Numerical Simulation of Liquid Sprays for Jet Engine Applications

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1 ABSTRACT

Improving combustion is critical for the next generation of aircraft in order to lower the fuel consumption and reduce the emissions of greenhouse gases. During the hydrocarbon fuel combustion, liquid fuels must undergo a series of processes including the aerodynamic-induced liquid film atomisation – primary and secondary breakup – into a spray of droplets, and its further evaporation. But the primary breakup process of two-phase flows is not yet well understood. An improved understanding of the liquid fuel injection and atomisation in jet engines is essential to allow for a cleaner, more efficient and better-controlled combustion process. Increasing our understanding of the physical phenomenon via experimental investigations involves many trials and errors at the expense of time and cost for industries. Therefore, adequate modelling of injector and combustor behaviour requires computational fluid dynamics (CFD). Recent numerical progress in CFD has allowed significant improvements to be made on current industrial spray models and suggest that a significant breakthrough could be achieved numerically. My research programme sets out to provide a systematic, qualitative and quantitative assessment of the phenomenology observed during primary atomisation of two-phase flows using a novel in-house state-of-the-art multiphase flow modelling capability, in conjunction with a thorough comparison with the available experimental data and linear and non-linear stability analyses. Ultimately, the outcome of this analysis will provide the aero-engine industry with a complete theory to describe the hydrodynamic and aerodynamic processes involved when liquid fuel disintegration occurs under various take-off and cruise conditions.
2 INTRODUCTION

2.1 BACKGROUND

In the commercial and military aircraft industry, aero-engines generally rely on fuel preparation systems known as atomisers to inject the liquid kerosene in combustion chambers. Atomisers eject a liquid bulk that disintegrates into isolated liquid structures – primary breakup – which will further break up into the desired fuel spray – secondary breakup (Fig. 2.1). The atomisation of the bulk liquid fuel produces a spray of small drops whose ratio of surface area to volume is increased, resulting in enhanced heat and mass transfer rates for the subsequent combustion [1]. Most of the systems now in service are of airblast prefilming type, in which a cylindrical liquid sheet of fuel is exposed on both sides to separate annular air flow passages, to allow high-velocity air to impact both sides of the liquid sheet for atomisation. The airblast atomiser function is to employ the kinetic energy of a flowing airstream to shatter the fuel sheet into drops. One example is shown in Fig. 3.1, designed to operate in the gas turbines of Rolls-Royce engines.

Atomisation is one of the most decisive steps in fuel preparation. Atomisation is the mechanism from which all subsequent spray processes originate (evaporation and combustion). Fuel injectors are thus central to the nature of the primary zone flow field in combustion chambers and the chemical reactions happening within it.

During the past decades, there has been a tremendous expansion of interest in the science and technology of atomisation as the aviation industry is exploring the environmental factors related to the sustainable growth of air traffic, with the greatest attention being devoted to the reduction of pollutant emissions (NO\textsubscript{X}, CO\textsubscript{X}, soot and unburned hydrocarbons) as well as improvements in the engine performance.

To increase the engine performance and efficiency, combustion chambers operate at always higher local pressure and temperature, at the expense of more thermal NO\textsubscript{X} production. To prevent this, engines normally operate below the stoichiometric fuel-to-air ratio to limit the peak flame temperature in the combustion chamber and thus operate at a temperature where thermal NO\textsubscript{X} production is greatly reduced [1]. The resulting drawback from a lower flame temperature environment is poorer flame stability [2]. Yet, a better control over the fuel droplet sizes and spatial distribution in the combustion chamber can improve flame stability. This is because discrete liquid drops have a range of sizes and move in different directions with different velocities to that of the main gas stream. It leads to irregularities in the propagation of the flame front due to the lack of uniformity in the unburnt mixture. The literature also reveals that the achieved degree of mixing of the fuel droplets with the oxidant has an important influence on flame stability and pollutant emissions along with burning rates and heat release per unit volume [1]. The question is how to manage fast, thorough mixing with complete combustion resulting in minimum polluted exhaust gases [3]. A good homogeneous mixing of the fuel and air is a direct consequence of a fine atomisation and fast vapourisation and thus a consequence of an optimised fuel injection. A controlled atomisation is needed (in terms of droplet size and droplet spatial distribution) so that the fuel vapourises and mixes more quickly with the oxidant. The finer the drops and the more controlled is their spatial arrangement in the combustion chamber, the better the mixing efficiency. As a result, the
Figure 2.1: Different regimes for airblasted liquid sheet oscillations observed by Lozano and Barreras [4].
fuel would burn more quickly and within a smaller lengthscale, leading to an increase in the combustion rate and ultimately allowing combustion chambers to be more compact. The overall effect is a better efficiency performance – i.e. an increased heat release per unit volume maximises the performance of the gas turbine – and less pollutant.

The compliance with stricter emissions regulations from the International Air Transport Association and the International Civil Aviation Organisation, as well as the aviation industry exploring enhancement in engine performance, has assumed greater significance in all aspects of spray combustion [1] and therefore demands a deeper, more complete, physical understanding of the liquid fuel fragmentation processes and resulting final fuel spray character [5]. In this regard, development in the liquid-fuelled gas turbine combustors sector has become increasingly striking.

2.2 AIMS AND OBJECTIVES IN PRIMARY ATOMISATION RESEARCH

It is important to know which type of atomiser is best suited for any given application. It is now clear that important spray characteristics, such as mean drop size and drop size distribution, are dependent on a large number of variables such as nozzle geometry, the physical properties of the liquid being atomised and physical properties, turbulence characteristics and flow conditions in the surrounding gas [6]. Despite their importance and numerous advances, the exact mechanisms responsible for liquid-film injection, especially primary breakup, and the nature of the spray produced remain unresolved to this day.

The current experimental understanding in the field is limited because of the difficulty in observing and measuring flow properties in the dense spray region near the injection point. During the past few decades, numerous experimental studies of airblast atomisers have been carried out and this has led to the evolution of empirical correlations to express the relationship between the mean drop size in a spray and the variables of liquid and gas properties, flow conditions and nozzle design features. Many of the correlations obtained apply solely to a specific nozzle design over a narrow range of test conditions (mostly at sea level ambient conditions) [7].

Moreover, until recently, computational limitations have curbed the research growth in the field as the mechanisms responsible for primary breakup could not possibly be explicitly modelled; rather, they are replaced by simplified instability mechanisms and adjustable constants. The design of injectors relies therefore heavily on testing as no numerical methods has so far been able to provide validated quantitative results on a real airblast atomiser geometry.

If the basic mechanisms involved in airblast atomisation and their changes with the ambient conditions were fully understood, then, for any given application, it should be possible to design an atomiser of optimum performance commensurate with other requirements such as minimum cost and complexity [5].

With recent numerical developments in 3-D CFD, current industrial spray models have come closer to simulating the atomisation process and can successfully make adequate evaluation of fuel injection in gas turbine combustion chambers, without the need to resort to current black-box primary breakup models. The numerical approaches dedicated to the understanding of the mechanisms of liquid atomisation are diverse [8, 9, 10, 11]. This major field of research is now accompanied by a proliferation of laser diagnostics for spray analysis, which serve in
validating the numerical results [12, 2, 13].

3 Methodology

The following sections present the numerical formulation for two incompressible isothermal immiscible fluids – in the absence of phase change – with relevance to primary breakup.

Navier-Stokes Equations  The Navier-Stokes equations are a set of partial differential equations that describe the motion of fluids as a relationship between momentum and pressure. In multiphase flows, with the additional surface tension force along the interface between the gas phase and the liquid phase, the two fluids are governed by one single set of Navier-Stokes equations, expressed over the whole multiphase domain, given by equation (3.1). In addition, the continuity equation ensures mass conservation (3.2).

\[
\frac{\partial (\rho u)}{\partial t} = \rho f + \nabla \cdot (T - \rho u \otimes u) \tag{3.1}
\]

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \tag{3.2}
\]

where \( f \) is the sum of body forces (essentially gravity \( g \)). Gravity is ignored in the context of primary atomisation as it has no effect over the lengthscales and timescales involved. \( T \) is the stress tensor. It comprises normal stresses (pressure \( p \)) and shear stresses for viscous fluids. Stokes postulated the viscous contribution to the stress tensor for Newtonian incompressible fluids to be: \( T = -pI + S \), where \( I \) is the identity matrix and \( S \) is the shear stress tensor:

\[
S = 2\mu \mathcal{D} = 2\mu \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)_{i,j=1,2,3} \tag{3.3}
\]

We note that the shear stress tensor also accounts for normal stresses when \( i = j \).

Most primary atomisation applications involve low Mach number everywhere in the domain considered, i.e. the speed of the flow is much lower than the speed of sound. Solving the Navier-Stokes equations and the continuity equation in the incompressible limit is thus perceived as a valid assumption and is the approach chosen here. For incompressible fluids the momentum equations and the continuity equation become,

\[
\frac{\partial}{\partial t} (\rho u) + (u \cdot \nabla)(\rho u) = -\nabla p + \rho f + \nabla \cdot (2\mu \mathcal{D}) \tag{3.4}
\]

\[
\nabla \cdot u = 0 \tag{3.5}
\]

The numerical solver employs finite-volume discretisation for the solution of the two-phase flow equations. The flow variables are cell centred, but face interpolated values are also used in the solution procedure as part of the flux calculation.
SURFACE TENSION AND CAPILLARY FORCES

The interface thickness is comparable to the molecular scale, across which density jumps are of several orders of magnitude. Thus, the sharp interface represents a continuous, but very steep change of the properties (density, viscosity, etc...) of the two fluids. In terms of momentum conservation, and given the forces in play, the surface tension force must balance the jump in the stress tensor \([\mathbf{T}]_\Gamma\) (normal and tangential components) along the fluid interface. Thus the dynamics of the interface at each timestep is determined by the following balance condition:

\[
[-p \mathbf{I} + \mathbf{S}]_\Gamma \cdot \mathbf{n}_\Gamma = \sigma \kappa \mathbf{n}_\Gamma + \nabla_\Gamma \sigma \tag{3.6}
\]

where \([-1]: \) jumps across the interface

\[\mathbf{n}_\Gamma: \) the normal to the interface

\[-p \mathbf{I} + \mathbf{S}]_\Gamma: \) the jump of the stress tensor across the interface

\[\kappa: \) the curvature of the interface

\[\sigma: \) the surface tension coefficient

This is the Young-Laplace junction condition, a law for pressure discontinuity across the interface due to surface tension and related to the shape of the interface. The term on the right-hand side is effectively the source term in the Navier-Stokes equations for the singular capillary forces:

\[
f_\Gamma = \sigma \kappa \delta_\Gamma + (\nabla_\Gamma \sigma) \delta_\Gamma \tag{3.7}
\]

where \(\delta_\Gamma\) denotes a distribution concentrated on the interface. In general, \(\sigma\) is assumed constant along the interface and the gradient operator \(\nabla_\Gamma\), restricted to the surface, results in \(\nabla_\Gamma \sigma = 0\) and:

\[
f_\Gamma = \sigma \kappa \delta_\Gamma. \tag{3.8}
\]

In addition, capillary forces are only present on the nearly infinitely thin interface and are therefore singular. It results that a major complexity of modelling multiphase flows is the numerical handling of the phase boundary as an extension of capillary forces. This is why hydrodynamic breakup and atomisation studies, and more generally multiphase flows studies, challenge the development of highly resolved simulations where the gas-liquid interface has to be sharply captured.

Pringuey and Cant [10, 11] pursued the development of a new state-of-the-art multiphase flow modelling capability, RCLSfoam (Robust Conservative Level-Set), based in the OpenFOAM® environment to simulate the atomisation process during fuel injection in real engine combustion chambers. They developed a robust highly accurate numerical scheme for solving the Navier-Stokes equations in high-density ratio interfacial regions. In addition, an efficient level set method captures and transports the liquid-gas interface accurately while conserving mass.

FORMULATION OF THE CONSERVATIVE LEVEL-SET METHOD
The level set (LS) formulation, originally formulated in Osher and Sethian [14], is based on the transport of a continuous function \(\phi(x, t)\) in the computational domain, by the velocity field. The level set of the interface
is represented by \( \phi_{\Gamma} = 0 \) and \( \phi \) takes values below zero in one fluid and above zero in the other. The function \( \phi \) is generally taken as the signed distance function from the interface such that:

\[
|\nabla \phi| = 1. \tag{3.9}
\]

In the present numerical framework of Pringuey and Cant [11], the Conservative Level Set (CLS) method proposed by Olsson and Kreiss [15], based on an alternative definition of the level set function, is employed. Instead of transporting a signed distance function, the method transports a hyperbolic tangent function \( \psi(x, t) \) that can be initialised with the signed distance function as follows:

\[
\psi = \frac{1}{2} \left( \tanh \left( \frac{\phi}{2 \epsilon} \right) + 1 \right). \tag{3.10}
\]

The conservative level set \( \psi \) goes smoothly from 0 (in the gas phase) to 1 (in the liquid phase). It takes values between 0 and 1 in the transition region. The location of the interface is given by the level set \( \psi_{\Gamma} = 0.5 \). All the volume encompassed by that surface can be considered as filled with liquid. In this framework, the hyperbolic tangent function resembles a smeared out/smoothed liquid volume fraction. In (3.10), \( \epsilon \) is introduced by Olsson and Kreiss [15] as a control parameter over the thickness of the interface, which is kept constant once defined. Olsson and Kreiss [15] recommend to characterise \( \epsilon = \Delta x/2 \), where \( \Delta x \) is the mesh spacing.

The function \( \psi \) is first advected in a zero-divergence velocity field:

\[
\frac{\partial \psi}{\partial t} + \nabla \cdot (u \psi) = 0 \tag{3.11}
\]

in a conservative manner such that it remains conserved to machine accuracy. The above equation is solved with a high-order WENO numerical schemes. WENO schemes have the unique ability to preserve the required sharpness of the interface in front-propagating problems and to cope efficiently with the large gradients associated with jumps in material properties of several orders of magnitude, resulting from the presence of the phase boundary. The resulting method conserves mass to machine accuracy and its ability to capture the physics of the atomisation was demonstrated in Pringuey and Cant [11]. In addition, a n-halo parallelisation method has been implemented in OpenFOAM® to perform the computations at the expected order of accuracy. Finally, a droplet transfer algorithm is applied to allow for input conditions into a secondary breakup sub-model for combustion modelling purposes.

**Numerical Set Up and Flow Configuration**  
We investigate a geometrical variant to the modelled atomiser in Pringuey and Cant [11] with the intent to mimic the prefilming airblast atomiser in the experimental studies by Gepperth et al. [12, 2] and Bhayaraju and Hassa [13]. In this manner, numerical simulations can be calibrated and validated against experimental results.

In this design (Fig. 3.1), the fuel injector has, in order from radially inner to outer, a coaxial arrangement of an inner swirler air passage, an annular fuel passage, an annular outer swirler air passage. The fuel passage extends to a prefilming lip where the fuel is spread out in a thin continuous sheet of uniform thickness before being subjected to the atomising action of high-velocity air and being discharged at the atomising lip. At the exit of the atomiser,

Figure 3.2: Computational domain for the simulation of atomisation representing the 2-D geometrical abstraction of Fig. 3.1 and the experimental apparatus of Gepperth et al. [12, 2].
at the atomising lip, the two airflows merge with the fuel liquid sheet and convey the fuel spray stream into the combustion zone. In order to reduce the configuration complexity and enhance optical accessibility for measurements [12, 2, 13], the realistic annular airblast atomiser geometry is simplified into a 2-D abstraction representing a planar geometry for academic configurations.

The flow conditions chosen for this study are listed in Table 3.1 and 3.2. All test cases use room temperature material properties. Two sets of air and liquid parameters are used: air at atmospheric conditions together with Jet-A1 type fuel at atmospheric conditions; and air at elevated combustion chamber pressure at cruise altitude together with kerosene at elevated pressure.

Table 3.1: Operating conditions for the spray calculations at cruise altitude operating conditions used in Pringuey and Cant [11] with Jet-A1 type fuel. High-pressure combustion chamber at room temperature.

<table>
<thead>
<tr>
<th></th>
<th>Fuel</th>
<th>Gas</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density $\rho$</td>
<td>840.0 kgm$^{-3}$</td>
<td>20.0</td>
</tr>
<tr>
<td>Viscosity $\nu$</td>
<td>5.952 × $10^{-6}$ m$^2$s$^{-1}$</td>
<td>8.5 × $10^{-7}$</td>
</tr>
<tr>
<td>Liquid surface tension $\sigma$</td>
<td>0.0261 Nm$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>Mean inlet velocity $\bar{u}$</td>
<td>4.0 ms$^{-1}$</td>
<td>40.0</td>
</tr>
</tbody>
</table>

Table 3.2: Operating conditions for the spray calculations at operating sea level conditions from Gepperth et al. [12, 2] with Jet-A1 type fuel Shellsoll D100.

<table>
<thead>
<tr>
<th></th>
<th>Fuel</th>
<th>Gas</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density $\rho$</td>
<td>777.0 kgm$^{-3}$</td>
<td>1.21</td>
</tr>
<tr>
<td>Viscosity $\nu$</td>
<td>3.02 × $10^{-6}$ m$^2$s$^{-1}$</td>
<td>1.5 × $10^{-5}$</td>
</tr>
<tr>
<td>Liquid surface tension $\sigma$</td>
<td>0.0283 Nm$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>Mean inlet velocity $\bar{u}$</td>
<td>4.0, 12.5 ms$^{-1}$</td>
<td>40.0, 60.0</td>
</tr>
</tbody>
</table>

4 RESULTS SO FAR

We have performed a set of preliminary transient calculations of the free surface problem that represents the primary breakup of liquid fuel inside a modern aero-engine airblast fuel injector. The calculations picked up the growth of Kelvin-Helmholtz longitudinal instabilities along the phase interface, which are the result of the aerodynamic forces from the high speed co-flowing gas. When aerodynamic forces on the liquid core are significant, i.e. when the top gas-stream speed is large enough, they expand the liquid film against the contracting effect of surface tension, as predicted by the stability analysis theory and weakly non-linear theories.

In addition to longitudinal undulations, transverse instabilities appear, as observed in all experimental works [4, 12, 2, 13]. We also note the development of both spanwise and streamwise ligaments disintegrating into smaller liquid structures under aerodynamic tearing (Figure
4.1). It is clear from Figure 4.3 (middle) that the “cell-like” structures forming between the ligaments are the precursors of groups of ligaments elongated in the longitudinal direction, reaching for the injector edge. As ligaments start stretching away from the liquid core rim, in the streamwise direction, they pinch off into irregularly shaped liquid structures, shedding liquid blobs. Fragmentation of the ligaments starts along the streamwise direction when ligaments have been generated and elongated in the streamwise direction – under aerodynamics tearing due to the strong streamwise air velocity field – whereas ligaments seem to be mostly unstable due to capillary effects – Plateau-Rayleigh instability – and break apart in the transverse direction when first generated in the transverse direction, in accordance with experimental findings.

A parametric study revealed the influence of the shear stress on the development of surface instabilities by varying the operating conditions and the air velocity profile [16]. At high altitude cruise conditions the liquid film is subject to a higher shear than at sea level conditions, as there is an enhancement in the difference in viscosities between the two phases. This results in stronger topology changes and simultaneous atomisation events than at sea-level ambient conditions (Figure 4.1, top-right and Figure 4.3, left). At ambient conditions, the decrease in air density is synonymous with a stronger surface tension force, rendering the bulk liquid less conducive to atomisation. An increase in air velocity induces higher aerodynamic forces. Those forces act on the ligaments and cause them to be destabilised faster and thus lead to earlier fragmentation, compared to the previous computation.

The air velocity in the top channel was then given a parabolic profile, more representative of the air velocity profile in real injectors. The results are shown in Figure 4.1(bottom-right) and Figure 4.3(right). Significant change in the development of surface instabilities occurs. The direction of propagation of the surface wave crests is eventually reversed. The air velocity profile seems to not entrain the liquid film forward anymore, but rather drags it backwards. Linear stability properties have changed in this new flow configuration. The resulting shear forces (Figure 4.4) acting in the tangential direction to the interface affect the atomisation process, in which liquid blobs are now shed upstream.

5 Future work

We aim to make an informed qualitative and quantitative assessment of the topological variations of the phase interface through dynamical and statistical analysis; and investigating the whole domain of operating conditions both for sea-level experimental data and aero-engine injection conditions relevant to industry. The question remains as to whether the onset of shear-driven instabilities has any effect on the resulting spray at certain operating conditions, as the interaction of both velocity fields, and as a result, the shear stress, are believed to play a significant role in the atomisation process. Also, the impact on primary breakup (spray analysis) due to a varying inlet velocity profile of the fuel and air phases will be tested. In addition, our work intends to question the role and strength of turbulence in the early development of surface instabilities and the primary atomisation process as a whole. In particular, the authors are planning on mimicking the flow configuration of Gepperth et al. [2] and Bhayaraju and Hassa [13] to test and validate our numerical framework.
The fuel is not entrained downstream as fast as at high pressure. Instead of elongating and thinning downstream under aerodynamic forces, the bulk liquid grows in size as more fuel is fed in. The main role of a higher gas viscosity is to inhibit the development of instabilities in the liquid sheet and to delay the onset of atomisation. This delay causes atomisation to occur further downstream from the injection channel, which is not observable yet at the end of our simulation, at $t = 13\text{ms}$. Streamwise ligaments are able to grow bigger and the liquid bulk is more stabilised, for longer. This was also experimentally observed by [6].

**Figure 4.1**: Simulation of flat sheet breakup – Liquid phase iso-volumes and centerline velocity field. Top left – ($u_g = 40\text{m/s}, u_f = 4\text{m/s}$) cruise conditions at $t = 13\text{ms}$; top right – ($u_g = 40\text{m/s}, u_f = 4\text{m/s}$) ambient conditions at $t = 13\text{ms}$; bottom left – ($u_g = 60\text{m/s}, u_f = 12.5\text{m/s}$) ambient conditions at $t = 13\text{ms}$; bottom right – ($u_g = 40\text{m/s}, u_f = 4\text{m/s}$) cruise conditions at $t = 17.5\text{ms}$. 
Figure 4.2: Simulation of flat sheet breakup at flight conditions ($u_g = 40\text{m/s}$, $u_f = 4\text{m/s}$) and uniform air velocity profile – Time development of the interface location coloured by streamwise fuel speed. From left to right: $t = 4\text{ms}, 6.5\text{ms}, 13\text{ms}$. 
Figure 6. Simulation of flat sheet breakup with interFoam – Interface location coloured by streamwise fuel speed. From left to right: $u_g = 40\text{m/s}$, $u_f = 4\text{m/s}$ at ambient conditions at $t=13\text{ms}$; $u_g = 60\text{m/s}$, $u_f = 12.5\text{m/s}$ at ambient conditions at $t=13\text{ms}$; $u_g = 40\text{m/s}$, $u_f = 4\text{m/s}$ at cruise conditions and parabolic air velocity profile at $t = 17.5\text{ms}$.

Figure 7. Simulation of flat sheet breakup with interFoam at flight conditions ($u_g = 40\text{m/s}$, $u_f = 4\text{m/s}$): left – uniform air velocity profile; bottom at $t = 13\text{ms}$; right – parabolic air velocity profile at $t = 17.5\text{ms}$. Interface location coloured by shear stress $\sigma_{xy} = \frac{du_y}{dy}$.
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REFERENCES


