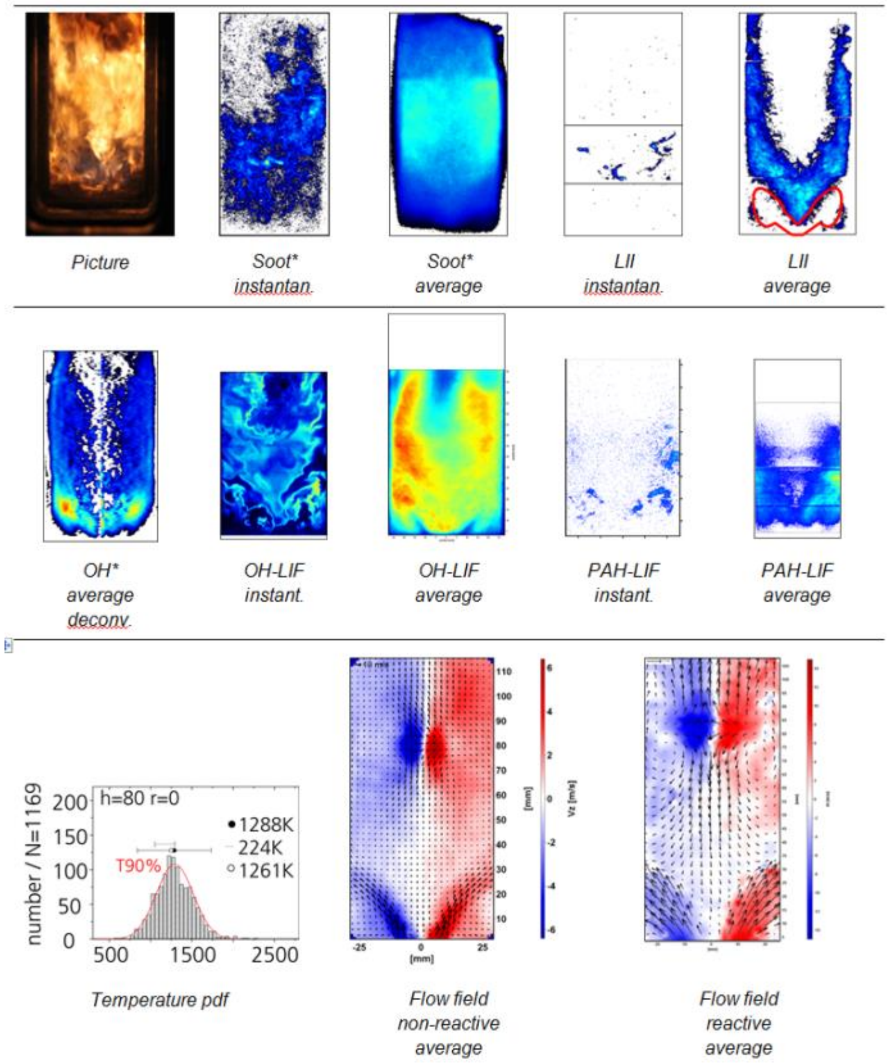


Figure 39: Burner geometry, nozzle details and cross section at the height of oxidation air injection, with the laser sheet and CARS measurement positions introduced.



Picture

Soot* instantan.

Soot* average

LII instantan.

LII average

OH* average deconv.

OH-LIF instant.

OH-LIF average

PAH-LIF instant.

PAH-LIF average

Temperature pdf

Flow field non-reactive average

Flow field reactive average

Figure 40: Different diagnostics applied to reference operating condition. The OH* chemiluminescence distribution is added as contour into the averaged soot distribution (LII), showing a complementary behaviour

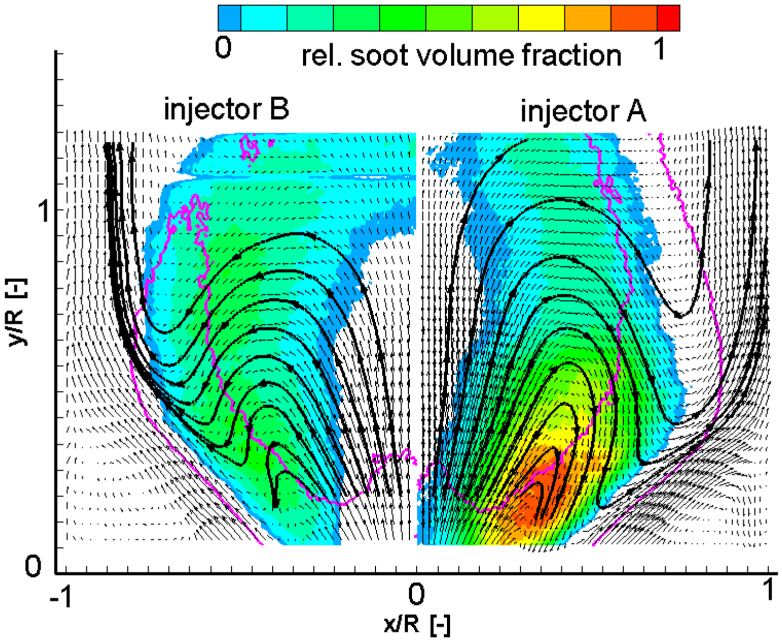


Figure 41: Velocity filed and soot distribution (false color) for injectors A and B at rich conditions. Magenta contour lines show heat release regions

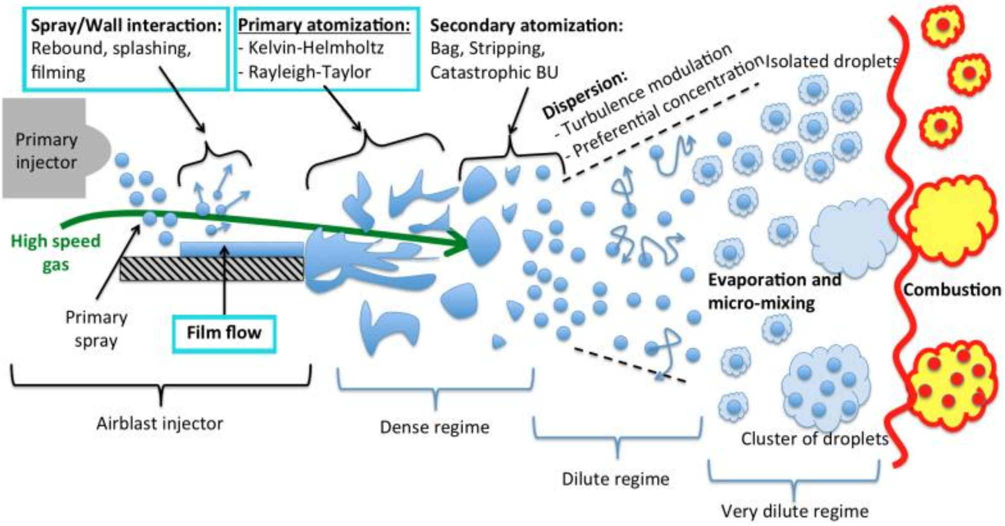


Figure 42: Main liquid phase phenomena in a combustion chamber supplied by an airblast atomizer

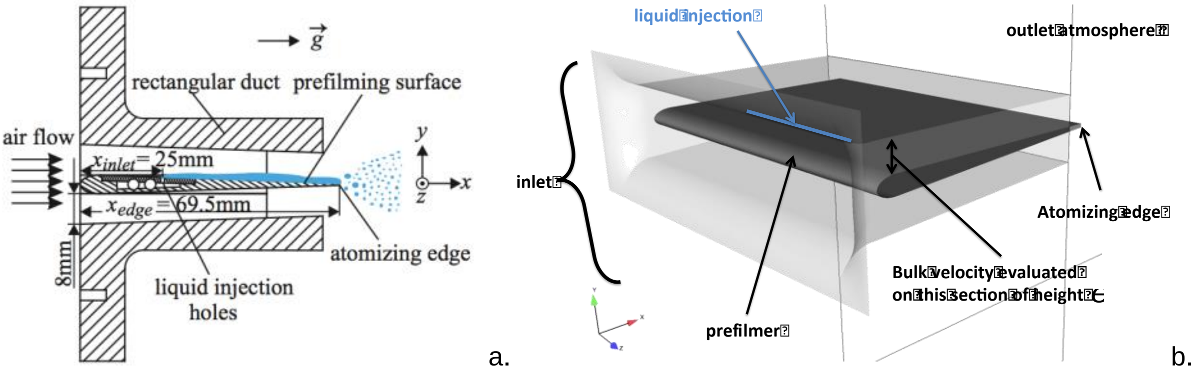


Figure 43: a. Schematics of the KIT-ITS experiment. b. Computational domain – zoom on the prefilmer

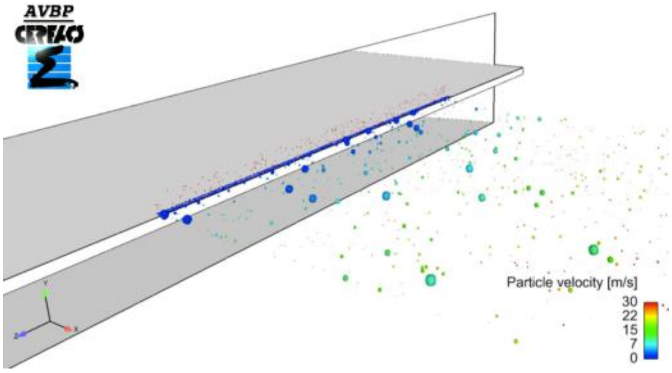


Figure 44: Instantaneous distribution of droplets downstream the atomizing edge in the KIT-ITS prefilming configuration

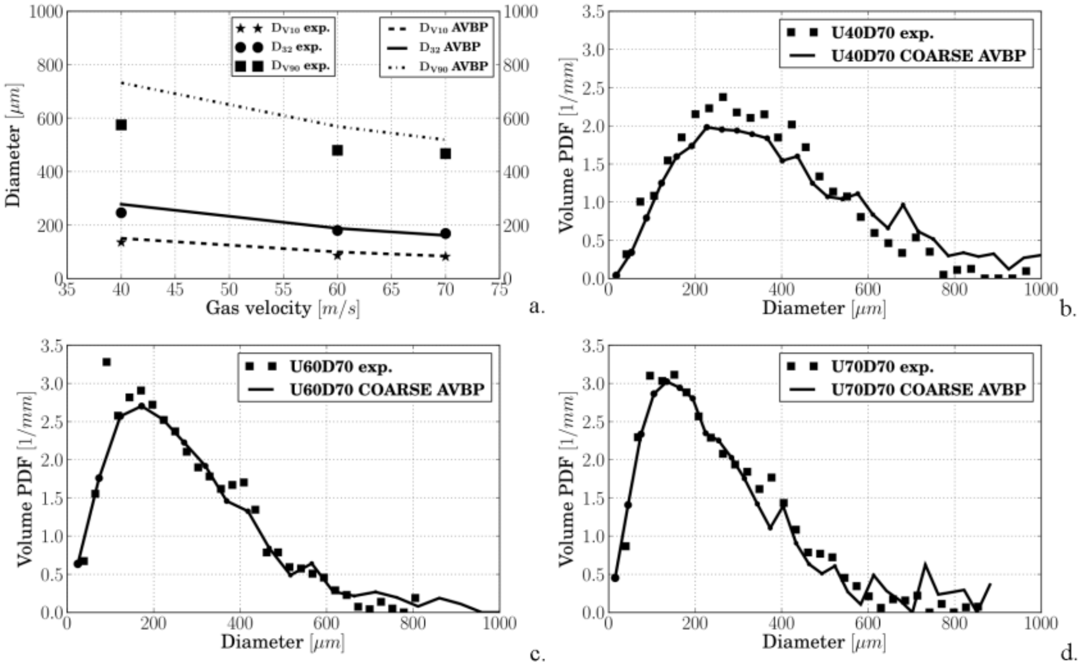


Figure 45: Characterization of the spray generated downstream the atomizing edge. Comparison between experiments (symbols) and LES (lines). a. Mean diameter versus gas velocity. b.-d. Diameter distribution for three gas velocities.

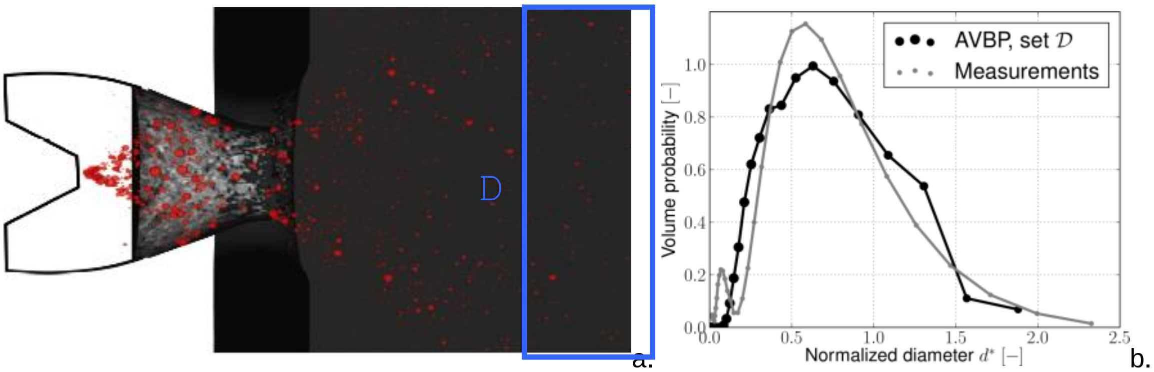


Figure 46: a. Topology of the liquid phase in the Safran Turbomeca combustion chamber (film droplets are hidden for the sake of clarity). b. Comparison between experiments and LES of volume distribution in the `D` volume sketched in blue in a.

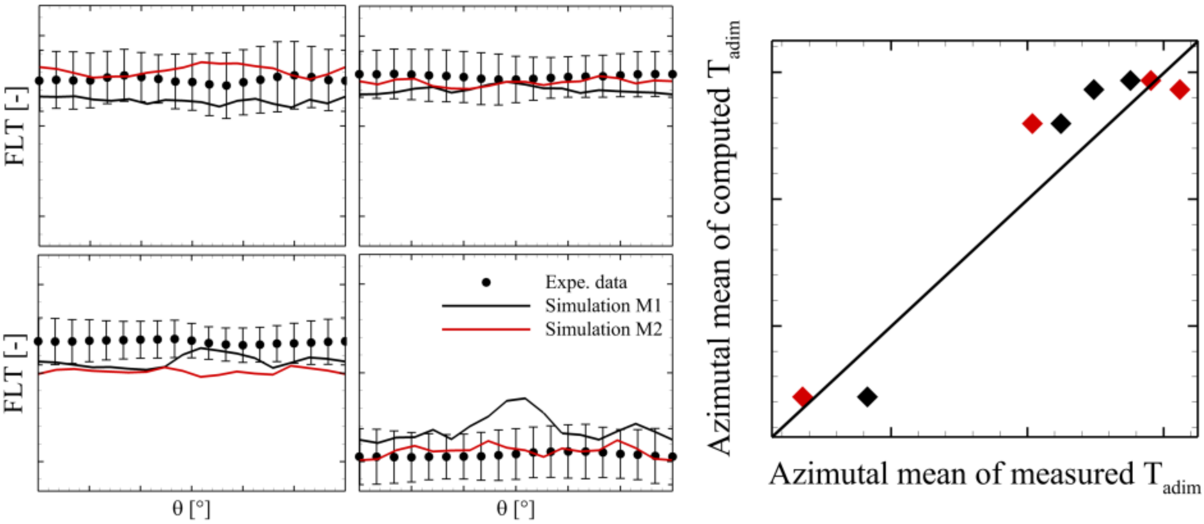
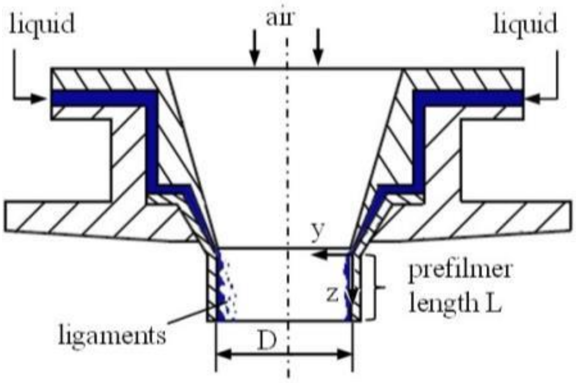


Figure 47: Simulations results compared with experimental data for a helicopter combustion chamber operating at max take off conditions



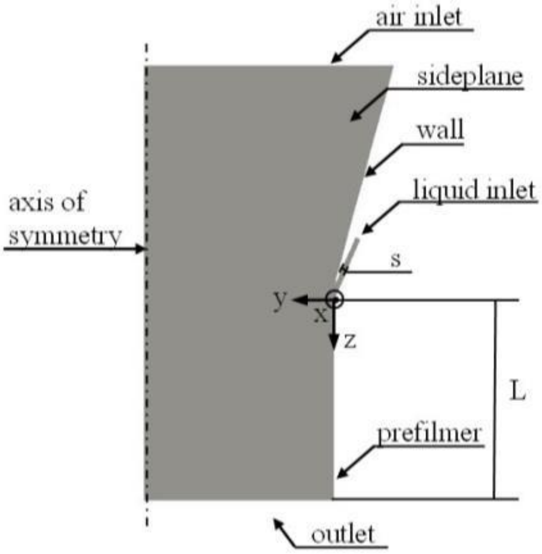


Figure 48: Model injector scheme (l.h.s) and simplified numerical model (r.h.s)

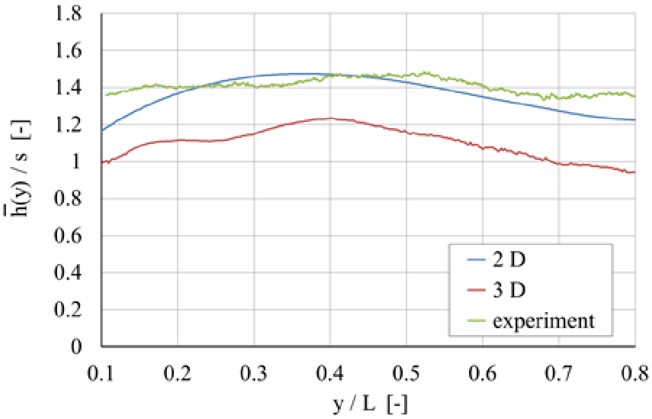


Figure 49: Temporarily averaged film thickness distribution along the prefilmer length: experimental data vs. numerical results of 2D and 3D modelling for M=3.1

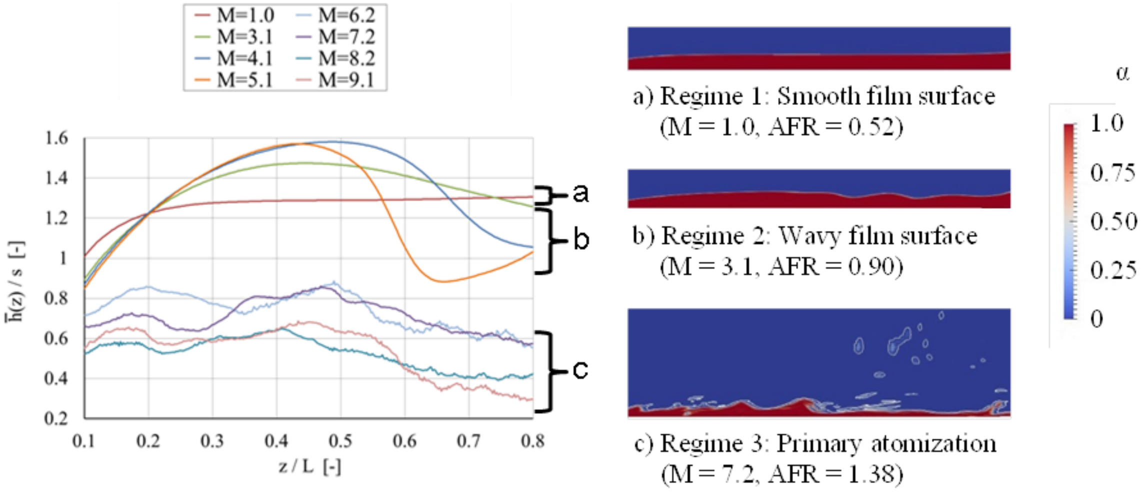


Figure 50: Regimes identified in the interface interaction

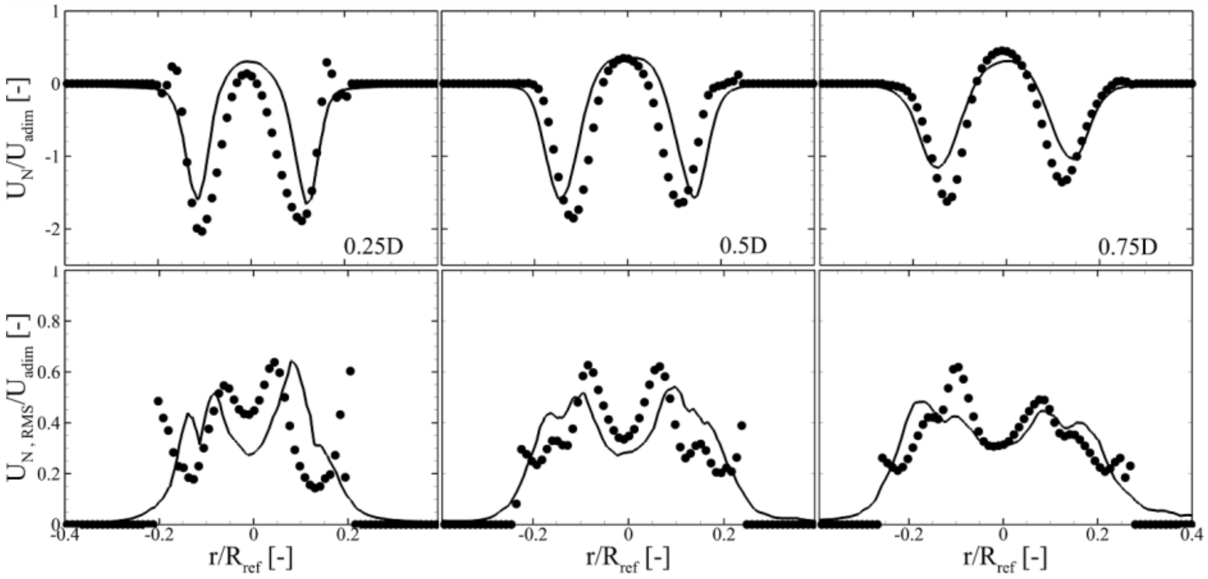


Figure 51: Profiles of mean (up) and rms (down) velocity components along three axial positions for configuration C2. The symbols represent experimental data and the solid line the aerodynamic simulation. Left: 0.25D; center: 0.5D; right: 0.75D.

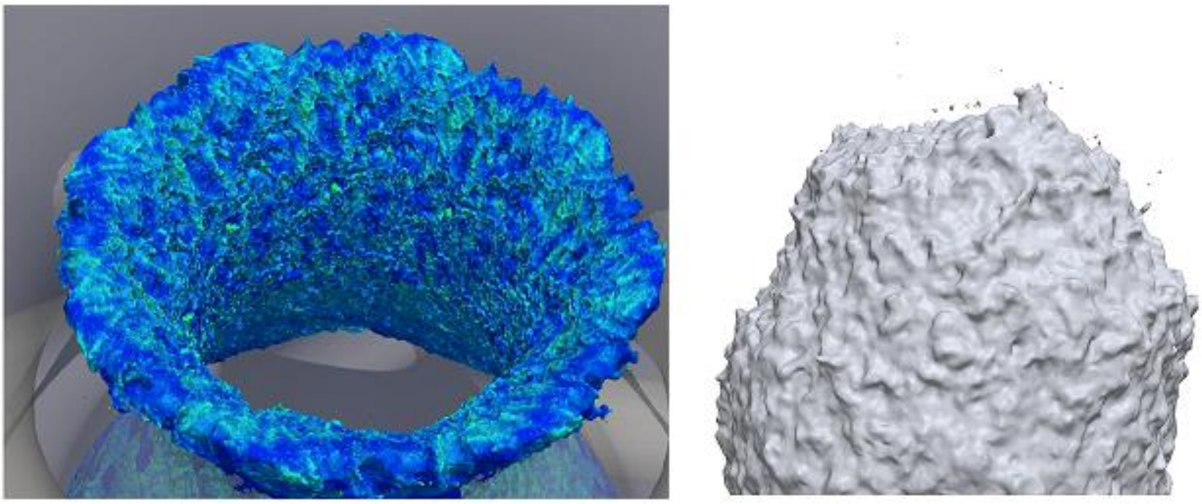


Figure 52: Iso-surface of level-set function for the two investigated industrial injectors. Left: configuration C1; right: configuration C2.

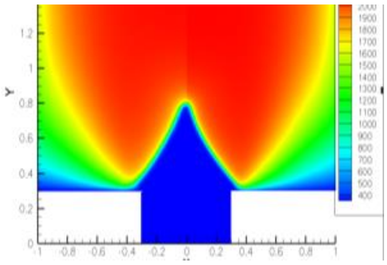


Figure 53: Temperature result using Lamfla2D (TUE, van Oijen), left and PRECISE-UNS using the DLR detailed chemistry model (right).

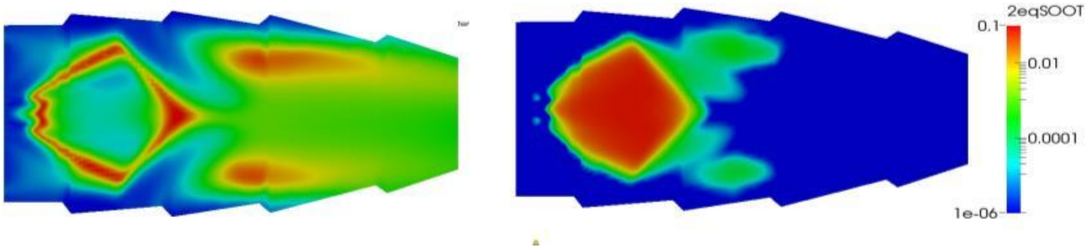


Figure 54: Temperature and soot field computed with DLR's chemistry and soot model for the small combustor

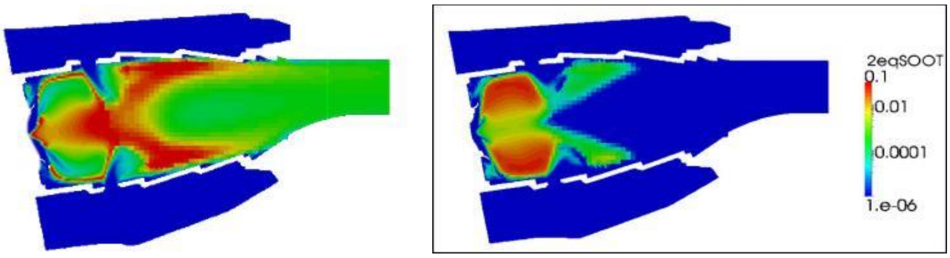


Figure 55: Temperature and soot field computed with DLRs chemistry and soot model for the large combustor.

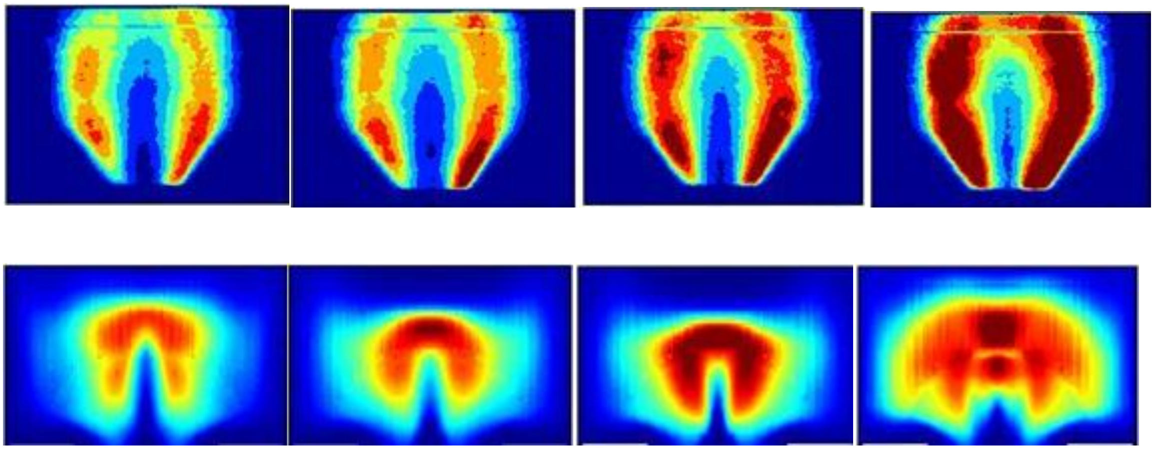


Figure 56: Measured soot concentrations of a lean injector (top). From left to right the AFR decreases and computed soot results.

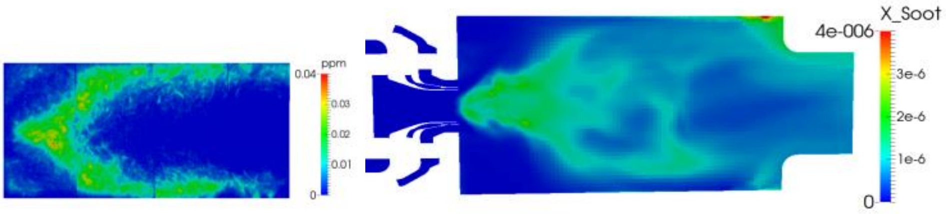


Figure 57: Measured (left) and LES results (right) soot more fraction.

4. Part 4: Potential impact, main dissemination activities and exploitation of results

Summary impact at project level:

The impact of the FIRST project is through the development of new substantial and critical new tools, and the improvements of existing methods, for the investigation, design and optimisation of combustion systems for environmentally sustainable air transport. The capability to model fuel sprays and soot emissions in the gas turbine engine combustor will accelerate the EU industry's effort to achieve the ACARE goals and reducing NOx, CO_2 and soot emissions.

Through the improved measurement and modelling capabilities, both in fuel spray and in soot formation, FIRST directly contributes to the more rapid development of more affordable, cleaner and reliable engine products therefore helping Aviation moving one step closer to achieving the ACARE goals for a greener, safer environment.

The US competition in air transport propulsion is benefitting from substantial funding of their own. The innovative solutions and technologies developed in FIRST will enhance the competitiveness of EU aero-engine industries by offering new technologies to the growing market demand for cleaner engines. This has in turn potential to generate new job creations and increase employment throughout Europe.

Through the research network established for the project, FIRST directly contributed to education, training and knowledge/competence sharing throughout Europe. At least six theses were written within the project, with to date three confirmed successful PhD degrees. Some results have already been used in a lecture within a course at the Von Karman Institute in Belgium. New research collaborations were established between universities, between academic and industrial partners and between SMEs and industry. This has already resulted in plans for further research with new applications for grants while some results are being passed onto the Clean Sky and Clean Sky 2 programmes for further development. New links with the automotive industry were created: through concrete transfers of knowledge from one industry to the other, the FIRST project could have a potential impact not only on the aerospace transport, but also on transport at large wherever fuel injector and combustors are used. When considering spray measurement, modelling and prediction capabilities, the new modelling technologies developed in FIRST could have a potential, beneficial input on a vast number of domains, for example in medical equipments in health, although links with other industries are yet to be made. Further research will be needed for extension of the impacts.

Below is a detailed report of the potential impact, the main dissemination activities and exploitation of results. FIRST had a prolific dissemination activity over the four years of research (over 70 publications), and the complete list is available on the public website here.

Detailed impact at Work-Package level:

4.1 WP2

As a result of the FIRST project, significant improvements have been achieved for the Direct Interface Simulations for primary atomization by CORIA, KIT, ONERA and UPMC. It is now possible to simulate the full process at least for academic configurations and in the near future for more industrial ones.

Two main issues were overcome: the first one is related to high liquid to gas density ratio simulations, the second one to the smallest droplet formation. All the main approaches dealing with interfacial flows were considered in this package: interface capturing methods like VoF, coupled VoF-level-set, meshless like SPH, conservative level-set on unstructured grid and finally diffuse interface methods. Several multi-scale strategies were developed to capture and follow the smallest droplets generated in the primary atomization process. First comparisons with experiments also conducted in the FIRST project show good agreement. The interest of such accurate direct interfacial simulations is twofold. Firstly, it can be considered as a numerical experiment that provides reliable insight on the physic of primary atomization. Secondly, the results can be employed to design large scale models for industrial LES two-phase flows computations as well as supplying accurate and unsteady boundary conditions for the spray. It is worthwhile mentioning that a specific workshop entitled **Investigation of Assisted Atomization in Industrial Application** was held last summer in Toulouse

Concerning sub-scale models for droplet formation, some effort was put on the prediction of droplets characteristics in the case of hollow cone pressure injector. In the context of RANS simulations, the atomisation model developed by UNIBG for hollow cone sprays is capable of determining the dominant mechanism responsible for primary break-up and the most crucial parameters affecting the process. Under the selected operating conditions, suitable for aero-engine applications, the liquid lamella thickness at the nozzle exit and the fuel injection rate appear to be the most sensitive parameters to the evaluation of the d_{30} mean diameter of the spray generated after the break-up of the liquid jet, confirming the crucial influence of internal nozzle flow development on spray formation. With regard to droplet behaviour in LES computations, IMPERIAL established the groundwork for the development of the dispersion and clustering models, through the evaluation of the current Eulerian-Lagrangian capabilities of open-source CFD packages. It indicated the fields requiring further development, resulting in the development of additional custom solvers and boundary conditions for use in this type of simulations. Another contribution was the generation of detailed computational datasets for heavily particle-laden flows at high *Re* numbers in LES and RANS frameworks for a variety of particle sizes. The purpose of the said datasets was the evaluation of the respective framework capabilities as well as the investigation of mechanisms pertinent to the phenomenon of particle preferential concentration.

With a decade of experience in soot modelling DLR is known to provide detailed soot models with a certain predictive capability which is achieved by continuous model validation based on test cases at different levels of complexity. During FIRST, significant model improvements have been achieved and deeper insights regarding soot evolution in laminar and turbulent combustion were gained. Respective dissemination activities are in progress. In the near future, the model improvements obtained in FIRST will be used for high-fidelity large-eddy simulations of technical combustors at various operating conditions as investigated experimentally within FIRST, thereby, supporting future combustor design.

At IMPERIAL, the use of ab initio methods to address long-standing problems affecting calculation methods for practical fuels is a major step towards addressing the societal challenge of particulate emissions from propulsion devices. The starting point for the soot modelling approach was developed with EU FP6 funding to provide critical information on nano-scale soot particle size distributions for SOFC applications in order to prevent stack damage. Subsequent research support from Scania for low emission Diesel engines and for aero-engine specific challenges (FIRST) resulted in archival joint dissemination and contributions to a new international group of leading universities. It also provides the basis for a bilateral collaboration with the Rolls-Royce Commonwealth Center for Aerospace Propulsion Systems (CCAPS) and the currently EU funded DREAMCODE project.

4.2 WP3

Regarding the development of experimental diagnostic tools, a novel fibre optic probe technique was successfully implemented in a fully functional measurement system. This could benefit the entire scientific community dealing with fine and dense sprays. This method was compared with other techniques, and should assure potential users to adopt it in addition to their traditional tools. In terms of employment, the commercialization of this new product should lead to the creation of 2 or 3 positions within the A2PS Company in the next 3 years (now composed of three persons). The most significant impact of the A2PS participation in the FIRST project is probably the fact that this small high technology company is now known and “referenced” by opinion leaders and major players dealing with sprays, within and outside the FIRST project. From a different perspective, Imperial College successfully combined the simultaneous application of two novel optical diagnostic techniques for the first time on a complicated academic geometry, namely a swirling axisymmetric prefilming atomizer. The technique provided a significantly improved method for evaluating the primary breakup length and allowed the concurrent measurement of the downstream droplet sizes and velocities. The simultaneous measurements permit the generation of insightful correlations between the primary breakup and the downstream droplet evolution.

Fundamental injector experiments allowed better understanding of the physics of atomization. Excellent progress has been achieved by CNRS-LEGI with the resolution of a more than 15 years controversy about the nature and the prediction of axial instabilities arising in air-assisted atomization. In addition, new issues have been unveiled by demonstrating the role of “hidden” parameters on the unstable behaviour of such systems: these new findings open the way to more refined investigations, and also would be quite challenging for direct numerical simulation. These academic experiments performed by ONERA and CNRS-LEGI also provided a large amount of experimental data bases that will be crucial in validating and improving present and future numerical simulations. These experiments have put forward the importance of boundary conditions on the atomization process, which is of paramount importance for numerical simulations. The data collected and the improved understanding of mechanisms provide guidelines for an optimal design of injectors. Also, some ways to (partly) control the atomization process have been unveiled through preliminary experiments. The main issue, however, will be to pursue the comparison between experiments and direct numerical simulations. The improvements required here a range from accessing more refined or extra variables in experiments to significantly increasing the physical time accessible to computations, the ultimate goal being to get direct numerical simulation of gas-assisted atomization process that are both reliable and numerically efficient to be routinely used by engineers. Much of this work was published in international peer-reviewed journals and presented during symposiums.

Simplified injector experiments were carried out by ONERA and Imperial College. These experiments have shown the usefulness and quantify the presence of a swirl on injection systems. The data obtained will facilitate the improvement of numerical simulation that will help in the design of future industrial injection systems. Also, the detailed measurements performed for a wide range of gas and liquid flow rates and for two different film thicknesses in a swirling axisymmetric prefilming atomizer will provide a valuable tool for evaluating the performance of existing computational tools and the development of new ones.

For understanding the physics of the atomization process and to provide experimental validation data, engine injector experiments were performed by DLR, Loughborough University, RRUK and SCITEK. Work carried out by Loughborough University provides aerodynamically representative data relating to the internal flow field within a modern low emission, injector. This will accelerate the development of airblast atomisers, both experimentally and in terms of numerical predictions. The data set has already been utilised within FIRST, providing both boundary conditions and validation data for numerical predictions. The work has been presented in several forums including various technical review meetings with Rolls-Royce, and at ASME Turbo Expo 2014. The new film thickness measurement technique developed was able to spatially and temporally resolve the fuel film in an aerodynamically representative geometry and, as measurements have not previously been available, this data will facilitate improved numerical methods. Furthermore, the technique has been demonstrated at a pressure of 4 bar which improves scalability towards engine conditions. The technique is now being employed within a UK funded research program utilising multiple advanced diagnostic techniques for two-phase flows at elevated pressure.

The measurements provided by SCITEK have allowed the improvement and validation of Rolls-Royce CFD models that will be used in the design process of future combustors designed for lower emissions. The improvements will aid the transition of RR combustor technology from rich burn to lean burn combustors substantially reducing emissions of NOx and smoke. They will also enable more accurate predictions of temperature profiles and increase cooling efficiencies leading to longer combustor and engine life. Furthermore, these improvements for better combustion design tools will increase European competitiveness against American companies which already have lean burn technology in service. The funding provided in the project has made employment more secure in both companies working on this task helping to subsidise salaries while ensuring essential research and development work is conducted to mature the design process of aero combustors.

KIT performed work investigating the surface stripping at realistic geometries. A model injector was investigated which possesses the main geometrical features of a real prefilming airblast nozzle and the ability to impose swirl on the air flow. The prefilmer is accessible for an optical measurement technique in order to measure the liquid film thickness. A new method for the evaluation of the film thickness was developed which considers the total reflection effect at the air-liquid interface. The main result of this work is that a great part of the film disintegrates before it reaches the atomising lip. This result is very important for further investigations because the position of the film disintegration influences the droplet dispersion and so the heat release distribution in the combustor. Furthermore, the results can be used for validation of CFD codes for 2 phase flows. The investigation of the influence of further important parameters (surface tension, geometry factor) is required in future for fully understanding the phenomena. Also, KIT developed a new method for the determination of the global SMD generated by an Airblast atomizer. The new method is based on the combination of PDA with a patternator measurement technique. Based on this methodology the effect of scaling factor and boundary conditions on the atomisation was investigated. The results of the current investigation show that at constant We-number the influence of air velocity is much greater than the influence of geometrical scaling. The linear downscaling of the atomizer shows marginal effect on the spray as compared with the prototype at constant air velocity. However, previous research works observed that for constant air velocity the SMD decreases with decreasing airblast atomizer diameter. The achieved results can be used to validate CFD codes due to the prediction of the droplet dispersion which highly influences the combustion process. The results were published at ILASS2013.

Activities in FIRST extended diagnostic capabilities towards not only quantitative measurements of soot distributions in realistic aeroengine combustors, but also complementary measurements of reaction zones and flow fields. This allowed correlations to be established between relevant phenomena and improved the understanding of soot forming processes and their parametric dependencies. Diagnostic methods for soot measurements developed in FIRST formed the basis for application in rich burn combustors. The data generated feed into the development strategies of RRD for both lean burn and rich burn technologies. The work performed in FIRST lead to a continued cooperation between DLR and RRD / RRUK on a broader basis by extension of diagnostic repertoire. Diagnostic methods developed in FIRST will be (and are currently) applied within IMPACT A.E., LEMCOTEC and German national programmes. The results of DLR's activity feed into the Lean Direct Injector Development which is a part of the combustor development effected in the Clean Sky 1 and 2 engine programmes. Regarding dissemination, results from DLR's work were presented at the IMPACT A.E. Workshop, (Dec.10-11, 2014, in Florence, Italy), and included in the Proceedings of ASME Turbo Expo 2013 (GT2013 June 3-7, 2013, San Antonio, Texas, USA, paper No. GT2013-94796). Furthermore, results were published in Journal of Engineering for Gas Turbines and Power Vol. 135 (2013)

Lastly, Work Package 3 was also focused on the creation of soot validation data sets. DLR provided a highly valuable validation data set for combustion emission modellers. This data from the FIRST project is now in use by partners throughout the academic and industrial community and includes researchers from Clean Sky projects. This confirms DLR's position as provider of high quality data characterizing combustors exhibiting technical features. The extensive use of this data and the comparison of model results achieved by the different approaches and groups, in research and industry, will certainly serve to bring soot modelling in combustors to a higher maturity, thus supporting future combustor design. Beyond others using our data set, DLR has identified several features contributing to a better understanding of soot formation and oxidation in technical combustors directly from the experiments. DLR is confident that future use of the burner developed within FIRST will find funding to follow those indications. This shall include development of other diagnostics to further complement the data set, and application of various diagnostics simultaneously.

4.3 WP4

Work Package 4 performed detailed validation of different numerical models and achieved some significant improvements of the numerical tools of the partners involved. For example, the phenomenological model for liquid injection through airblast atomizer has been implemented in the LES solver AVBP and distributed to SAFRAN engineers. From an industrial point of view, the model is now used by SAFRAN engineers in real combustion chambers to better understand the impact of fuel injection on the flame structure, the temperature profile at the combustion chamber outlet and the pollutant emission levels. The partners published the comprehensive work through a presentation at the 25th European Conference on Liquid Atomization and Spray Systems in Chania, Crete in September 2013, and one article submitted to the International Journal of Multiphase Flow.

The commercial code Ansys® CFX had not been verified in the aerospace sector as a tool to study the atomisation breakup process as all models implemented were developed for the automotive combustion. The secondary break-up model testing at different operating conditions with a real aerospace GE Avio combustor geometry validated the applicability of these models for the aviation sector. Moreover, the most recent developed secondary atomization models have been implemented in OpenFOAM and compared with the commercial code.

The phenomenological model to specify spray boundary conditions at the injector tip is based on spray measurements downstream of the injection plane and inverse methods. As it is not specific to the Snecma injector system used in the subtask, it can be easily generalised to any type of atomizers, especially to multipoint systems that are used more and more nowadays, providing spray measurements downstream of the injection system are available. The comparisons between numerical and experimental results downstream of the injector show good agreement in terms of droplet velocity and diameter distribution showing the validity of the method. As advanced numerical methods to account for complex liquid injection phenomena are far from being in everyday use in simulations of real geometries, this method of building a phenomenological injection model will certainly be used both by academia and industry to improve the reliability of the simulations of injection systems.

The phenomenological droplet cluster model proposed, developed and evaluated successfully in WP4 is not limited to the aero-combustor field. Rather, it is equally suited to a wide range of industrial and environmental applications, whether these are related to the internal combustion engine, spray drying process or pollutant transportation. This belief is reaffirmed from the successful application of the model, and the promising results it yielded on the industrial geometries of subtask 5.1.7. In this task the Reynolds numbers increased by an order of magnitude and the complexity of the flow was significantly increased through the introduction of multiple recirculation zones and high rates of shear in the azimuthal direction. In the near future the developed model will be tested on environmental scale problems and furthermore investigations will be carried out, once the required modifications have been made, to determine the applicability of the model for use in anisotropic flows.

The systematic cross-comparison of simulations in 2D and 3D of a sheared plane liquid sheet contributes to the validation of the codes recently developed with the latest experimental results within FIRST. This work has an impact on other research activities in the area of spray combustion. The results of the cross-comparison are helpful in the simulation of primary atomization and stripping, and in some measure also in the simulation of the large scale breakup, which provide the initial droplet size and velocity distribution in a combustion chamber. These droplet-size and velocity distributions will help improve codes that predict behaviour on the scale of the combustion chamber. The next stage is improvement of these kinds of results, as computational cost is still high and quantitative agreement is not yet reached. The various partners will thus actively search for improvements in the efficiency and accuracy of their simulations.

The soot formation modelling was improved significantly within WP4. With a decade of experience in soot modelling, the DLR could provide detailed soot models with a certain predictive capability which is achieved by continuous model validation based on test cases at different levels of complexity. To extend the predictive capability, unsteady Reynolds averaged Navier-Stokes simulations (URANS) and large eddy simulations (LES) of an unprecedentedly well-characterized aero-engine combustor were performed in FIRST and detailed insight into transient soot evolution at complex combustion conditions was gained and published. Even though soot was reasonably predicted, possibilities for further model improvement could be deduced and realized by implementation of a reversible soot precursor model.

The successful simulations of the TLC combustor at ONERA indicate that the multipoint injectors are efficient to prevent soot emission at take off conditions. They also deliver the scientific information that the soot yield has not a monotonic evolution as a function of the kerosene droplet size, although the biggest droplets give rise to the largest soot formation rate as expected. Both partners, DLR and ONERA, successfully published their comprehensive results in conference and journal papers of high quality.

4.4 WP5

The work with the film model used in task 5.1.2 in combustion calculations allows Snecma to better predict the behaviour of the combustors in some critical regimes as close to extinction or in high altitude relight condition.

The promising results obtained in task 5.1.3 by TM with the developments of the models in the FIRST project encourage TM to continue to use these modeling approaches for combustion chamber simulations. As the numerical simulations are becoming a crucial tool to design new technologies, TM will benefit from the results of FIRST by applying the models to design new eco-friendly combustion chambers in the framework of CleanSky2 project and to reach ACARE goals.

In task 5.1.4 the OPENFOAM computations performed by MTU showed a significant liquid mass transfer during the onset of ligament formation observed already inside the model injector. Standard modelling approaches of fuel injection nowadays do not take into account such an early ligament formation, but start from a droplet distribution at the combustor inlet. The numerical result indicates that this definition may have to be updated to take the ligament formation inside the injector into account. Further studies in the future have to be conducted and combined with emission testing to identify the impact of the early primary atomization on the fuel distribution and, as consequence, the flame stabilization inside the combustion chamber. This future work may show potential to improve combustor design by the significant improvement of numerical predictions of local heat release and temperature loads on combustor walls. The latest test data of the experimental task includes measurements at elevated pressures and with a non-swirled and swirled flow configuration of the model injector. This data base will be the starting point for future investigations regarding the applicability of the model approach to real engine conditions. The results of the numerical study will be published at the ASME IGTI 2015 conference.

The contribution of Task 5.1.5 in the FIRST project has enabled the investigation of the effects of the liquid film developing on the pre-filming air-blast on the global combustor performance by means of fast and robust CFD analysis suitable for industrial applications. Prefilming injector geometry with an additional pressure swirler pilot injection (provided by GE Avio) was considered in a tubular configuration simplified to obtain axisymmetric computations. Results indicate that fuel evolution is deeply impacted in the injector region by liquid film formation especially in case droplets from the pilot injector impinge on the film. Furthermore, the OpenFOAM toolbox is now upgraded to provide reliable simulations of other pre-filming air-blast atomizers or of the same injector in other configurations.

Work on this model, together with similar contributions from other partners, University of Bergamo and EnginSoft, have improved reactive computations of spray flame in an industrial configuration.

The numerical methodology developed by UNIBG in task 5.1.6 has been refined at a level that the predicted variability due to the numerical method is well below the differences among the results obtained using well known empirical correlations available in the literature and usually implemented for spray calculations. This suggests that the methodology can be used to improve the performances of spray atomisation models and consequently the design of such injectors. The methodology developed by means of an Artificial Neural Network allows GE Avio to evaluate the spray characteristics in any physical condition with the accurate computations of only a reduced number of operative points with benefit on time and electricity consumption saving. The procedure is considered part of the future development for a “high fidelity virtual combustor”, where the algorithms used must be more consistent with the physics and the empirical correlations are no longer considered sufficient.

The work performed in task 5.1.7 has contributed significantly to improved methods for the design of rich and lean burn fuel injectors. While the typical computational resources available in industry prevent application of advanced two-phase flow techniques for prediction of spray size distributions, the approach explored in FIRST will be utilised to support injector design, ultimately leading to faster and better solutions, which in turn will deliver more competitive and environmentally friendly combustors and engines.

The results obtained at TM in task 5.1.8 with the developments of the methodologies in the FIRST project push TM to continue to support development of modelling approaches by academic partners for combustion chamber injector simulations. As the numerical simulations are becoming a crucial tool to design new technologies, TM aims at benefiting from the results of FIRST by using in the near future the approaches developed by academic partners to design new injectors in the framework of CleanSky2 project. This work will be supported by a PhD thesis funded by Safran, which started at CORIA in 2014.

The development and implementation of the soot models in task 5.2.1 based on detailed chemistry provides a framework to perform soot predictions based on state of the art detailed kinetic models. It has been shown that further development of the soot chemistry model is required when used on a gas turbine conditions configuration, particularly it is the modelling of the soot oxidation that has to be improved. However, when making any updates to the chemistry model no code development is required to apply this. Therefore, the development as performed within FIRST is a step towards a more accurate and reliable soot predicting capability.

Furthermore in task 5.2.2 the results of CFD simulations on aero gas turbine combustors have shown that the oxidation of soot in these combustors is over-predicted. Therefore, some further work on the development of the soot model is required. However, the development and implementation of this soot model based on detailed chemistry provides a framework to perform soot predictions based on state of the art detailed kinetic models. However, when the chemistry model is being updated, no code development is required to apply this. Therefore, the development as performed within FIRST is a step towards a more accurate and reliable soot predicting capability.

For additional information on exploitable foreground and the impact over the State-of-the-Art, please refer to the Annex *'FIRST Project Summary of Achievements: Advancements in Spray & Soot Research'*. This brochure also contains a directory of researchers involved in the FIRST project.

5. Annex: FIRST Project Summary of Achievements: Advancements in Spray & Soot Research

FIRST Project Participants

A2 Photonic Sensors (A2PS)

ARTTIC (ARTTIC)

Centre Europeen de Recherche et de Formation Avancee en Calcul Scientifique (CERFACS)

Centre National de la Recherche Scientifique (CNRS-CORIA / CNRS-LEGI)

EnginSoft (EST)

GE AVIO (Avio Aero)

German Aerospace Center (DLR)

Imperial College of Science, Technology and Medicine (IMPERIAL)

Karlsruher Institut fuer Technologie (KIT)

Loughborough University (LU)

MTU Aero Engines AG (MTU)

Office National d'Etudes et de Recherches Aerospatiales (ONERA)

Rolls-Royce Deutschland (RRD)

Rolls-Royce PLC (RRUK)

SCITEK Consultants (SCITEK)

SNECMA (SN)

TURBOMECA (TM)

Universita Degli Studi Di Bergamo (UNIBG)

Universita Degli Studi Di Firenze (UNIFI)

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FIRST
Fuel Injector Research for Sustainable Transport

FIRST Project Summary of Achievements:

Advancements in Spray & Soot Research

Introduction

The FIRST project (Fuel Injector Research for Sustainable Transport) was a collaborative project that ran for 48 months from December 2010 to 2014. Its 7.2M euros budget was partly funded by the European Union 7th Framework Programme and the 20 industrial and academic project partners.

Aviation's environmental impact must be reduced to allow sustainable growth to benefit European industry and society. This is captured in ACARE's 2020 goals of reducing CO2 by 50%, NOx by 80% and in SRA1/2 proposed reductions in soot and the development of alternative fuels.

Consequently, the aims of the FIRST project were to deliver key enabling technologies for combustion emissions reduction by developing improved design tools and techniques for modelling and controlling fuel sprays and predicting soot emissions. CFD simulations have for many years relied upon over-simplistic definitions of the fuel spray for model boundary conditions. By understanding and controlling the complex physics of fuel atomisation and the subsequent mixing the emissions predictions can be directly improved leading to more competitive aero combustor designs.

The FIRST project has delivered a step change in the detail and accuracy of the fuel spray boundary conditions and the propagation to downstream conditions. This has been achieved through the implementation of advanced experimental diagnostic measurements, the development of novel physics based modelling techniques and the derivation of sophisticated correlations.

FIRST has also delivered improved CFD soot models, thereby, enabling the reduction of soot in aero-engine combustors. These calculations require the improved fuel spray boundary conditions provided within the project and also need the higher fidelity physical and chemical models describing the soot production and consumption processes provided from FIRST.

The potential use of future alternative aero fuels will be enhanced by the FIRST project as it has provided information for performing predictions and measurements of both fuel sprays and soot across a number of different alternative fuel types.

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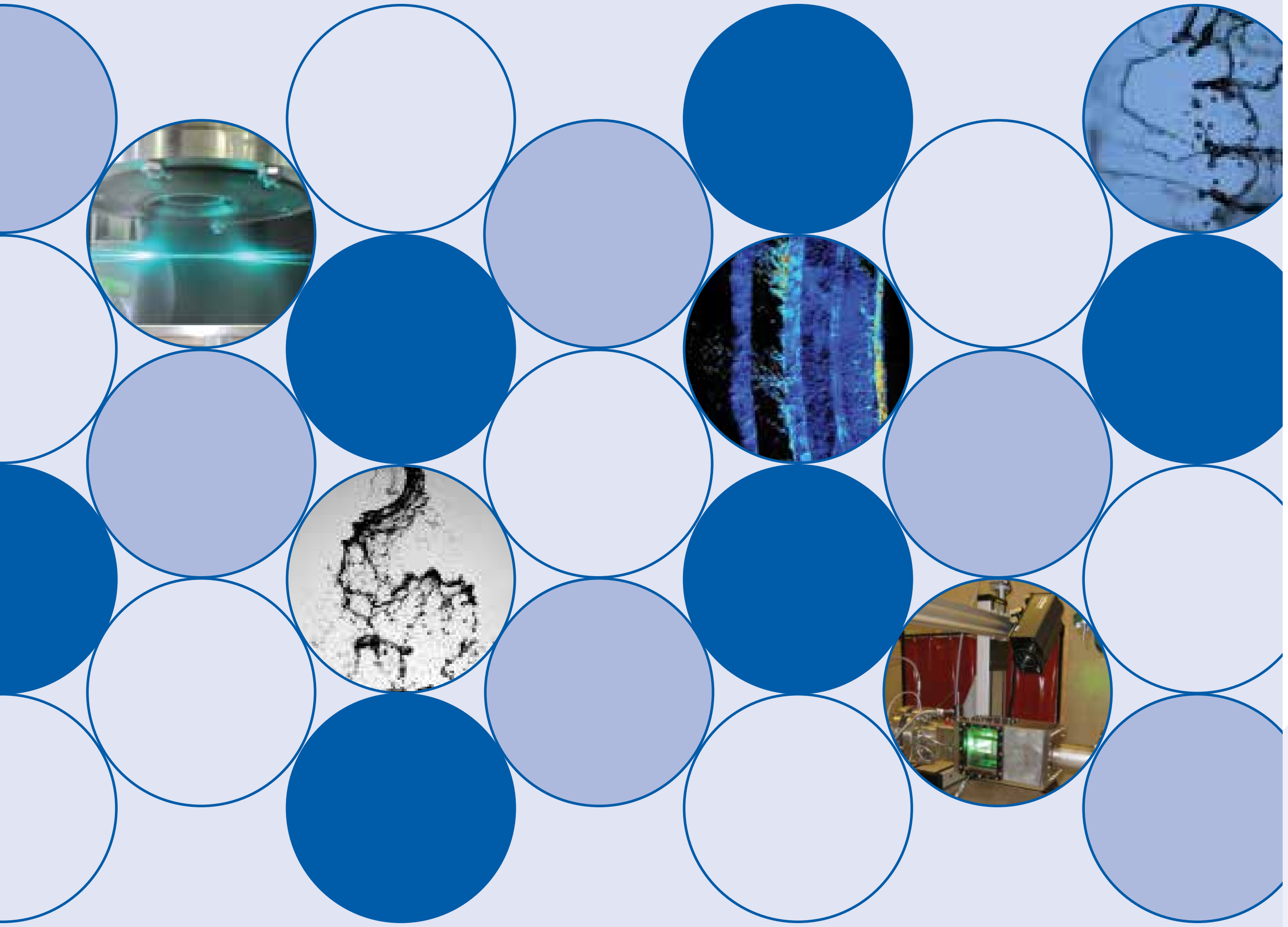
Glossary

AMR	Adaptive mesh refinement
CARS	Coherent Anti-Stokes Raman Scattering
CFD	Computational Fluid Dynamics
CPU	Central Processing Unit
DFT	Density Functional Theory
DNS	Direct Numerical Simulation
EE/EL	Eularian/Lagrangian
FGM	Flamelet Generated Manifold
GSMD	Global Sauter Mean Diameter
ILIDS	Interferometric Laser Imaging Droplet Sizing
KS	Kinematic Simulation
LES	Large Eddy Simulation
LIF	Laser-Induced Fluorescence
LII	Laser-Induced Incandescence
nPB	n-Propyl Benzene
OC	Optical Connectivity
OH	Hydroxyl Radical
PAH	Poly-cyclic Aromatic Hydrocarbon
PDA	Phase Doppler Anenometer
PDF	Probability Density Function
PFR	Plug-Flow Reactor
PSD(s)	Particle Size Distribution
PSR/JSR	Perfectly Stirred Reactor / Jet-Stirred Reactor
RANS	Reynolds Average Navier Stokes
RDF	Radial Distribution Function
SMD	Sauter Mean Diameter
SPH	Smoothed Particle Hydrodynamics or Spherical Particle Hydrodynamics
ULN	Ultra Low Nox
VOF	Volume of Fluid
WSR	Well-Stirred Reactor



Sprays:

Experimental Measurements

Fundamental mechanisms of assisted atomisation and spray characteristics (CNRS-LEGI)

1. State of the Art before the FIRST project

Assisted atomisation is widely exploited for fuel injection in aero-engines, but the involved complex break-up phenomena are only partly understood. Prior to the FIRST project, some data and a few phenomenological models were available to evaluate the size of drops formed by stripping. Much less was known on the large-scale instabilities of jets.

2. Research & Development Activities Performed

Extensive finely controlled experiments were performed to identify the influence of flow conditions and of injection geometrical parameters on spray characteristics. Dedicated measuring techniques were developed together with stability and/or phenomenological analysis. These activities also benefited from advances in phase detection probes and in direct simulations as developed by partners of the FIRST project.

3. Advancement of Capability due to the FIRST project

Beside the production of a data base over a wide range of flow conditions and more than 10 injector geometries, our understanding of atomisation process has been significantly improved. In particular, quantitative agreements between stability theory and experiments have been obtained for the first time on the interfacial instabilities leading to the stripping of drops off the liquid film. The size of drops due to stripping remains strongly controlled by internal injector design, with a diameter evolving from a few (at high gas velocities representative of take-off) up to 20 (at low gas velocity representative of cruise regime) times the gas vorticity thickness at injection. For large scale instability, new data were gathered on flapping frequency, size distributions, fluxes and their evolution with control parameters: the corresponding drops happen to be typically ten times larger than those due to stripping. Moreover, hidden parameters acting on the axial instability that open the way to new atomisation control strategies were also unveiled. These advances provide useful guidelines for optimal injector design and the data bases are helpful to test DNS or to feed numerical codes.

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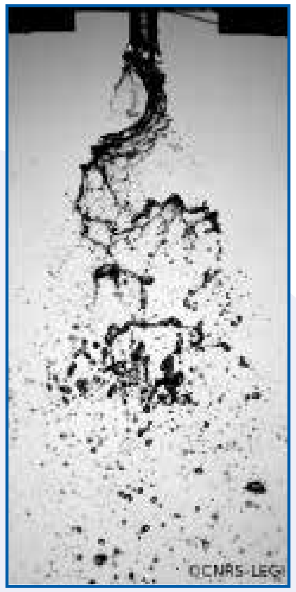

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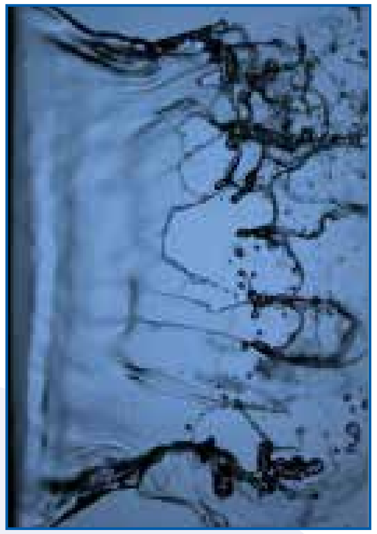
4. Additional information

Application: Fuel injection in aero-engines
Research area: Fundamental mechanisms controlling assisted atomisation
Technology readiness level: 3
Owner of IPR: CNRS – LEGI
FIRST Task: T3.1.1
Main author and contact: Alain Cartellier, CNRS

Planar liquid sheet atomisation (ONERA)

1. State of the Art before the FIRST project



Before the start of the FIRST project there was a lack of information about the influence of air thickness and air ambient pressure on a liquid sheet behaviour and atomization.

2. Research & Development Activities Performed

ONERA conducted an experiment on liquid sheet atomization with variable air flow around a liquid sheet and investigated this under pressure.

Different measurement techniques were used to characterise the liquid sheet atomization. The use of optical techniques based on visualisation and image analysis coupled with conventional techniques of fluid mechanics, hot wire or Pitot allowed information obtained to be merged from the gas phase and the liquid phase to improve knowledge on this phenomena.

3. Advancement of Capability due to the FIRST project

The most important results were obtained on the influence of the surrounding air, specifically its thickness and the characteristics of the resulting boundary layer. As expected the role of the boundary layer is of primary importance on the liquid sheet behaviour. Differences in the flapping frequencies and on the breakup length linked to the type of air boundary layer, laminar or turbulent, at the beginning of the liquid sheet were shown. The wall shear stress seemed to be an important parameter but not the only one.

To examine the pressure influence on atomization study it is necessary to work in a confined environment. In these conditions, the droplet size measurements are difficult and the systems currently used are not able to give primary droplets sizes due to their non spherical shape. The pressure effect on final drop size is visible and it improves the atomization process, but it is difficult to determine where the effect is greater, on primary or on secondary atomization due to the lack of information on primary breakup.

4. Additional information

Application: Fuel injection
Research area: Liquid film atomization
Technology readiness level: 3
Owner of IPR: ONERA
FIRST Task: T3.1.1
Main author and contact: Pierre Berthoumieu, ONERA

Fiber optic sensor for sprays: improvements and performance (A2PS)

1. State of the Art before the FIRST project

The technology of fiber optic probe for bubbly flow spray characterisation (liquid concentration, bubble/drop size and velocity) was initially developed in the 90s by an academic lab then transferred in 2007 to the company A2 Photonic Sensors for improvement, industrialisation and commercialisation. Commonly used in bubbly flows, this sensor was also used in sprays, but was limited to the analysis of droplets no smaller than 15 μm and drop velocities no higher than 25 m/s, and was therefore not fully responding to the requirements of turbomachinery and aeronautic engine injector studies.

2. Research & Development Activities Performed

A2PS has improved its spray analysis fiber optic sensor by optimising the sensing element, improving the data analysis algorithm and implementing it with easy-to-use software. In addition, a large part of the activities were dedicated to testing and qualifying the sensor performance in terms of small drop size detection capabilities and maximum velocity reachable, as well as testing the sensor in spray conditions representative of real engine injector study case.

3. Advancement of Capability due to the FIRST project

Improvement of the optical probe technique led to a measurement system fully functional in unidirectional sprays with droplet sizes down to 10 μm and velocity up to 60 m/s. The capability to measure precise flow rate and flux was demonstrated even with a very high droplet number per volume (very dense spray). In addition, a comparison with a PDA system showed good results agreement and more importantly, a clear advantage to the optical probe system due to its user-friendliness with its very short installation time and very easy set-up and use. As a result, A2PS are convinced that the optical probe technique will become an essential instrument for spray analysis in addition to already existing techniques.

4. Additional information

Application: Fuel injector and nozzle of aero combustors
Research area: Spray and atomization measurements: drop size & velocity, flux
Technology readiness level: 7 or 8
Owner of IPR: A2PS
FIRST Task: T3.1.1 & T3.1.3
Patent: none
Main author and contact: Stéphane Gluck, A2PS

Combined Break-Up Length and Droplet Size and Velocity Distribution Measurements (IMPERIAL)

1. State of the Art before the FIRST project

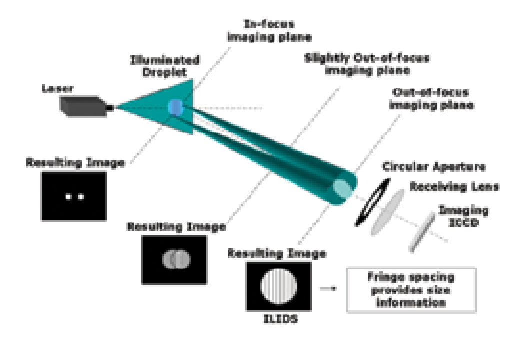
Prior to FIRST, ILIDS for the simultaneous measurement of droplet size and velocity had only been performed on automotive fuel injectors. While the OC technique for determining the break-up length had never been applied to pre-filming atomizers.

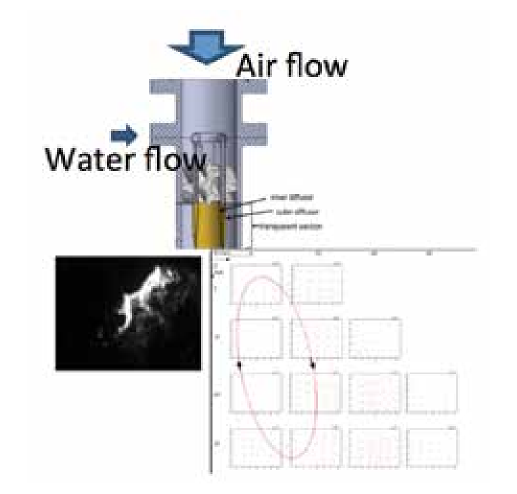
2. Research & Development Activities Performed

IC was the first to apply the ILIDS and OC techniques on a prefilming airblast atomiser, typically found in aero-engine combustion systems and pioneered the concurrent application of both techniques. Instrumentation and data processing algorithms were developed for the simultaneous collection of measurements and their interpretation. The spray characteristics of two prefilming atomizers (designed at IC and ONERA) were reported. Experiments were performed for different air and water flow test conditions.

3. Advancement of Capability due to the FIRST project

ILIDS measurements were reported for different axial and radial positions away from the nozzle exit and axis respectively. The increase in SMD of droplets towards the spray edge for both atomizers was explained on the basis of larger centrifugal force acting on the bigger size droplets due to the swirling flow. The average droplet velocity plots in case of the model atomizer showed the presence of an induced vortical flow structure causing flow reversal near nozzle axis, which arose due to the swirling motion of the air. Away from the nozzle axis, the droplet velocity was downward and increased till the droplets lost momentum near the edge of the spray. Apart from the basic velocity statistics, the spatial droplet-droplet velocity correlations (Rdd) and RDF are presented for different droplet size classes. Measurements of Rdd quantified the strength of the intra-phase coupling of the droplet flow field in both the axial and radial directions. The RDF for the different droplet size classes indicated that the larger droplets (45-60 μm) showed greater tendency to form instantaneous droplet clusters in the sprays. The average cluster dimension decreased towards the spray edge. The break-up length of the liquid sheet was measured by the LIF technique, and the measurements were reported for different Reynolds number of water flow for the same air flow rate. Finally, the statistics including the fluctuations of droplet concentration and its correlation with the droplet velocity, which are vital for understanding the droplet cluster formation, were measured.





4. Additional information

Application: Fuel injector for aero combustors
Research area: Combined Break-Up Length and Droplet Size and Velocity Measurements
Technology readiness level: 3
Owner of IPR: Imperial College London
FIRST Task: T3.2.2
Main author and contact: Yannis Hardalupas, Imperial College

Experimental investigation of the onset of film breakup in an annular prefilmer (KIT)

1. State of the Art before the FIRST project

Prior to FIRST, experimental investigations of the onset of film breakup in an annular prefilmer were difficult to perform. The reasons were the poor homogeneity in the circumferential direction of the liquid film flowing through the annular prefilmer for small liquid mass flow rates and incorrect arrangements of laser sheet and camera position.

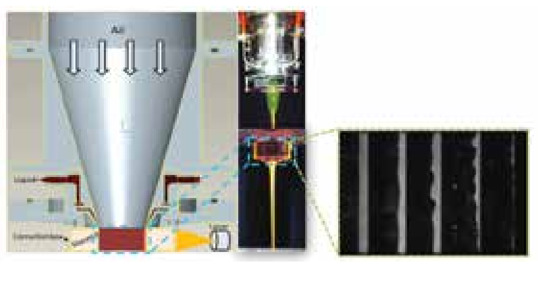
2. Research & Development Activities Performed

The Engler-Bunte-Institute (EBI) of KIT has designed a model research nozzle which generates homogeneous laminar film flow without any support of air flow and developed a measurement technique to determine the film thickness and detect the onset of the film breakup. One of the crucial points in detecting the film thickness was the position of the camera capturing the film at the illuminated surface with a light source.

The simulation and experimental investigation performed for different positions of the camera have proved that different positions of the camera gave different results for a predefined film thickness at the same boundary conditions. These investigations lead to the fixing of an arrangement of laser sheet and camera position which detects a predefined film flow precisely. Based on this validated arrangement, investigations of film breakup were performed with two main results. The first one concerns the Momentum Ratio (MR) between air and liquid flow. In contrast to existing research on film breakup we found that MR is not sufficient to characterise the beginning of primary atomization. The second one deals with the comparison of swirling and not swirling air flow. For the same air pressure drop the swirling flow generates a thinner liquid film thickness.

3. Advancement of Capability due to the FIRST project

During the FIRST Project a model research nozzle which produces a homogeneous laminar liquid film flow was designed and a measurement technique to capture the liquid film thickness was developed. The generated experimental data can be used in order to validate software programs calculating film flows. Furthermore, the experimental facility can be used for future research work in order to extend the experimental data base.



4. Additional information

Application: Fuel injector of aero combustors
Research area: Experimental study on primary breakup
Technology readiness level: 3
Owner of IPR: KIT
FIRST Task: T3.2.3.1
Main author and contact: Mulubrhan Gebretsadik, KIT

Effect of linear geometrical scaling and aerodynamic boundary conditions of a double swirl airblast atomizer on GSMD (KIT)

1. State of the Art before the FIRST project

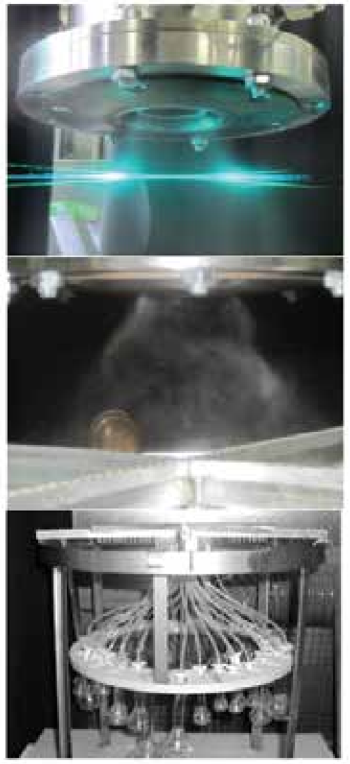
The evaluation of the GSMD for the whole spray is very difficult because it requires the radial SMD and liquid mass flow distribution. Therefore, the existing data base on GSMD for different performance conditions is very limited. Based on this limited experimental data base the developed correlations predict the GSMD as a function of the Weber number (We = (ρu2·D)/ρ́.

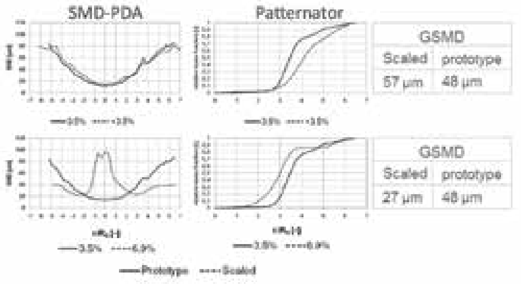
2. Research & Development Activities Performed

The Engler-Bunte-Institute (EBI) of Karlsruhe Institute of technology (KIT) has developed a method to evaluate the GSMD of a spray produced by double swirl airblast atomizer by a combination of two measurement techniques. The radial distribution of the liquid mass flow is captured by a patternator, whilst the radial distribution of the SMD is evaluated from PDA data. A prototype and a scaled version of the prototype injector with a linear geometric scaling factor of two were investigated at different boundary conditions to determine the effect of different parameters explicitly on GSMD.

3. Advancement of Capability due to the FIRST project

The combined experimental investigation of patternator and PDA within the FIRST project has enabled the evaluation of the GSMD for the whole spray produced by a specific boundary condition in double swirl airblast atomizer. This helps to compare effects of different parameters on the spray. The combined measurement technique reveals that the impacts of the variables in the We-Number in predicting the GSMD are different. The air velocity, which is calculated from the pressure drop, has much higher impact on the GSMD than the characteristic length at constant air to fuel ratio (AFR), surface tension and density.





4. Additional information

Application: Fuel injector of aero combustors
Research area: Experimental study on spray
Technology readiness level: 3
Owner of IPR: KIT
FIRST Task: T3.2.3.2
Main Author and Contact: Mulubrhan Gebretsadik, KIT

Characterisation of the Pre-filming Inlet Velocity Field (LU)

1. State of the Art before the FIRST project

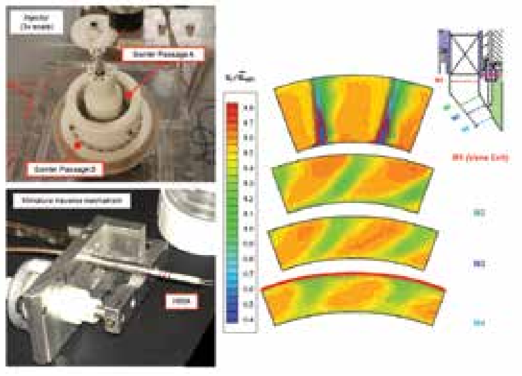
Modern fuel injectors often incorporate a pre-filmer surface onto which liquid fuel is introduced. Both computational and experimental studies were done which examine the development of the liquid film and its subsequent break-up. However, these studies have invariably utilised simplified geometries which may not capture the significant aerodynamic flow features present within a representative injector geometry. Such aerodynamic features were thought to be prominent in the development of the two phase flow field and therefore should be resolved.

2. Research & Development Activities Performed

A large scale representative fuel injector geometry was designed and manufactured. This facilitated detailed 2-D aerodynamic measurements at multiple planes within the pre-filming passage. Mean and fluctuating measurements were acquired, with and without fuel present, capturing the development of the aerodynamic flowfield within the pre-filming passage.

3. Advancement of Capability due to the FIRST project

An aerodynamically representative data set was generated which captures key flow features along the pre-filmer passage. These include the influence of fuel blockage, vane wake stretching and migration, resultant variations in mean velocity and turbulence adjacent to the pre-filmer and total pressure loss development. The data provides inlet boundary conditions for numerical (CFD) predictions relating to fuel injector flows. As the data charts the flowfield development along the pre-filming passage, it also provide a means of validating the numerical predictions.



4. Additional information

Application: Fuel injector of aero combustors
Research area: Internal Velocity Field Characterisation
Technology readiness level: 2
Owner of IPR: Rolls-Royce
FIRST Task: T3.3.2
Main author and contact: Ashley Barker, Loughborough University

Time-Resolved Measurements of Fuel Film Thickness on Representative Fuel Injector Geometries (LU)

1. State of the Art before the FIRST project

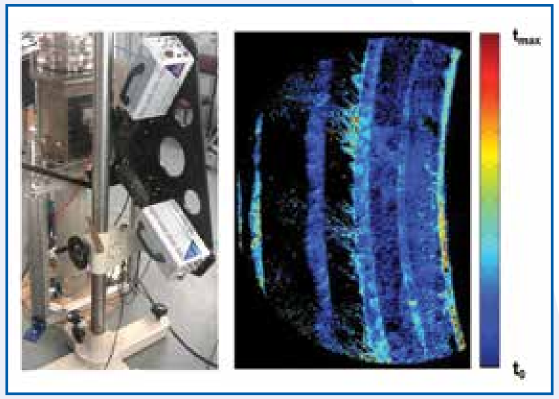
Prior to FIRST, 2-D measurements of fuel film thickness had been made on an engine representative injector at atmospheric conditions. They were obtained using a prototype instrumentation assembly which successfully demonstrated the capability, but was unrefined and did not temporally resolve the dynamics of liquid structures on the pre-filming surface.

2. Research & Development Activities Performed

LU has developed the instrumentation to make it more robust, increase portability and enable time-resolved measurements of fuel film thickness. Parametric studies were completed to better understand the effects of dye concentrations, optical filter choice, laser power/uniformity and substrate surface finish. Software development has facilitated rapid processing of the large quantities of data associated with such a measurement.

3. Advancement of Capability due to the FIRST project

Development of the instrumentation technique within FIRST enabled refinement of the opto-mechanical setup, culminating in a robust portable system capable of high-speed fuel film thickness measurements. The technique has been demonstrated at ambient pressure and at 4 Bar, and such measurements will improve the identification and understanding of significant factors affecting the development of the liquid fuel film and thus the downstream two-phase flow field. As measurements have not previously been available, this data will also facilitate improved methods for predicting such flow fields. Factors have been identified which will facilitate further advancement through acquisition of appropriate hardware, such as improved temporal resolution using higher powered lasers.



4. Additional information

Application: Fuel injector of aero combustors
Research area: Liquid film thickness measurements
Technology readiness level: 2
Owner of IPR: Rolls-Royce
FIRST Task: T3.3.2
Main author and contact: Ashley Barker, Loughborough University

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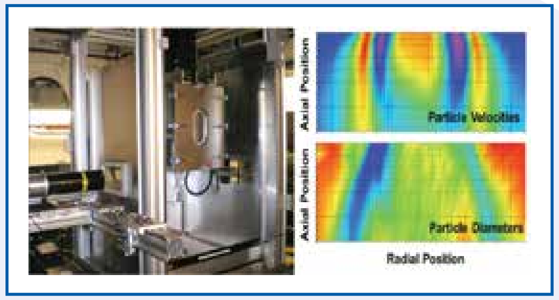
Engine Injector Spray Characterisation (RRUK, SCITEK)

1. State of the Art before the FIRST project

Before the FIRST project there was very little information available to describe the properties of atomisation from Rolls-Royce aero engine rich and lean burn fuel injectors. Lefebvre correlations were typically used to estimate the fuel spray boundary conditions for CFD modelling of these injectors in combustor flows. This coarse method used for numerical modelling made accurate prediction of combustor flow fields, and consequently emissions, difficult. Actual measurements of the fuel particle sizes and velocities were required before further progress could be made in improving modelling techniques.

2. Research & Development Activities Performed

A new test facility was built in the combustion laboratories in Rolls-Royce Derby that was specifically designed to enable PDA measurements of fuel sprays from engine injectors. All PDA and flow visualisation measurements were performed by SCITEK. Test geometries were designed and made that represented a single sector of an engine combustor so that the spray conditions were more closely representative of reality. Lean and rich burn fuel injectors were tested at a range of conditions relevant to their respective engine cycles and detailed measurements of droplet sizes and velocities were made at numerous locations. The work was extended to include sprays from alternative fuels as a comparison to a standard kerosene spray.

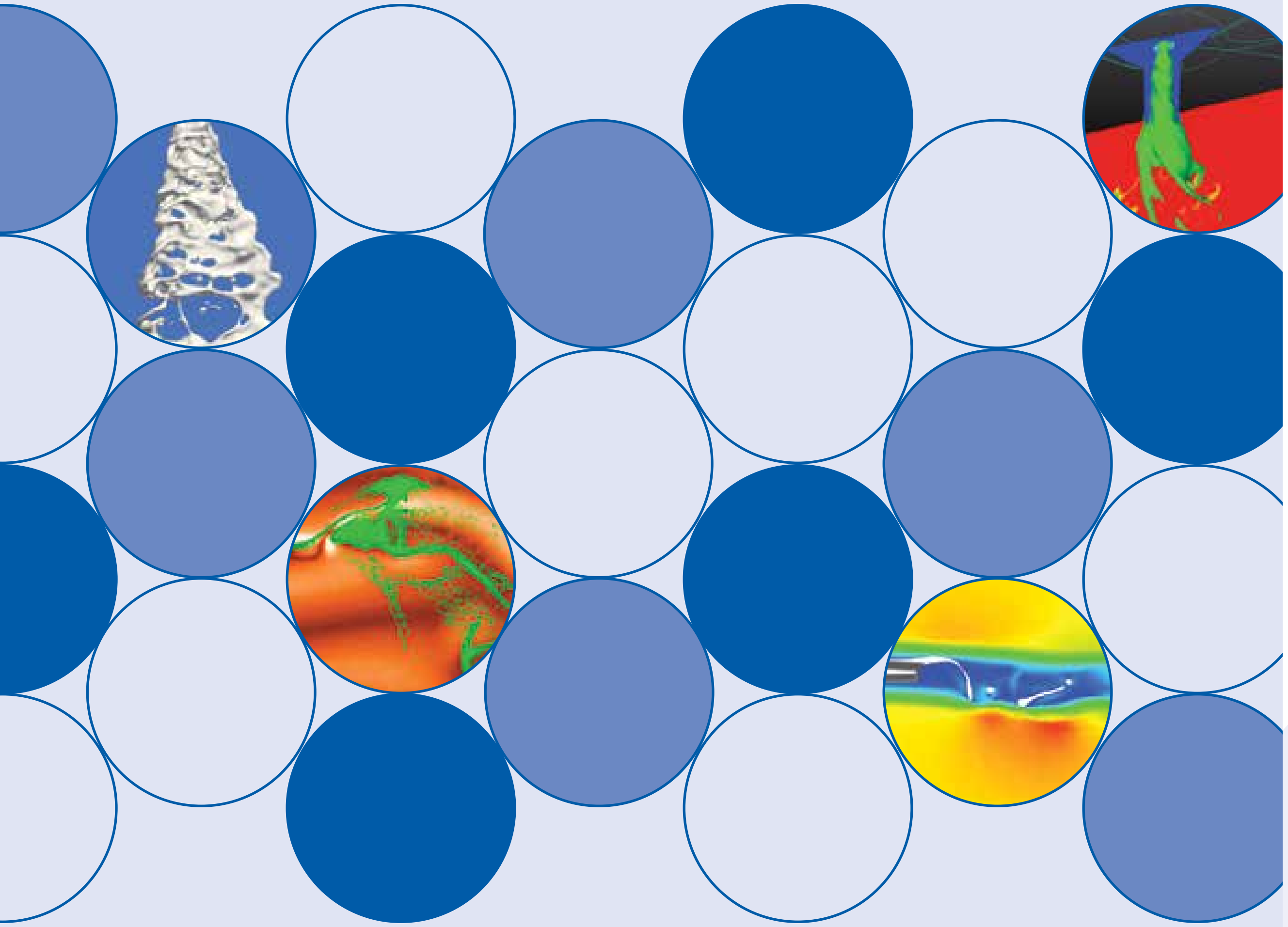


3. Advancement of Capability due to the FIRST project

The measurements of the spray from the fuel injectors have now provided the boundary conditions required for CFD modelling of Rolls-Royce engine combustors and has described the progression of the atomisation process as the flow moves downstream away from the fuel injectors. This is vital information for the improvement of numerical models to predict engine reacting flows. The CFD models can now be validated against the spray measurements for a wide range of geometries and conditions and a step change in modelling accuracy will be the result. Future designs of aero engine combustors and fuel injectors will benefit from the improved modelling accuracy.

4. Additional information

Application: Measurements of engine injector sprays for validating CFD modelling
Research area: Spray measurements from engine injectors
Technology readiness level: 3
Owner of IPR: RRUK
FIRST Task: Task 3.3.3
Main author and contact: Darren Luff, Rolls-Royce UK



Sprays:

Numerical Modelling of Academic Configurations

Development and evaluation of numerical methods for the simulation of primary atomization in aeronautical injection systems (CNRS)

1. State of the Art before the FIRST project

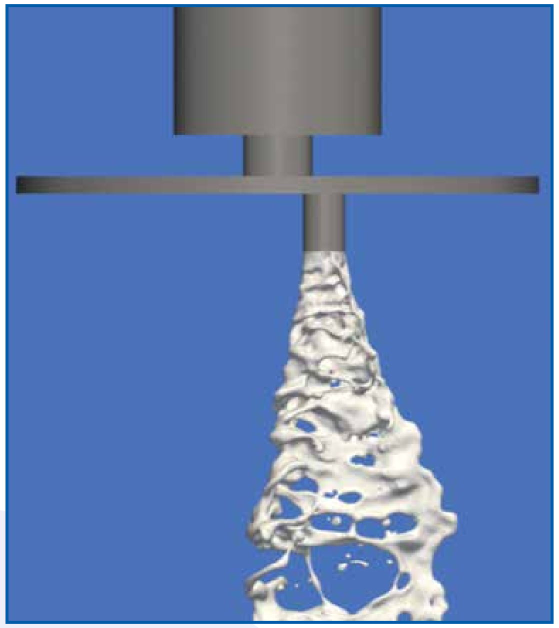
Primary atomization modelling has been an active research topic over the last two decades with the development of various numerical techniques for the tracking of the interface motion (Volume-Of-Fluid, Level Set) and for the capturing of the jump conditions at the interface (Continuous Force, Ghost-Fluid Method). All these techniques have been largely validated for academic two-phase flows and very few attempts have been conducted for realistic geometries such as aeronautical injection systems.

2. Research & Development Activities Performed

In the FIRST project, CORIA researchers have developed and applied numerical methods for primary atomization to realistic injectors. The aim of these simulations was twofold: i) validate the numerical strategy in terms of accuracy and robustness, ii) identify the bottlenecks and the potential improvements. The simulations of the triple injector, of the ONERA liquid sheet with swirl and of the Turbomeca injector, highlighted the need for high mesh resolution at the air/liquid interface. Such resolution may only be obtained through manual or automatic local mesh adaptation.

3. Advancement of Capability due to the FIRST project

During the project, various numerical techniques were developed in order to improve the fidelity of the simulations and enhance their comparison with experiments. Two major new capabilities of the simulation tools are parallel adaptive mesh refinement and segmentation techniques for the calculation of droplet size distribution. All these capabilities have been designed for massively parallel LES with more than 10,000 cores of modern super-computers. These simulations tools are now used by industrial partners in the FIRST project to improve their understanding of primary atomization.



4. Additional information

Application: Liquid fuel injection in aeronautical burners

Research area: Primary atomization modelling

Technology readiness level: 2

Owner of IPR: CORIA - CNRS

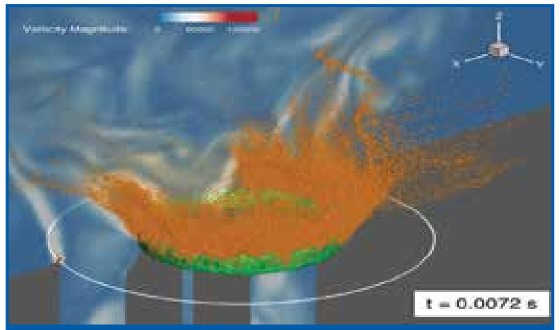
FIRST Task: T2.2.2

Main author and contact: Vincent Moureau, CNRS-CORIA

A Multi-Scale Approach For Primary Atomization Modelling (ONERA)

1. State of the Art before the FIRST project

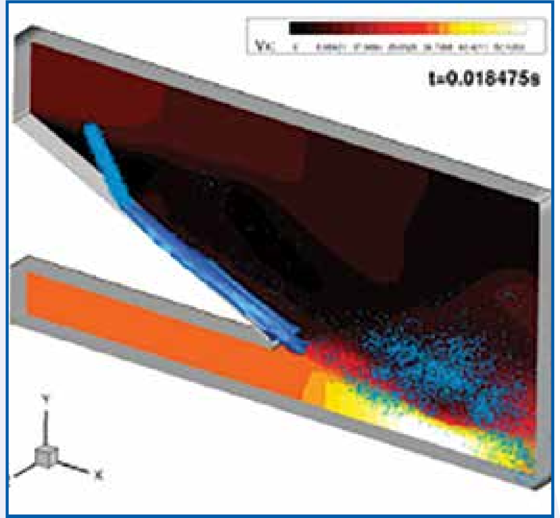
Today most advanced LES simulations of aeronautical combustors are performed with dispersed phase approaches for the fuel. The numerical droplets are directly injected by fixed numerical injectors whose characteristics are obtained by empirical correlations. These correlations demand an a priori knowledge of the injector, defeating the purpose of predictive computations.



Simulation of a sheared planar liquid sheet. Turquoise: resolved liquid core; green: Lagrangian droplets.

2. Research & Development Activities Performed

ONERA has developed a new approach for large-scale unsteady simulations of primary atomization. It consists of a coupled multi-fluid solver for the simulation of the liquid core and a dispersed phase approach for the generated cloud of droplets. This approach has been tested on different configurations, such as atomization of a sheared planar liquid sheet, film formation and re-atomization and a realistic circular swirled injector.



Simulation of droplet impact on a wall and subsequent film re-atomization.

3. Advancement of Capability due to the FIRST project

Current industrial numerical simulations of combustion chambers cannot resolve the small-scale mechanisms of primary atomization. Injection of droplets is done by fixed injection points. The ONERA multi-fluid method is able to reproduce the large scale instabilities of primary atomization such as flapping motion and largest ligaments formation. The developed atomization model is able to detect the zone where the droplets are most likely to appear and to act subsequently as an advanced numerical injector, transferring the resolved liquid to an appropriate distribution of numerical droplets. Taking account of the instabilities of the injection, it gives a more accurate initial position and velocity of each particle. The model naturally respects the resolved liquid core and performs the conversion at realistic break-up lengths. The reciprocal model of droplets impact on resolved liquid structures or wall has been developed as well. Implementation of the solvers and the model is straightforward in any unstructured mesh finite volume framework.

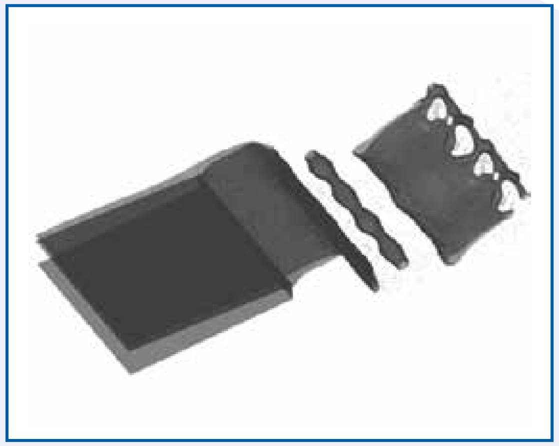
4. Additional information

Application: Fuel injector of aero combustors
Research area: LES simulation of combustors injection
Technology readiness level: 2
Owner of IPR: ONERA
FIRST Task: T2.2.4.1
Main Author and Contact: Davide Zuzio, ONERA

Primary break-up modelling using SPH (KIT)

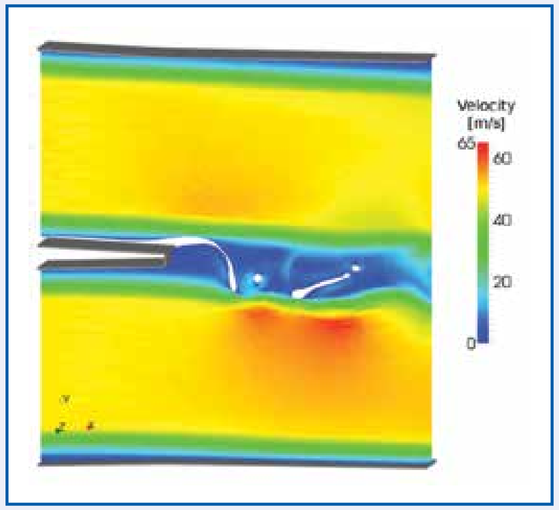
1. State of the Art before the FIRST project

Before FIRST, reliable predictions of the fuel atomisation in aero combustors were not feasible using conventional grid based simulation techniques. By introducing the particle based method SPH, such simulations including multiple fluids can be performed more easily. Prior to FIRST, the method lacked some basic boundary treatment capabilities such as generalised periodic boundaries and suitable inlet/outlet boundary conditions.



2. Research & Development Activities Performed

KIT has implemented a massively parallel software based on the standard SPH methodology and developed robust inlet/outlet boundary conditions and generic periodic boundaries. Some physical models were adjusted in order to handle fluid pairings with high density and momentum ratios correctly. 2D and 3D simulations of an academic air-blast atomizer were performed and results have been validated by experiments. Additional software has been developed for data reduction and visualisation of the results, even on a standard PC.



3. Advancement of Capability due to the FIRST project

The advancement of the SPH method within FIRST enabled its applicability to the simulation of air assisted atomizers. Detailed simulations, including very fine spatial resolutions and large data sets are possible due to the low memory requirements of the method and the highly parallelized code. The simulation of an academic atomizer at ambient pressure has been performed. The implemented additional post-processing software facilitates and speeds up the analysis of simulation results. The simulations help to understand the complex phenomenon of primary atomization, which in turn is a prerequisite for the development of more environmentally friendly combustion processes.

4. Additional information

Application: Fuel injection in aero combustors
Research area: Liquid fuel atomization modelling
Technology readiness level: 3
Owner of IPR: KIT
FIRST Task: T2.2.4.2
Main author and contact: Samuel Braun, KIT-ITS

Modelling of liquid jet primary break-up in swirl atomisers (UNIBG)

1. State of the Art before the FIRST project

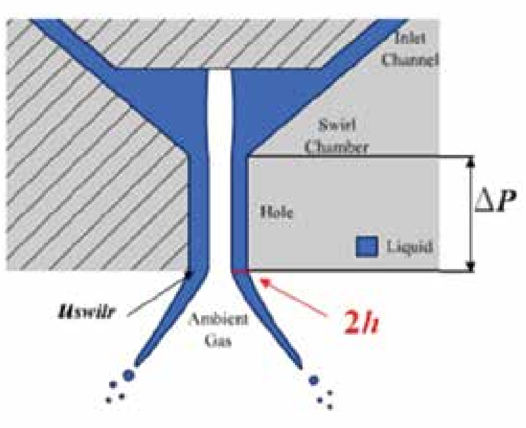
Prior to FIRST the primary break-up models available in the literature for hollow cone sprays did not account for the effect of turbulence on primary atomisation.

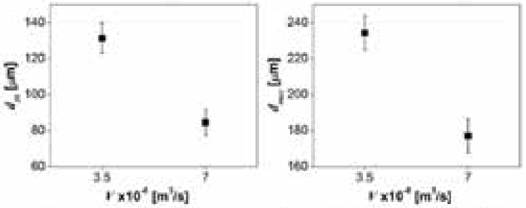
2. Research & Development Activities Performed

A novel formulation of the primary atomisation model has been developed by UNIBG for hollow cone swirling jets, under operating conditions suitable for aeronautic applications and explicitly accounting for turbulence and aerodynamic effects on the liquid break-up. The input conditions of the model have been provided by the simulations performed by UNIBG within the project. The model determines the dominant mechanism responsible for liquid jet break-up and the mean, maximum and drop size distribution of the newly formed spray.

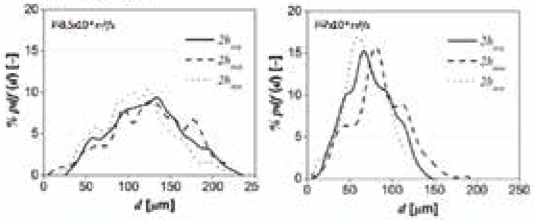
3. Advancement of Capability due to the FIRST project

The atomisation model developed by UNIBG within the framework of the FIRST project for hollow cone sprays is capable of determining the dominant mechanism responsible for primary break-up and the most crucial parameters affecting the process. Under the selected operating conditions, suitable for aero-engine applications, the liquid lamella thickness at the nozzle exit and the fuel injection rate prove to be the most sensitive parameters to the evaluation of the d30 mean diameter of the spray generated after the break-up of the liquid jet. This confirms the crucial influence of internal nozzle flow development on spray formation.





Effect of fuel injection flow rate on drop mean and maximum diameters after primary break-up



PDF distribution of drop diameter after primary break-up, function of the average, min and maximum values of the lamella thickness as predicted by 3D VOF simulations.

4. Additional information

Application: Fuel injector of aero combustors

Research area: Liquid film atomisation

Technology readiness level: 2

Owner of IPR: Università degli studi di Bergamo

FIRST Task: T2.2.6

Main Author and Contact: Gianpietro Cossali, UNIBG

Modelling of spray formation in a ULN injector (UNIBG, AVIO)

1. State of the Art before the FIRST project

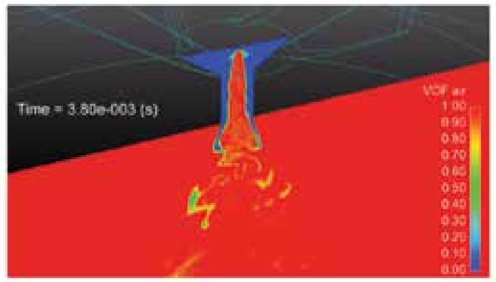
Prior to FIRST the input conditions of the primary atomisation models predicting the jet break-up for aero-engine applications were provided by semi-empirical correlation available in the scientific literature.

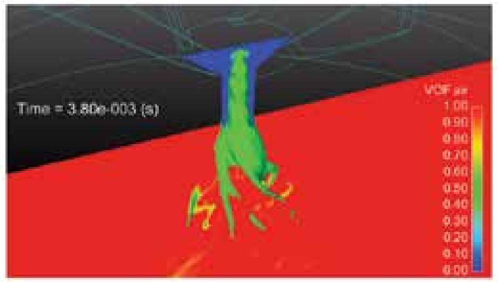
2. Research & Development Activities Performed

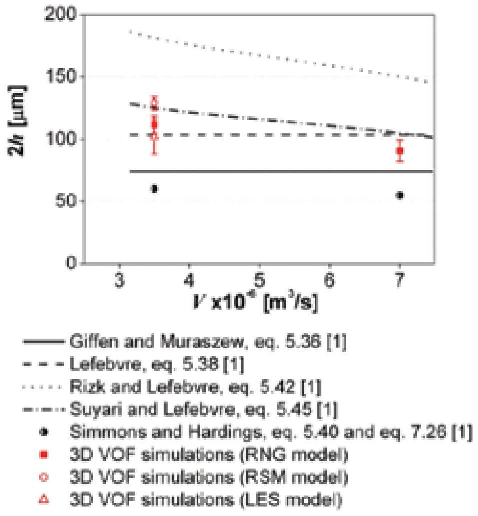
The internal flow and the liquid structure exiting the nozzle have been investigated by UNIBG in a typical pressure swirl atomizer for aero-engine applications under isothermal non reacting environment, using a combination of single and two-phase flow Eulerian models implemented in-house and commercial CFD codes. A numerical methodology has been developed to provide the necessary input conditions for successive atomisation modelling.

3. Advancement of Capability due to the FIRST project

The work performed by UNIBG during the FIRST project has evidenced that the liquid lamella thickness at the nozzle exit results to be the most crucial parameter affecting the successive primary atomisation modelling. The proposed methodology has been refined at a level that the predicted variability due to the numerical method is well below the differences found in the results obtained using well known empirical correlations available in the literature and usually implemented for spray calculations, suggesting that it can be used to improve the performances of primary atomisation models.







[1] Lefebvre, A. H., 1989, Atomization and Sprays.

4. Additional information

Application: Fuel injection in aero combustors

Research area: Internal nozzle flow simulations

Technology readiness level: 2

Owner of IPR: Università degli studi di Bergamo, GE Avio

FIRST Task: T2.2.5 and T5.1.6

Main author and contact: Gianpietro Cossali, UNIBG

A Phenomenological Model for Droplet Dispersion and Clustering (IMPERIAL)

1. State of the Art before the FIRST project

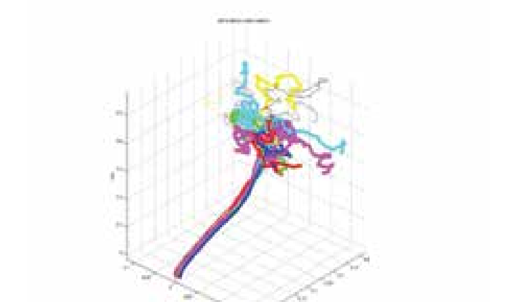
The stimulus for this work is the inability of the currently available RANS modelling tools to predict certain phenomena, experimentally observed, within the dispersed phase. Namely, particle/droplet preferential concentration and droplet trajectories in recirculation zones and regions of flow separation. The consequences of these limitations are that the instantaneous non-uniformity/homogeneity of droplet concentration spatial distributions observed experimentally at high Reynolds number flows cannot be observed in the corresponding modelling efforts.

2. Research & Development Activities Performed

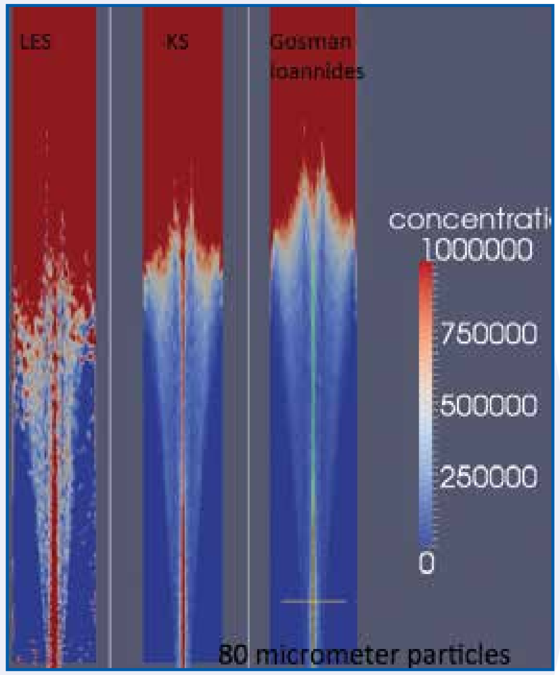
IMPERIAL developed fully coupled incompressible EE/EL solvers for use within the openFOAM modelling package. In addition a phenomenological model for particle dispersion that uses KS was developed to model the smaller scales of the dispersed flow in a RANS framework. The model was tested on an axi-symmetric sudden expansion test case for two distinct particle class sizes and several mass loadings. Results were compared to LES calculations performed and to RANS simulations employing the commonly used dispersion model as well as against experimental data.

3. Advancement of Capability due to the FIRST project

The limitation of current RANS Lagrangian tracking dispersion models may be traced back to the fact that the 'computed' instantaneous flow eddies in Monte-Carlo models are only prescribed from the local values of the turbulent kinetic energy and the local dissipation rate of the flow field from which a fluctuating component of velocity is assigned to the particle. There is no physical flow structure information contained within these 'constructed' eddies. The developed model uses the standard (u)RANS technique for modelling the bulk of the flow field but then employs KS within each 'computationally constructed' eddy in order to introduce a more realistic flow structure for the smaller scales of the flow, which are not computed in a typical RANS calculation. Performance of the developed model is improved over the existing models and, for certain regions of the flow, predictions are very similar to the LES results but is still limited by the RANS framework it was designed for. The developed model is not restricted to the aero-combustor sector but is equally suited for use in a wide range of fields from biological modelling to environmental flows.

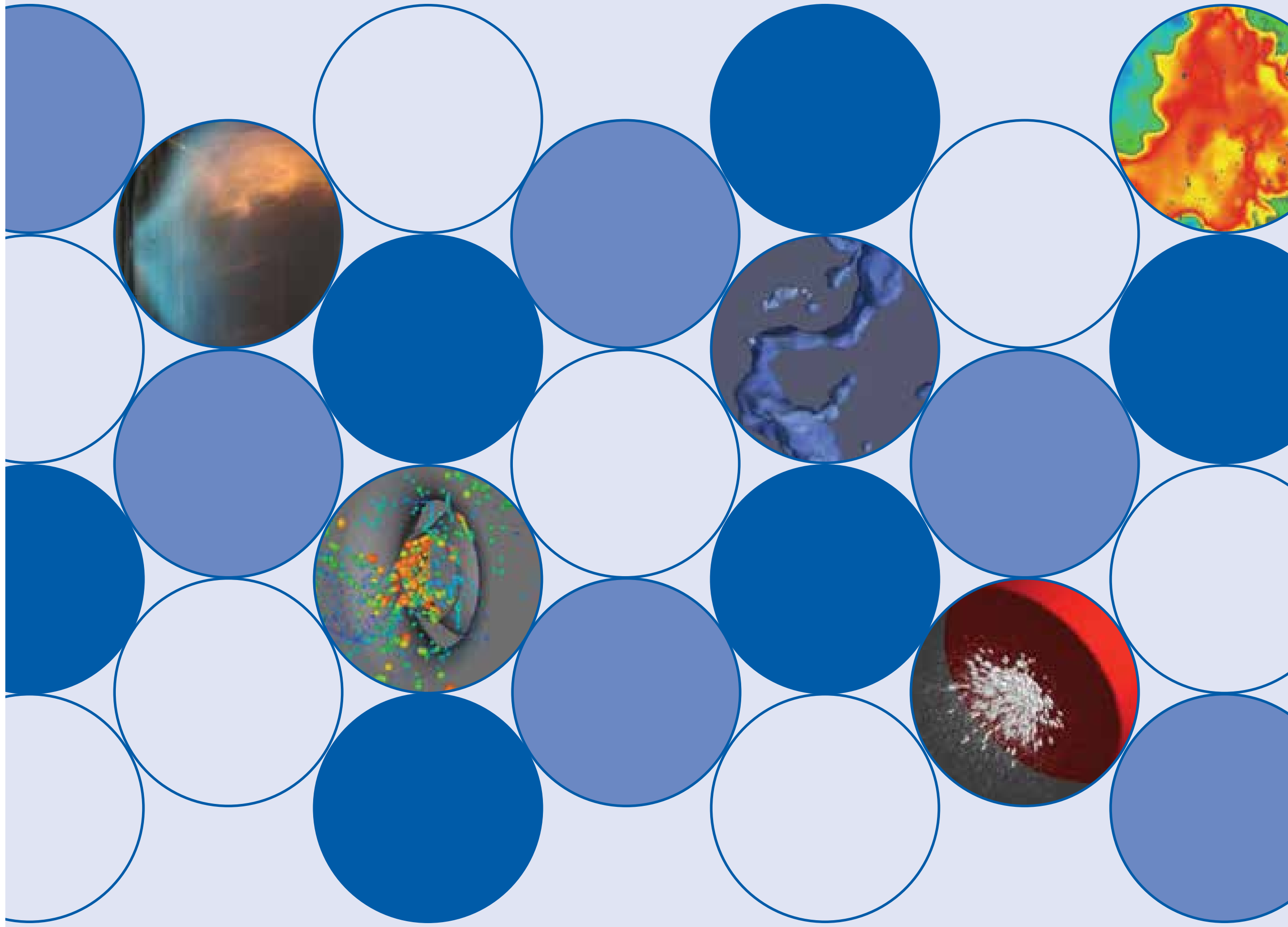


Dispersion of a cluster of fluid particles in KS flow field



4. Additional information

Application: Fuel injector for aero combustors
Research area: Spray Modelling
Technology readiness level: 2
Owner of IPR: Imperial College London
FIRST Task: T2.2.3 & T4.2.2
Main Author and Contact: Koulis Resvanis, IMPERIAL College



Sprays:

Numerical Modelling of Ideal and Real Injectors

Secondary breakup CFD models (EST, UNIFI, AVIO)

1. State of the Art before the FIRST project

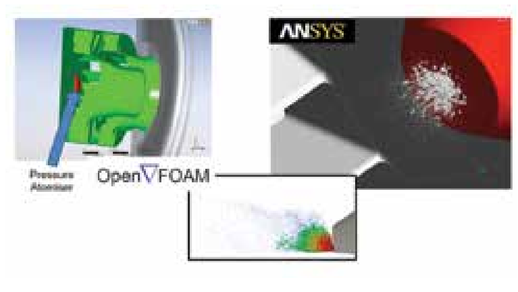
Before FIRST, recent developed secondary atomization models were not available in the OpenFOAM suite and the commercial code Ansys CFX had not been verified in the aerospace sector as a tool to study the breakup process. All available models had only been tested in the automotive field.

2. Research & Development Activities Performed

In order to test the accuracy and reliability of selected secondary breakup and droplets coalescence/ interaction models in Ansys CFX, different operating conditions were investigated. The cases considered were characterised by different values of pressure and temperature for the chamber and different flow rates. In the FIRST project, UNIBG performed numerical simulations of the injector using the VOF method in order to provide a text file with droplets position, velocity and diameter as a function of time after primary breakup for each case. These files were used as droplets boundary conditions for calculations in the project. Global and local criteria have been used to evaluate the process. The behaviour of the models is very similar in the global criteria and some differences are only visible in the local distribution of diameters. Selected secondary breakup models have been implemented in the OpenFOAM suite. To test the accuracy and reliability of the implemented models, a selected case was investigated with different breakup models and the results compared with Ansys CFX. The behaviour of the models is similar in normal penetration and spray angle. Some differences are visible in axial penetration.

3. Advancement of Capability due to the FIRST project

The FIRST project has enabled investigation of secondary breakup models in different operating conditions for a real injector developed by GE Avio using the commercial code Ansys CFX. The results indicate that the available models are almost equivalent in the evaluation of the global characteristics of the spray (penetrations and angle), but differ enough in the local diameter distribution. In addition, the FIRST project has enabled the implementation and exploitation in OpenFOAM of recently developed secondary breakup models.



4. Additional information

Application: Secondary atomization using commercial and open source CFD codes
Research area: CFD analysis of injection zone
Technology readiness level: 2
Owner of IPR: EnginSoft, Università degli Studi di Firenze, GE Avio
FIRST Task: T4.1.1
Main Author and Contact: Michele Andreoli, EnginSoft

Numerical methods to compute dense spray inside the injector (CERFACS)

1. State of the Art before the FIRST project

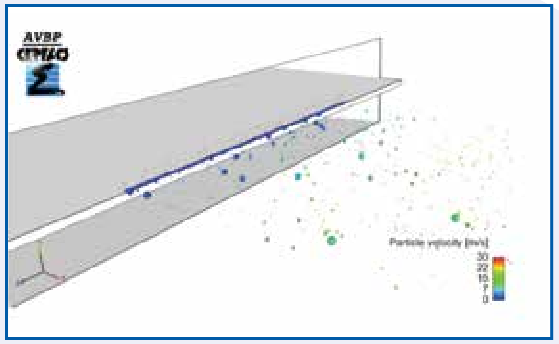
Fuel injection models such as FIMUR developed by CERFACS only describe the spray issued from a pilot injector. However in many real engines, the spray generated by the central nozzle impacts the walls of the diffuser, forming a liquid film that re-atomizes downstream at the tip of the diffuser to create a secondary spray that has very different features. The objective was to develop a model for Spray-Wall Interaction (SWI), capable of describing the film forming, flowing and atomization.

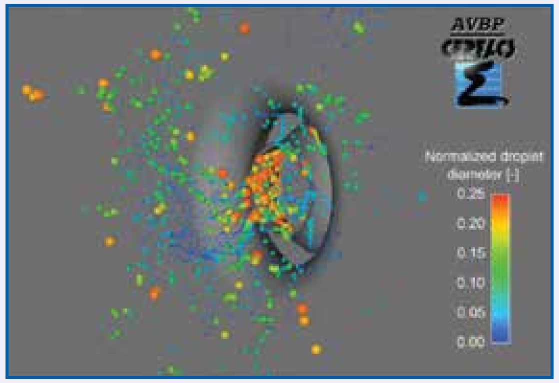
2. Research & Development Activities Performed

A phenomenological model was developed based on the knowledge available in the literature. It describes the droplet impact, film flow and film atomization and was parameterised by the known two-phase flow characteristics and geometrical features. The implementation in the numerical code AVBP, using the Lagrangian framework, was validated against experimental results obtained in the KIAI project by KIT, before being applied to a real Turbomeca injector. The impact on the subsequent two-phase flow and flame in the combustion chamber was observed and analysed.

3. Advancement of Capability due to the FIRST project

This work allowed significant improvements of the representation of the complex physics of liquid injection in the code AVBP. The code has been equipped with a model for SWI and liquid film, that may now be used in other contexts than injection (SWI and liquid films may also exist inside the combustion chamber).





4. Additional information

Application: Spray-Wall interaction and liquid films
Research area: Two-phase flow modelling
Technology readiness level: 2
Owner of IPR: CERFACS
FIRST Task: T4.1.3
Main author and contact: Geoffroy Chaussonnet, CERFACS

Assisted atomisation process: advanced simulations and comparison with experiments (UPMC, CNRS, ONERA)

1. State of the Art before the FIRST project

Prior to the FIRST project, DNS of complex interfacial phenomena were already under development. Yet, they remained ineffective and numerically unstable for flow conditions encountered in aero-engines, namely high density (> 1000) and velocity (≥ 10 in favour of the gas).

2. Research & Development Activities Performed

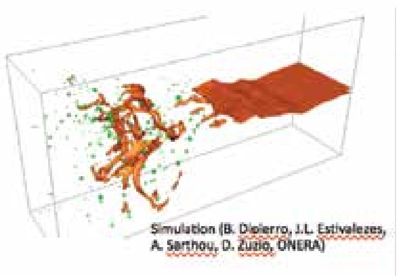
Detailed analysis of code limitation have led to the development and the implementation of new resolution schemes for DNS based on VOF and/or Level-Set methods. The spatio-temporal resolution as well as numerical performances of these codes were significantly improved, allowing to simulate laboratory experimental conditions. The combined investigation of atomisation processes by way of controlled experiments, simulations and theoretical analyses was also undertaken to test the ability of these codes, to accurately represent the elementary physical processes and to evaluate their reliability.

Simulation (A. Berlemont, T. Ménard, G. Vaudor, CNRS-CORIA)

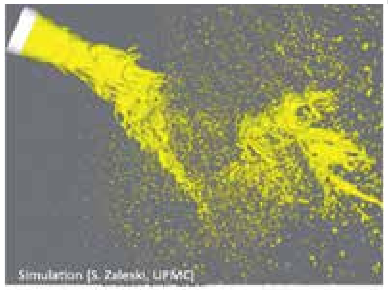
Experiment (A. Cartellier, A. Delon, J.P. Matas, CNRS-LEGI)

3. Advancement of Capability due to the FIRST project

DNS of assisted atomisation phenomena that were out of reach at the start of the project, are now available for flow conditions relevant for turbo-reactors. The codes developed are thus at the cutting edge. The combination of such advanced simulations and of experiments has led to a new understanding of the interfacial instabilities arising in assisted atomisation. In addition, quantitative agreements between experiments and simulations have been obtained on a number of physical quantities. In particular, preliminary comparisons between predicted and observed size distributions is quite encouraging. A further significant decrease of computation times that remain enormous - at the limit of today's computers – is required to fully ascertain the reliability of such tools in terms of drops size and flux.



Simulation (B. Dipierro, J.L. Estivalezes, A. Sarthou, D. Zuzio, ONERA)



Simulation (S. Zaleski, UPMC)

4. Additional information

Application: Prediction of spray characteristics in aero-engines
Research area: Fundamental mechanisms controlling assisted atomisation and their simulation
Technology readiness level: 3
Owner of IPR: UPMC, CNRS-CORIA, CNRS-LEGI, ONERA
FIRST Task: T4.1.4
Main Author and Contact: Alain Cartellier, CNRS

Identification of Spray Boundary Conditions from Measurements (ONERA)

1. State of the Art before the FIRST project

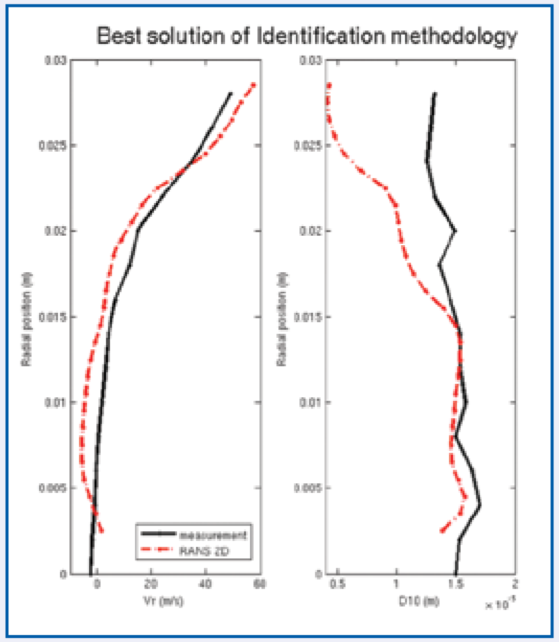
Two phase flow computations require the specification of the boundary conditions for the liquid phase. When they are not known but measurements not too far from the injection points are available, an approach based on the inverse problems can be implemented. The fuel injection model developed by CERFACS (FIMUR) provides the size and velocity distributions of the droplets at injection for a pressure-swirl atomizer. The purpose was to develop a methodology of identification for any type of atomizer.

2. Research & Development Activities Performed

Spray boundary conditions are a solution of an inverse problem which involves the minimisation of the distance between computed and measured distributions of size and velocity of the droplets at measurement section. This optimisation problem is solved as a results of a surrogate modelling approach and a genetic algorithm. Because of the high cost of two phase flow computations, the choice was made to use 2D-axisymmetrical computations with the ONERA code CEDRE. In order to validate the process, the boundary conditions obtained were then applied to 3D LES (code AVBP, CERFACS) and 3D RANS (code N3SNatur, SNECMA) computations.

3. Advancement of Capability due to the FIRST project

A methodology for boundary condition identification is now available as a result of the FIRST project. Moreover, the measurements necessary for its validation are issued from the project and have benefited from the setup improvements, by allowing the measurement section to be moved closer to the injection point. Although the TLC SNECMA injector chosen for the experimentation did not appear to have an axisymmetric behaviour, the application on this injector has shown that a valuable expertise can be obtained with this methodology.



Best solution of Identification methodology

4. Additional information

Application: Boundary conditions of liquid phase for two phase flow computations
Research area: Two-phase flow injection modelling
Technology readiness level: 2
Owner of IPR: ONERA
FIRST Task: T4.2.1
Main author and contact: Patricia Klotz, ONERA

Exploitation film model (SNECMA)

1. State of the Art before the FIRST project

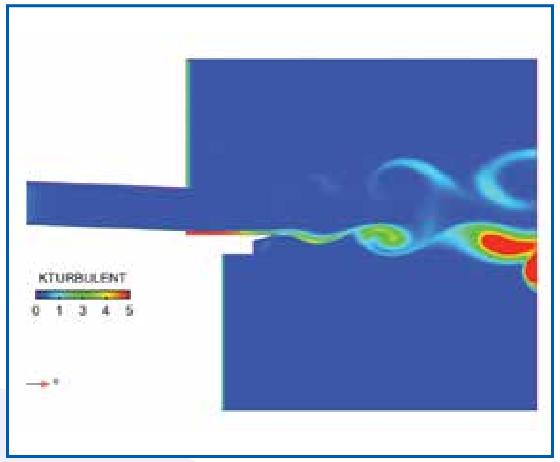
The numerical simulation of an aeronautical combustor requires a number of assumptions or simplifications. The formation of a film over the wall surrounding the injector which will then be atomized by the shear flow is in general not taken into account. To deal with the interaction of the droplet with the wall, a simple elastic or non elastic rebound is implemented in the solver. Numerically, the droplet never forms a film at the wall. By adopting this approach, an interesting physical behaviour that can modify the fuel distribution inside the combustor is lost. A film model accounting for those mechanisms was available in the Snecma in-house RANS solver but hadn't been validated.

2. Research & Development Activities Performed

In close collaboration with CNRS-LEGI, a planar film experiment was defined in order to provide data to validate the film model available in the Snecma in-house RANS solver and in particular the formation of droplets at the end of the injector wall (geometrical discontinuity). The liquid used in this experiment was water. Two operating conditions were agreed and LEGI provided the mean droplet characteristics at several radial and axial locations. Several calculations were made using the Snecma in-house film model to validate it against the available data.

3. Advancement of Capability due to the FIRST project

The Snecma in-house film model has been validated. The formation of a fuel film by the fuel droplets impacting the injector wall and the subsequent droplet formation at the wall end can now be included in combustor simulations. Nevertheless, this kind of RANS modelling is just one intermediate step in the path to the final use of more sophisticated and physics based models (Cerfacs and Coria work) to account for film and atomisation processes in computations.



4. Additional information

Application: Boundary conditions of liquid phase for two phase flow computations
Research area: Two-phase flow injection modelling
Technology readiness level: 2
Owner of IPR: SNECMA
FIRST Task: T5.1.2
Main Author and Contact: Juan Carlos Larroya Huguet, SNECMA

Exploitation of phenomenological models (SNECMA)

1. State of the Art before the FIRST project

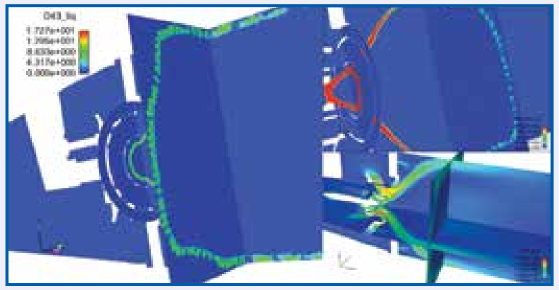
The simulation of two phase flow inside a combustor required the specification of the boundary conditions for the liquid phase. An experience based approach was available at Snecma to define these boundary conditions. Experimental characterisation of the injector was used to specify a pertinent ensemble of droplet classes as well as their initial velocities and injection locations close to the injector exit.

2. Research & Development Activities Performed

Snecma provided a TLC injector system to ONERA, who conducted the experimental characterisation of the spray. This information was used to feed an ONERA numerical tool devised to obtain a new and better set of boundary conditions for the liquid phase as output. Unfortunately, the experimental data has shown an unexplained asymmetric behaviour and the exploitation of this data by the ONERA tool was compromised. Partial data from TLC project on this injector was used to overcome this difficulty. ONERA provided a new set of boundary conditions for the liquid phase to Snecma and a back-to-back calculation was made in order to evaluate the result of applying the new methodology versus the old one.

3. Advancement of Capability due to the FIRST project

A new methodology for liquid phase boundary conditions identification is available as a result of the FIRST project. This methodology will be used to automate the generation of boundary conditions for the liquid phase and to improve the reliability of the combustor simulations. This kind of approach is just one intermediate step in the path to the final use of more sophisticated and physics based models (CERFACS and CNRS-CORIA work) to account for the liquid phase in simulations.



4. Additional information

Application: Boundary conditions of liquid phase for two phase flow computations
Research area: Two-phase flow injection modelling
Technology readiness level: 2
Owner of IPR: SNECMA
FIRST Task: T5.1.3.1
Main author and contact: Juan Carlos Larroya Huguet, SNECMA

Exploitation of phenomenological models (Turbomeca)

1. State of the Art before the FIRST project

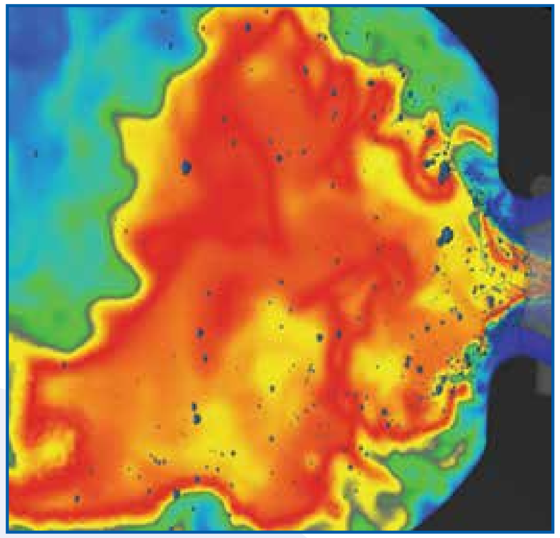
The specification of liquid injection properties can be of paramount importance when simulating a combustion chamber for reaction zone localization, pollutant formation, ignition or extinction processes. To specify such characteristics, Turbomeca employs the extrapolation of experimental measurements (velocity, droplets distributions) to reach realistic operating conditions.

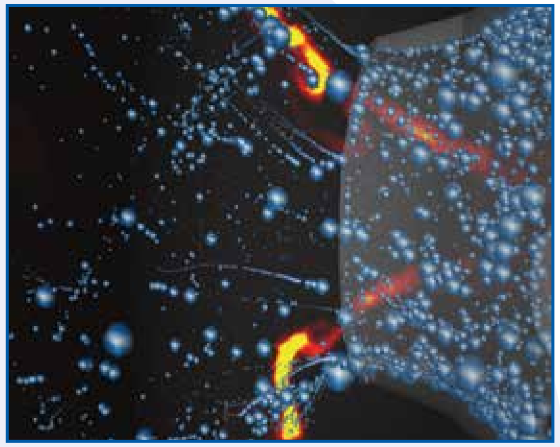
2. Research & Development Activities Performed

In the FIRST project, CERFACS developed liquid film and atomization models suited for the simulation of the dense-spray region inside an aeronautic combustion chamber equipped with airblast atomizers with film-wall interaction. CERFACS and Turbomeca performed reactive LES of a combustion chamber at two operating conditions, using different approaches to model the liquid boundary conditions.

3. Advancement of Capability due to the FIRST project

A new methodology for liquid phase boundary condition identification is available and requires no constraining parameters extrapolated from experimental data. This enables Turbomeca to confidently perform reactive two-phase LES at various operating conditions for a reasonable CPU cost. This kind of approach bridges the gap between very costly primary atomization simulations and cheap experimental correlations, which are not properly validated for a wide arrange of injection technologies and operating conditions.





4. Additional information

Application: Boundary conditions of liquid phase for two phase flow computations

Research area: Two-phase flow injection modelling

Technology readiness level: 2

Owner of IPR: Turbomeca

FIRST Task: T5.1.3.2

Main Author and Contact: Jean Lamouroux, Turbomeca

Validation of the VOF approach in regards to primary atomization in a model injector (MTU)

1. State of the Art before the FIRST project

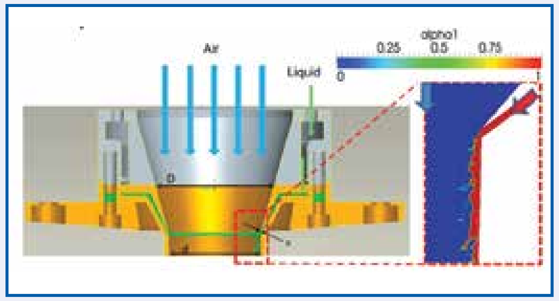
The volume of fluid (VOF) approach is a well known numerical method to simulate two-phase-flows. However, mainly due to the lack of detailed validation data, the applicability of VOF to predict the primary atomization in annular aero engine injectors could not be verified so far.

2. Research & Development Activities Performed

In cooperation with the Engler-Bunte-Institut (EBI) of the University of Karlsruhe, MTU performed a detailed comparison of numerical results with the experimental data base of a generic model injector. The analysis covered the comparison of the average film thickness as well as the local film thickness distribution. Through a comprehensive sensitivity study over a wide range of operation conditions, the occurrence of primary atomization inside the model injector was correlated to a minimum of momentum ratio of the liquid to gaseous flow.

3. Advancement of Capability due to the FIRST project

Using the validated numerical model, the parameter studies performed delivered a more detailed insight into the primary atomization occurring inside the model injector. The analysis of fuel mixed into the gaseous flow before leaving the injector nozzle and entering the combustion chamber indicates that the primary atomization influences the fuel distribution inside the reaction zone significantly. The simplification of ignoring the primary atomization inside the nozzles widely used in current modelling approaches may lead to incorrect fuel distribution predictions during design phases of combustion systems. The comprehensive sensitivity study revealed that the characterisation of the two phase interaction cannot be based only on the momentum ratio.



4. Additional information

Application: Fuel injector of aero combustors

Research area: Numerical investigation of primary atomization zone in fuel injectors

Technology readiness level: 2

Owner of IPR: MTU Aero Engines AG

FIRST Task: 5.1.4

Main author and contact: Marco Konle, MTU Aero Engines AG

Thin film model for prefilming airblast atomizers (UNIFI, AVIO)

1. State of the Art before the FIRST project

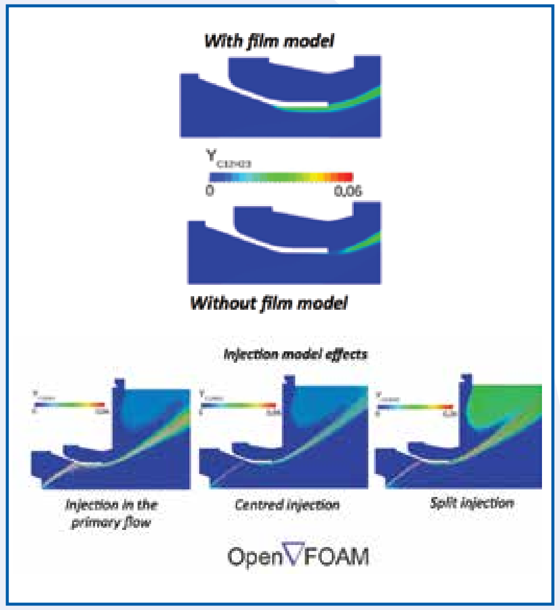
Before FIRST, computational techniques for liquid fuelled combustors based on Lagrangian tracking were not fully capable of dealing with liquid film development along the injector prefilming surface. This lack influenced both prefilming atomizer injection characterisation and parcel/wall interaction between prefilming surface and droplets coming from secondary injection (e.g. pressure atomizer functioning as pilot injector). For the former, modelling correlations were generally employed using a priori estimates of liquid film and gas flow field development, while for the latter, simple rebound models were often implemented neglecting the influence of liquid film development on droplet splashing.

2. Research & Development Activities Performed

A simplified model for the liquid film development along the prefilming atomizer surface coupled with a newly implemented steady-state Lagrangian tracking solver able to perform reactive simulations has been developed in the OpenFOAM suite. The model is based on the thin film approximation solving film conservation equations (film thickness, momentum and energy) with the Eulerian approach on a 2D mesh extruded normally from the wall. Coupling with the gas phase is achieved on the film/gas interface maintaining equal interface velocity and shear stress on both sides. Coupling with the Lagrangian tracking includes implementation of a splashing model (for droplet hitting the wet surface) and of injection models to account for the primary break-up. These injection models are based on available correlations which are solved with updated film and gas properties at each iteration to provide the required feedback from the film solver. Among the others, some of the implemented models are based on newly developed correlations developed in KIAI EU program by KIT for planar prefilming airblast atomizers.

3. Advancement of Capability due to the FIRST project

The FIRST project has enabled the investigation of the effects of the liquid film developing on the prefilming airblast on the global combustor performance by means of fast and robust CFD analysis suitable for industrial applications. A pre-filming injector geometry with an additional pressure swirler pilot injection (provided by GE Avio) was considered in a tubular configuration simplified to obtain axisymmetric computations. Results indicate that fuel evolution is deeply impacted in the injector region by liquid film formation, especially when droplets from the pilot injector impinge on the film. Furthermore the OpenFOAM toolbox is now upgraded to provide reliable simulations of other prefilming airblast atomizers or of the same injector in other configurations.



4. Additional information

Application: Thin film model for prefilming airblast atomizers
Research area: CFD analysis of injection zone
Technology readiness level: 2
Owner of IPR: Università degli Studi di Firenze, GE Avio
FIRST Task: T5.1.5
Main Author and Contact: Antonio Andreini, UNIFI

Expert system for liquid breakup (EST, AVIO)

1. State of the Art before the FIRST project

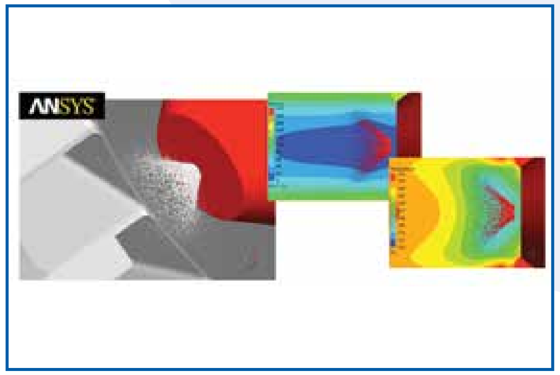
Before FIRST, the diameter distribution for sprays after the breakup process was computed by empirical expression.

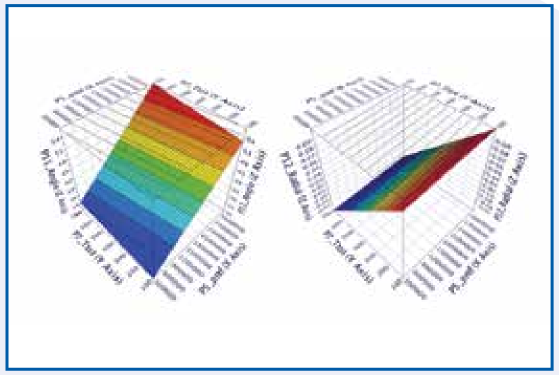
2. Research & Development Activities Performed

An expert system for the atomization scenario has been developed in order to characterise the breakup process in any physical scenario. Different operating conditions were considered and numerical simulations, including primary and secondary atomization have been computed using Ansys® CFX. The Design of Experiments (DoE) methodology was used to identify which input variables most affected the output variables. Starting from these results, response surfaces have been generated using the commercial code modeFrontier®.

3. Advancement of Capability due to the FIRST project

The FIRST project has enabled the prediction of diameter distribution for sprays after the breakup process in any scenario starting from the knowledge of the physical boundary condition. The accuracy of this method depends on the initial number of configurations used in the DoE, but can be considered more consistent with the physics compared to the empirical correlations used until now.





4. Additional information

Application: Response surface of breakup process
Research area: CFD analysis of injection zone
Technology readiness level: 2
Owner of IPR: EnginSoft, GE Avio
FIRST Task: T5.1.6
Main author and contact: Michele Andreoli, EnginSoft

Exploitation of spray models (IMPERIAL, RRUK, RRD)

1. State of the Art before the FIRST project

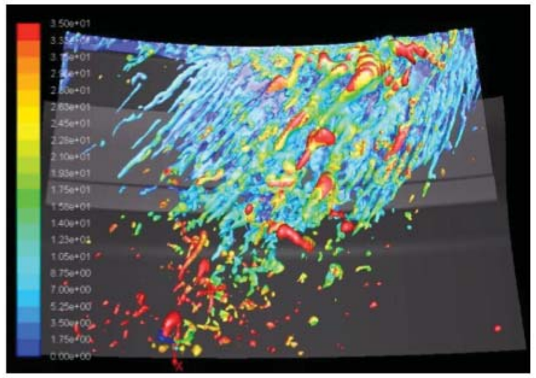
While CFD is widely used to simulate reacting flows in aero-engine combustors, spray boundary conditions have always been affected by significant uncertainty, which in turn can have a dramatic impact on a range of critical combustor performance parameters. In CFD simulations, spray is usually injected at a rather arbitrarily defined location downstream of the injector and particles tracked based on Lagrangian methods. Correlations derived in the past on geometries and conditions not necessarily representative of today's designs and pressure conditions have been used to define spray boundary conditions with mixed success. Limited understanding of the impact injector geometry has on spray quality has made injector design a highly empirical process with long development times, potentially leading to suboptimal solutions.

2. Research & Development Activities Performed

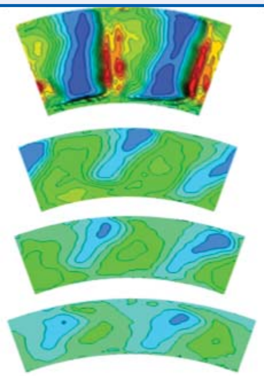
Detailed steady and unsteady simulations of an industrial lean burn fuel injector were carried out as part of FIRST, based on well resolved validation data provided by Loughborough University. The capability of single-phase LES methods to predict time-averaged and unsteady components for both the lean burn injector and a more conventional injector was assessed. Detailed simulation of the fuel passages enabled characterisation of the non-uniformity of fuel feed to the prefilmer of the lean burn injector. Furthermore, two-phase VOF simulations of an academic test case as well as the two injectors' film and primary break up were conducted. Eventually, an advanced dispersion model developed by Imperial College and based on the KS concept was implemented into the in-house code PRECISE and tested.

3. Advancement of Capability due to the FIRST project

The work done in FIRST has enabled to characterise the internal aerodynamics of a typical lean burn injector and validate the approach. In particular, an understanding has been obtained about the relative merits of LES over RANS within the injector design process. Moreover, a simple approach to simulating the fuel passages has proven beneficial to the definition of spray boundary conditions. While more research work will clearly be needed to make the two-phase flow methods for prediction of primary break up more accurate and computationally affordable, VOF has been proven to provide useful information about spatial and temporal distribution of fuel film on prefilming surfaces.



VoF LES of fuel film



LES of fuel injector air passages

4. Additional information

Application: Emissions, temperature and flow field predictions in aero engine combustors
Research area: Spray modelling
Technology readiness level: 2
Owner of IPR: Imperial College, Rolls-Royce plc and Rolls-Royce Deutschland
FIRST Task: T5.1.7, T5.1.1
Main Author and Contact: Marco Zedda, Rolls-Royce UK

Exploration and Exploitation of fundamental models (Turbomeca)

1. State of the Art before the FIRST project

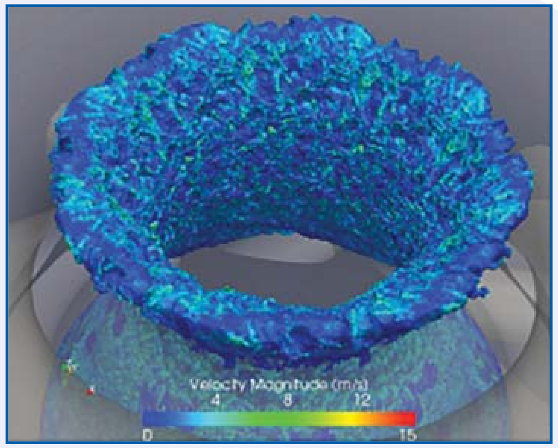
A wide range of methodologies on primary atomization modelling exist and numerous validations of these techniques are performed on academic configurations. However, due to the high CPU cost and to the complexity of primary atomization simulation, CFD computations of real industrial injectors are solely focused on aerodynamics at Turbomeca. The computations are used in the early stages of design, and correlations and experimental analyses are used in conjunction to develop the injectors.

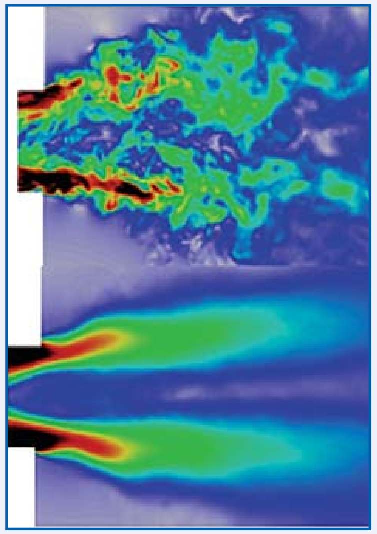
2. Research & Development Activities Performed

In the FIRST project, CNRS-CORIA researchers developed numerical methods for primary atomization adapted to large and complex geometries. Turbomeca assessed the feasibility of the simulation of one of its aerodynamic atomizer injectors where film-wall interactions are present by performing aerodynamic computations of the configuration. Turbomeca provided CORIA with one geometry and the associated experimental data for the primary atomization simulation using homogeneous mesh refinement methods. The simulations showed that the prediction of atomization using this approach was not compatible with industrial needs in terms of CPU costs, and highlighted the need for the development of heterogeneous mesh refinement methodologies.

3. Advancement of Capability due to the FIRST project

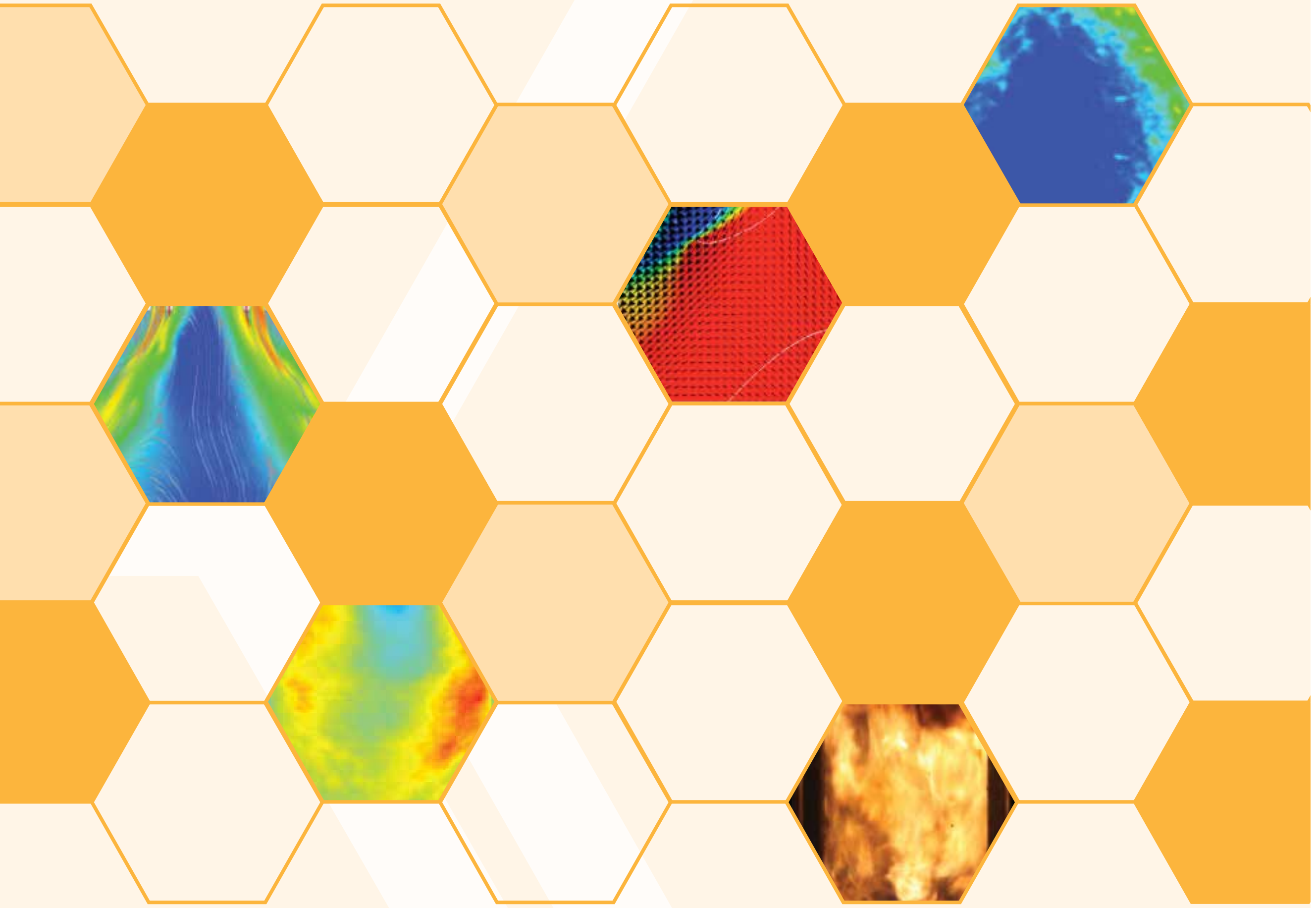
In the project, Turbomeca obtained knowledge and tools to simulate the atomization process for pressure atomizers. For air-assisted atomizers, CORIA developed heterogeneous mesh refinement and partitioning techniques, adapted to industrial geometries and CPU capacities. The Safran group is continuing to work on primary atomization with CORIA with the start of a PhD thesis in 2014.





4. Additional information

Application: Primary atomization computations of industrial injectors
Research area: Primary atomization modelling
Technology readiness level: 2
Owner of IPR: SAFRAN - Turbomeca
FIRST Task: T5.1.8
Main Author and Contact: Jean Lamouroux, Turbomeca



Soot:

Experimental and Numerical Investigation of Soot Production

Advanced modelling for complex combustion systems including PAH and soot BINs (DLR)

1. State of the Art before the FIRST project

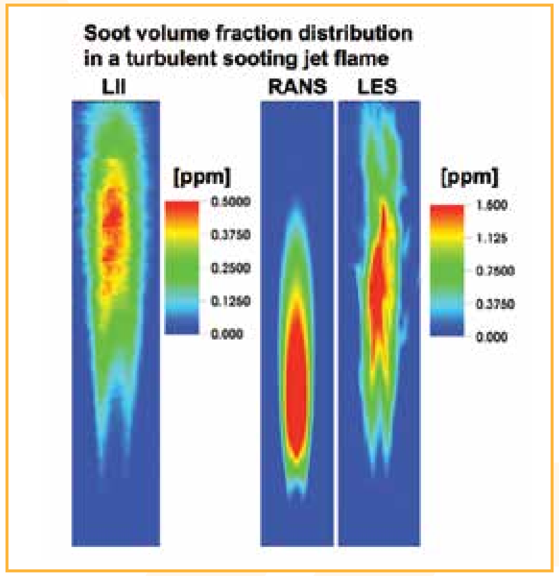
Before FIRST, the DLR soot model had been validated successfully for a wide range of different validation experiments (different fuels; laminar and turbulent; non-premixed, partially-premixed and premixed; atmospheric and high pressure conditions) with one set of model constants. However, the reversibility of surface chemistry was not considered in the soot model, yielding too fast soot formation compared to measurements. Turbulence was described by RANS turbulence models.

2. Research & Development Activities Performed

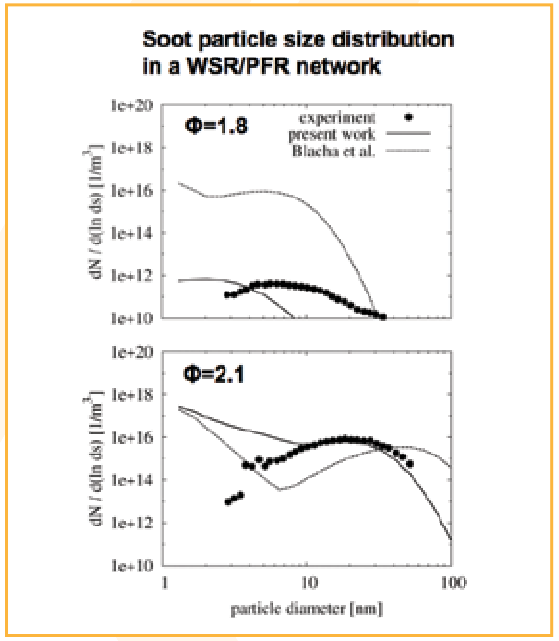
Within FIRST, the DLR soot model was coupled to LES turbulence models and LES simulations of a turbulent sooting jet flame were performed. Furthermore, a sectional soot precursor model which includes radical branches of PAH and reversible PAH surface chemistry has been developed and implemented in the DLR THETA code.

3. Advancement of Capability due to the FIRST project

The prediction of soot volume fractions in turbulent flames has been significantly improved by the coupling of the soot model with LES. The implementation of reversible soot precursor surface chemistry yielded a delayed soot formation and a better agreement on the validation of data. The sensitivity of the soot model to the equivalence ratio was improved, especially at equivalence ratios close to the sooting limit.



Soot volume fraction distribution in a turbulent sooting jet flame



Soot particle size distribution in a WSR/PFR network

4. Additional information

Application: Soot model development for turbulent pressurized combustion
Research area: Soot modelling
Technology readiness level: 2
Owner of IPR: DLR-ST
FIRST Task: T2.1.1
Main Author and Contact: Christian Eberle, DLR-ST

Improved Soot Nucleation and Oxidation Mechanisms and Links to Surrogate Fuel Chemistry (IMPERIAL)

1. State of the Art before the FIRST project

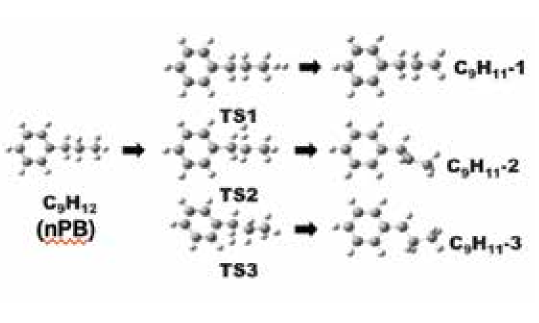
The formation and oxidation of aromatics is crucial in the context of links to surrogate fuel models used in combustor design calculations with nPB selected as a representative molecule in EU and US surrogate blends in order to modulate the sooting propensity. Prior to FIRST, the link between the chemistry of surrogate fuels and soot relied upon the application of reaction class, based estimation techniques with soot emissions typically computed using moment based or empirical methods, that do not provide PSDs.

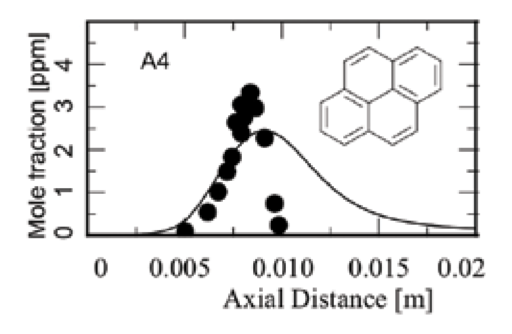
2. Research & Development Activities Performed

Ab initio methods at the G4, G4MP2 and G3B3 level were used to determine thermodynamic properties of 92 PAHs with up to 16 carbon atoms involved in soot nucleation and oxidation sequences. The recommended aromatic nPB component selected in the CFD4C programme (award: GRD1-1999-10325) was further studied through accurate ab initio methods with results obtained for six side-chain hydrogen abstraction reactions at the “gold standard” CCSD(T)/jun-cc-pVTZ//M06-2X/6-311++G(3df,3dp) level (bottom right image). More economical state of the art DFT methods were also evaluated. Test cases for laminar premixed flames, laminar diffusion flames and PSR/JSR geometries were computed and an evaluation of the PAH, soot formation and oxidation mechanisms performed in the context of computations coupled to sectional models capable of calculating full PSDs.

3. Advancement of Capability due to the FIRST project

The resulting chemical mechanism has been used to improve predictions of soot PSDs and particulate levels in premixed and diffusion flame environments through the further development of a mass and particle number density conserving sectional approach that links directly to the detailed PAH and soot inception chemistry. The ability of the devised approach to reproduce PAH concentrations up to pyrene (A4), used to define the smallest soot section via a dimerization, has been assessed using comparisons with laminar flame data (top right image). The prospects for simplifications of soot nucleation sequences has been evaluated along with the accuracy of computationally efficient DFT methods for larger molecules and recommendations made as to a suitable balance between accuracy and complexity.





4. Additional information

Application: Prediction of soot emissions from aero combustors

Research area: Surrogate fuels and link to soot particle size distributions

Technology readiness level: 2

Owner of IPR: Rolls-Royce

FIRST Task: T2.1.2

Main Author and Contact: Peter Lindstedt, IMPERIAL College

Characterisation of a Lean Burn Module Air Blast Pilot Injector with Laser Techniques (DLR)

1. State of the Art before the FIRST project

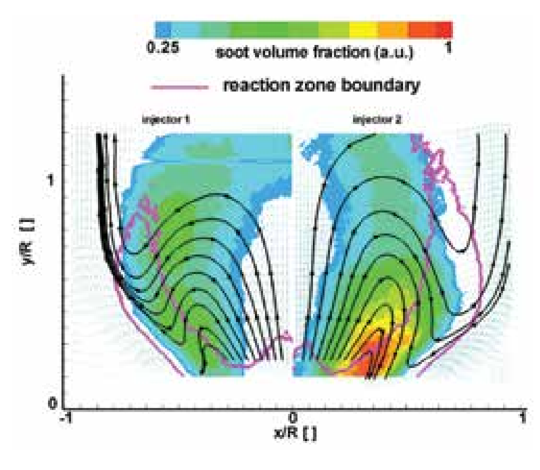
Pilot modules in staged lean burn fuel injectors exhibit a propensity to form soot at the upper power end of their operational envelope. Data on global smoke numbers at combustor exit and parametric dependence existed, but no detailed information on soot formation and its coupling to flow field and reaction zones inside the combustor were available. In particular, no validation data for CFD modelling of soot formation existed.

2. Research & Development Activities Performed

Data on velocities, soot volume fractions, reaction zone and fuel distributions, along with rig operation data, were obtained from a single sector combustor with optical access, equipped with a Rolls-Royce lean burn injector, by various optical methods under realistic operation conditions. The measurements allowed identification of soot forming regions inside the combustor and illustrated their dependence on flow field structures (through modified injector aerodynamics), equivalence ratio, temperature and pressure. These tests helped to obtain a qualitative understanding of the soot formation mechanisms. The data was provided to project partners for CFD validation.

3. Advancement of Capability due to the FIRST project

For the development of a virtual injector numerical tool, or more specifically soot formation predictive techniques, extensive databases with qualitative and quantitative measurements are necessary. For soot measurements, the LII technique was tested and applied under realistic operating conditions at idle and part load. Along with additional data on velocity field and reaction regions, these measurements form a database to validate the soot formation and transport models developed in FIRST.



4. Additional information

Application: Validation data for an industrial fuel injector; optical study of soot formation

Research area: Soot formation in lean burn injectors

Technology readiness level: 4

Owner of IPR: DLR

FIRST Task: T3.3.1

Main Author and Contact: Ulrich Meier, DLR

Validation data from sooting, turbulent flames (DLR)

1. State of the Art before the FIRST project

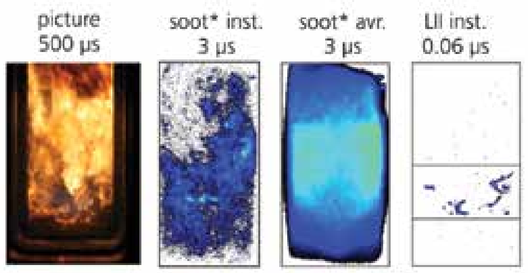
In literature no high quality validation data set is available at increased burner complexity. Soot model validation is mostly done using laminar flames or turbulent atmospheric jet flames. The only existing data set at increased pressure involving turbulence/swirl and oxidation air was good at that time but limited to soot concentration and few temperature measurement points for one single out of the set of flames (data set recorded during EU project Soot in Aeronautics, SiA).

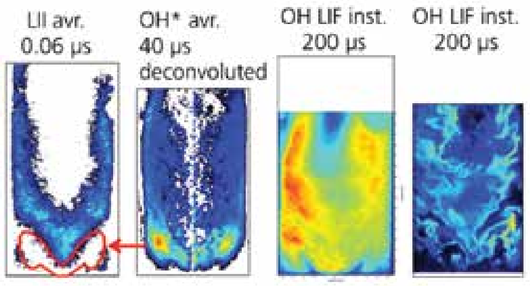
2. Research & Development Activities Performed

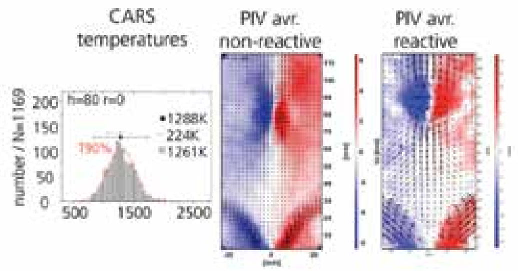
In addition to SiA, an optimised model combustor was developed with even better suiting simulation needs. A large suite of different optical and laser-based diagnostics was applied to this burner operating at increased pressure which resulted in a comprehensive data set. This data set includes soot concentration maps, a fine grid of CARS temperatures and statistics, OH distributions and velocity fields. In addition some instantaneous correlations were measured such as OH/soot and PAH/soot to show feasibility. Few flames were characterised in full detail, for others trends are available with a lesser degree of detail. The very sensitive influence of secondary air injection past the primary combustion zone provides an excellent test case for soot model validation, the comprehensive set of quantities being important to check different sub-models of CFD codes, i.e. cold flow, turbulent mixing, gas phase kinetics, and soot chemistry.

3. Advancement of Capability due to the FIRST project

A data set of unprecedented quality has already been used by CFD partners in the project and the scientific community was very interested (dissemination activities: publications, conferences) and requested access. The data was proposed as target flame in this year's International Sooting Flame Workshop ISF2. A combination of soot concentration with flow fields, temperatures and OH distributions was highly appreciated. New knowledge will be created by the comparison of model results with experiments. For this purpose, the use of correlated application of different diagnostics were made. This was not the main focus of the project and might be a task for future.







4. Additional information

Application: Soot formation and oxidation in pressurized turbulent flames

Research area: Understanding soot formation by detailed experimental data

Technology readiness level: 3

Owner of IPR: DLR-ST

FIRST Task: T3.4.1

Main Author and Contact: Klaus Peter Geigle, DLR

Validation of advanced soot modelling for complex combustion systems (DLR)

1. State of the Art before the FIRST project

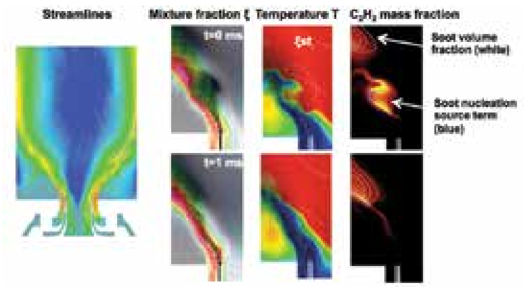
For complex combustion systems such as aero-engine combustors, quantitative validation of soot models was limited due to the lack of detailed experimental data. So far detailed validation data for sooting combustion was restricted to academic test cases like laminar flames or turbulent jet flames. Test cases which provide well defined boundary conditions and comprehensive validation data on one hand and feature technically relevant conditions as confined swirling flow and operation at elevated pressure on the other, were not available until recently.

2. Research & Development Activities Performed

This gap was closed by the measurements performed in the FIRST project, yielding a detailed characterisation of an aero-engine model combustor. Optical access to the combustion chamber via four quartz windows permitted the use of non-intrusive laser measurement techniques. This new data set provides an unprecedented opportunity to validate soot models at technically relevant conditions. Within FIRST, URANS and LES simulations of the model combustor using finite-rate chemistry and a two-equation soot model were performed successfully. Good agreement against experimental data was obtained and potential for further model development was deduced.

3. Advancement of Capability due to the FIRST project

The capability of the DLR soot model to predict soot distributions in complex combustion configurations has been demonstrated. It was shown by time-resolved data analysis that soot formation is highly unsteady and might be influenced by coherent flow field structures such as precessing vortex cores. Thus, time-resolved simulations are important for accurate soot predictions.



4. Additional information

Application: Soot model validation for complex combustion systems

Research area: Soot model validation for complex combustion systems

Technology readiness level: 2

Owner of IPR: DLR-ST

FIRST Task: T4.1.2

Main Author and Contact: Christian Eberle, DLR-ST

Cost-effective numerical simulation of soot formation (ONERA)

1. State of the Art before the FIRST project

Before the FIRST project soot modelling was either:

- very crude and with very low predictive accuracy when applied to technical scale devices;
- or complex and very expensive when applied to academic or semi-technical scale configurations, as most of the time it was used with simple turbulence modelling (RANS) to save CPU.

2. Research & Development Activities Performed

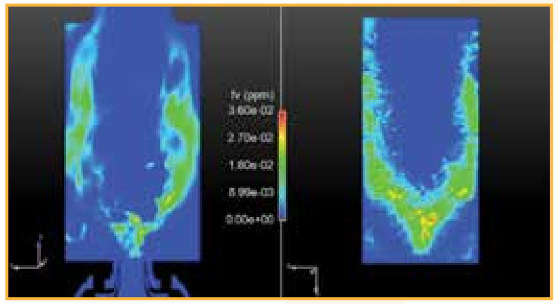
ONERA developed two complementary approaches in order to obtain a level of accuracy that significantly improved compared to the usual simple models, while keeping to an acceptable cost.

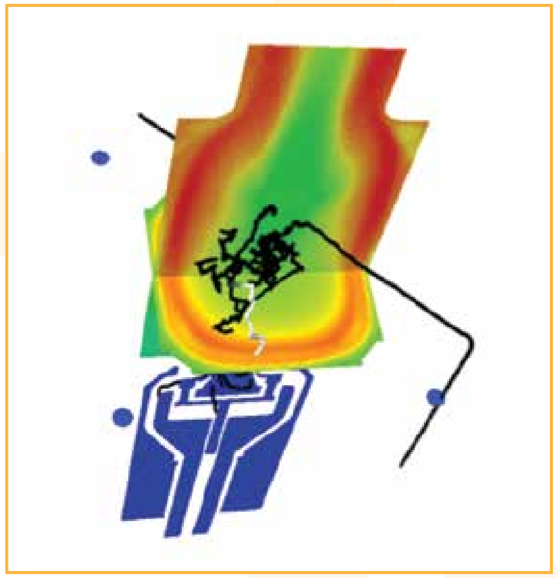
These new models are designed to be used in conjunction with LES and are applied to technical scale burners:

- 1st approach: The Soot model based on tabulated chemistry. This model is based on gaseous precursors like C2H2 instead of on total fuel as in simple models. Since all the chemical kinetics complexity is embedded in a pre-processed table, the CFD computation cost is significantly reduced compared to the “standard” approach, in which all the species are transported. Extracting species concentrations from the table gives the possibility of using rather accurate soot models;
- 2nd approach: The Hybrid EE/EL model with time-reversed trajectories. Soot characteristics are computed in post-processing with high accuracy only at points where information is required, which leads to low computation time despite the use of complex chemistry.

3. Advancement of Capability due to the FIRST project

These models were applied to the DLR burner. They successfully reproduced both topology of the soot field and magnitude of the soot mass-fraction. In the picture to the right, soot volume fractions computed with the tabulation-based soot model is reproduced on the left side of the image and compared with the experimental field obtained by LII, in the right side of the image. On the bottom image, trajectories of fluid particles are plotted, in order to illustrate the principle of the EE/EL method. The part of the trajectories where soot is produced is in white in the bottom picture.





4. Additional information

Application: Aero combustors
Research area: Soot modelling
Technology readiness level: 2
Owner of IPR: ONERA
FIRST Task: T4.1.5
Main Author and Contact: Nicolas Bertier, ONERA

Exploitation of soot models (RRD, RRUK, DLR)

1. State of the Art before the FIRST project

Prior to the FIRST project, rather simplified soot models were available within the Rolls-Royce in-house combustion CFD code. The reliability and predicting capability of these models were shown to be limited. Furthermore, the applied reaction mechanism for flamelet type combustion models like the FGM method, were based on reaction mechanism developed within the EU FP6 project CFD4C, and were not the state of the art anymore. Well documented and comprehensive databases were missing to validate the soot models.

2. Research & Development Activities Performed

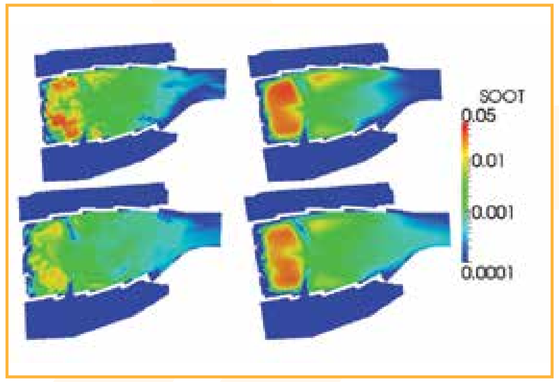
DLR-VT developed a soot model, which is based on detailed chemistry and includes all the required physics of soot production and oxidation processes. This detailed soot model was implemented into the Rolls-Royce in-house combustion CFD code PRECISE-UNS.

Furthermore, state of the art detailed chemistry models were developed by Imperial College London which describe the gas phase combustion process. This detailed chemistry model is used within the FGM combustion model used for combustor CFD applications.

DLR-VT generated a comprehensive validation data base of a generic combustor to validate the soot models.

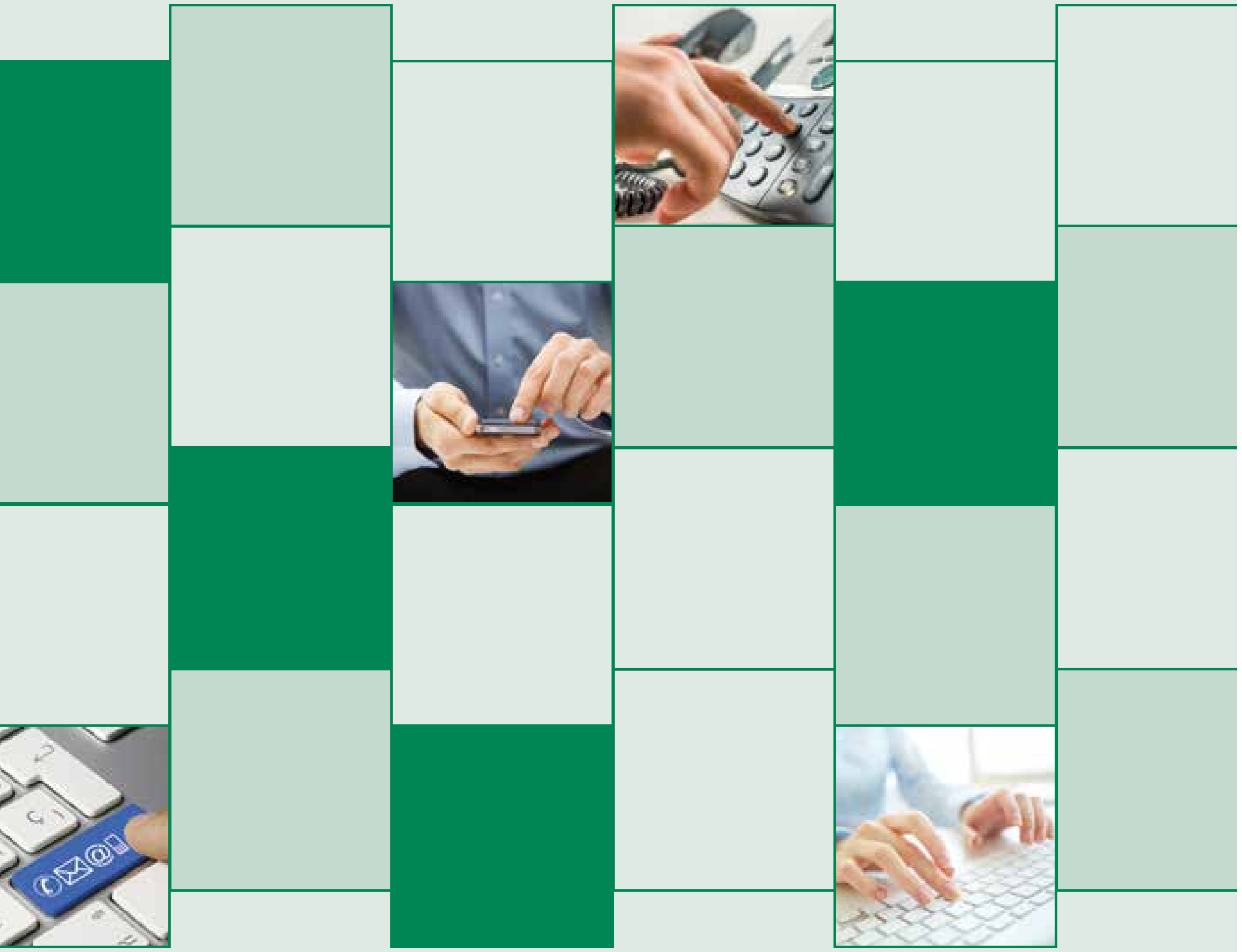
3. Advancement of Capability due to the FIRST project

The development and implementation of these reaction mechanisms and soot models provides a framework to perform soot predictions based on state of the art detailed kinetic models. Although further development and validation for aero gas turbine combustors is required, the developments performed within FIRST is a step towards a more accurate and reliable soot predicting capability.



4. Additional information

Application: Soot prediction in aero engines
Research area: Soot modelling, detailed chemistry models
Technology readiness level: 5
Owner of IPR: DLR-VT, Imperial College, Rolls-Royce plc and Rolls-Royce Deutschland
FIRST Task: T5.2.1, T5.2.2
Main Author and Contact: Ruud Eggels, Rolls-Royce DE



FIRST Project Participants Directory

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