

Article

Understanding Sub and Supercritical Cryogenic Fluid Dynamics in Conditions Relevant to Novel Ultra Low Emission Engines

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Abstract: In this paper we provide insight into the thermophysical properties and the dynamics of cryogenic jets. The motivation of the work is to optimise the use of cryogenic fluids in novel ultra low emission engines. For demonstration, we use conditions relevant to an internal combustion engine currently being developed by Dolphin N2 and the University of Brighton, the CryoPower recuperated split cycle engine (RSCE). The principle of this engine is a split-cycle combustion concept which can use cryogenic injection in the compression cylinder to achieve isothermal compression and thus help maximise the efficiency of the engine. Combined experimental and numerical findings are presented and the effects of atomisation dynamics of the LN₂ are explored at both sub- and supercritical conditions in order to cover different pressure and temperature conditions representative of the engine compression cycle. For subcritical regimes, we observe that the appearance of the jet coincides with the predicted atomisation regimes based on the Weber, Ohnesorge and Reynolds numbers for other common fluids. For the modelling of supercritical jets, a new methodology within OpenFoam which accounts for Real Fluid Thermodynamics has been developed and the jet behaviour under various pressure and temperature conditions has been investigated. To our knowledge this is the first study where a cryogenic spray process evolution is examined for conditions relevant to the ones prevailing in a compression chamber accounting for both sub and supercritical conditions.

Keywords: cryogenic injection and mixing; liquid nitrogen (LN₂); advanced internal combustion engines; supercritical; real fluids thermodynamics

1. Introduction

Liquified gases such as liquid air, liquid nitrogen (LN₂) or liquified natural gas (LNG) can serve as cost-effective energy vectors within power production units as well as transport “fuels” with zero emissions. For example, energy coming from renewable resources can be used in order to “cool” air or nitrogen, down to the point that they become liquids. Follow up injection of these liquids to a higher temperature environment causes rapid re-gasification and large expansion in volume. This can either drive a turbine or piston engine even without combustion (see for example the Dearman engine [1]) or be used in novel ultra-low emission combustion systems in order to optimise the compression stroke and reduce emissions as in the case of the Cryopower split-cycle engine [2–4]. Most importantly, because of the low boiling point of cryogenic liquids, low-grade or ambient heat can be used as a heat source, which otherwise is wasted. A better understanding and control of the injection dynamics of the

cryogenic fluids could boost the efficiency of the systems where these fluids are used and contribute to the reduction of emissions.

Recently, there has been an increased interest towards cryogenic technologies, however most studies have explored the physics of liquefaction [5] and energy storage [6] rather than the dynamics of cryogenic jets under compressed conditions. In the past, most of the existing scientific knowledge in the field of cryogenic injection was built upon experimental observations relevant to space applications (see for example [7–10]). Until now, limited studies have been performed for the potential use of these fluids in transportation and novel combustion systems. Experimental work has been focused on system level [4,11], while the specifics of injection have not yet been fully investigated, mostly because of the complexity of optical access and diagnostics. In internal combustion (IC) engines the injection process of cryogenics has different characteristics from those found in propulsion systems for space applications examined in the past. For example currently, to the best of our knowledge, research relevant to the behaviour of cryogenic jets under a pressure range corresponding to the compression stroke does not exist.

Although further experiments are necessary to obtain a clearer understanding of the dynamics of cryogenic jets at conditions relevant to IC engines, observations from the existing experiments for space applications [7–10] can still be used to explain some of the fundamental dynamics of cryogenic jets. At subcritical conditions right up to the critical pressure, presence of droplets and ligaments was observed, although a regime categorisation based on non dimensional numbers to confirm the observations was not performed. At supercritical pressures, cryogenic jets were reported to behave as diffusing gas jets into ambient gas and no droplets or ligaments were observed above the critical pressure. The lack of droplets is primarily due to lack of surface tension at supercritical pressures. With increase in supercritical pressure, cryogenic jets diffuse faster. Figure 1 by Chehroudi [9] neatly summarises the appearance of cryogenic jets at various sub and supercritical pressures and is included here for reference. The experiments in the figure were performed at constant chamber pressure. The wide range of pressures from low subcritical to high supercritical is particularly interesting for our study because the pressure in an IC engine compression chamber is expected to vary from atmospheric to a maximum of 17 MPa in some cases [12].

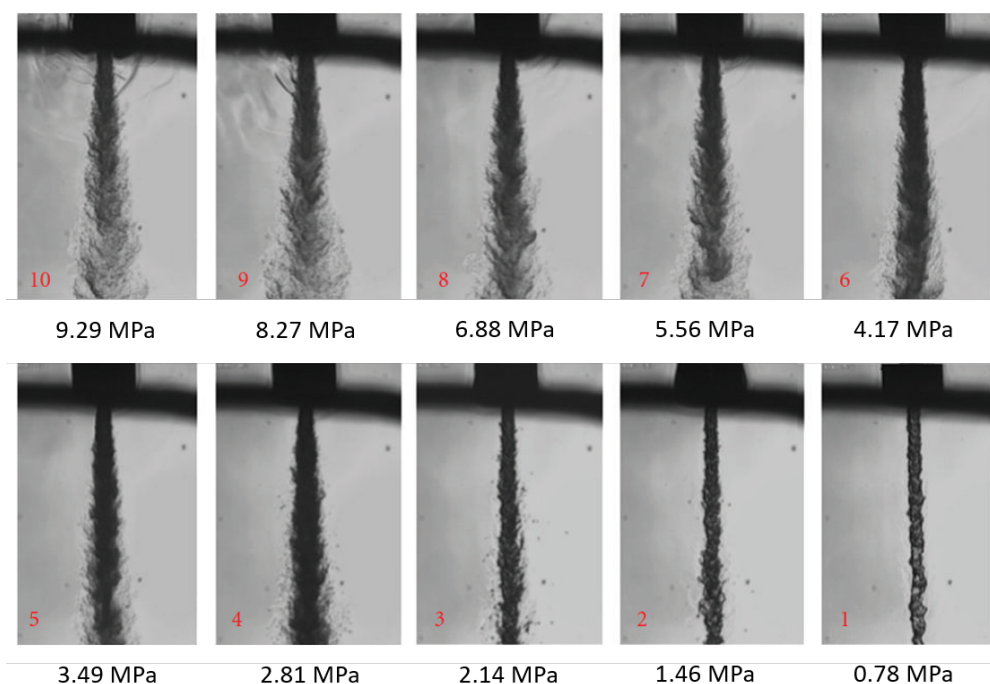


Figure 1. Injection of cryogenic nitrogen into gaseous nitrogen at various supercritical and subcritical pressures by Chehroudi [13].

Our paper aims to complement these previous studies by adding fundamental knowledge to the atomisation of liquefied gases, in order to significantly advance the technology required to efficiently control the “energy release” of cryogenic fluid injection in IC systems. We will focus on conditions relevant to the compression cycle of the Recuperated Split Cycle Engine (RSCE) currently under development by Dolphin N2 in collaboration with the University of Brighton (UoB) as a representative example of these systems. We chose this system as demonstrator since it has been partially developed in house and thus more complete information of its exact operating conditions are available. However, it should be pointed out that the main conclusions relevant to the fluid dynamics of these jets under various pressures resulting from the compression process are expected to hold for other systems based on similar operating principles.

The structure of the paper is as follows. We will initially present the basic principles of the RSCE focusing on linking the importance of the cryogenic injection dynamics in the compression chamber with the combustion dynamics and emissions in the combustion chamber (Section 2). Having defined the conditions prevailing in the compression chamber, we will then pick five indicative operating points (0.1, 3, 6, 10 and 17 MPa) corresponding to different injection timings during the compression and we will examine the cryogenic liquid thermodynamics behaviour in these conditions (Section 3). Two of the points correspond to injection conditions at subcritical conditions where droplets are formed and will be further investigated through experimental observations existent in the literature along with new ones from our in-house experiments (see Section 4.2). One of the novelty of this section is that for the first time we will present a categorisation of these jets according to the different break up regimes based on non-dimensional numbers. The other three operating points correspond to supercritical conditions which will be studied using computational fluid dynamics (CFD) (see Section 4.3). At the end the main conclusions will be presented. One important aspect of our work is that it includes both analysis of the thermophysical properties of the cryogenic fluid (LN_2) and its heat absorption potential decoupled from its dynamic characteristics as well as analysis of the mechanical forces acting on the cryogenic fluid when it is injected as a jet and how these forces affect the different phases. This is useful in order to quantify the combined effect of mechanics and thermodynamics in the evolution and disintegration of an entire cryogenic jet.

2. Working Principles of RSCE and the Importance of Cryogenic Injection

The working principles of RSCE, as well as how its efficiency is linked to cryogenic jet dynamics, is explained here with the support of a schematic diagram of RSCE in Figure 2. As it can be seen from this figure, ambient air is ingested and compressed in the compression chamber. Simultaneously during the compression, coolant (water or for better efficiency LN_2) is sprayed with the objective to make the compression process quasi-isothermal. This cool compressed air is then passed through a recuperator where some of the heat from the hot exhaust air is transferred. The compressed air which is now preheated is passed into the combustion chamber where fuel is injected. After the combustion process the exhaust gas is passed through the recuperator, so that some of the wasted heat is transferred back to the new pre-combustion air.

Using thermodynamic analysis, the efficiency of the RSCE is estimated to be over 55% and up to 60%, mainly due to the near-isothermal compression and the recuperation of wasted heat [11]. The additional work obtained from the RSCE can be understood by taking a look at the Figure 2 by Morgan [14] which represents the thermodynamic cycle of RSCE compared to a diesel engine. Past experiments with water to act as a coolant have achieved quasi-isothermal compression [15]. To achieve better isothermal compression and extract the maximum efficiency from an RSCE engine, cryogenic LN_2 was proposed to be used instead. LN_2 has been chosen as it is relatively inexpensive and abundant compared to other cryogenic fluids. A more detailed analysis of the suitability of LN_2 in terms of efficiency, availability and cost is presented by Jackson [15]. An additional advantage is that emissions can also be reduced through low temperature combustion (LTC), as the adiabatic flame temperature is reduced with the dilution of air with N_2 [2].

Further understanding as to how the LN_2 jet atomises in a compression cylinder is needed in order to control better the process of isothermal compression. When a cryogenic fluid is injected in an engine the penetration time of the jet into the cylinder is crucial. Introducing the cryogenic spray early on in the compression gives more time for atomisation and dispersion of the droplets and thus enhances mixing. However, most of the compression work (and hence heat generation) occurs at the end of the compression stroke. So if the cryogenic fluid is injected “too early”, the fluid will have already evaporated by the time a high heat transfer rate is most needed. On the other hand, since the density of the air increases during compression, droplets, which are injected late in the process, require more momentum to reach the centre of the cylinder and the process becomes less efficient.

An additional difficulty is that towards the end of the compression stroke the in-cylinder pressure is above the critical pressure of LN_2 and the injected fluid behaves as a supercritical liquid with reduced surface tension at the interface. There are no droplets and no boiling to take place. At these supercritical conditions, heat is absorbed over a range of temperatures which gradually transforms the fluid from liquid-like to gas-like. In contrast, at subcritical conditions the heat absorption is concentrated at the boiling point which transforms the fluid instantly from liquid to gas. Due to the inseparability of liquid and gas phase, and continuous change in the thermophysical properties of the cryogenic jet, the evolution of the cryogenic jet mimics the mixing of two fluids of similar phase and properties.

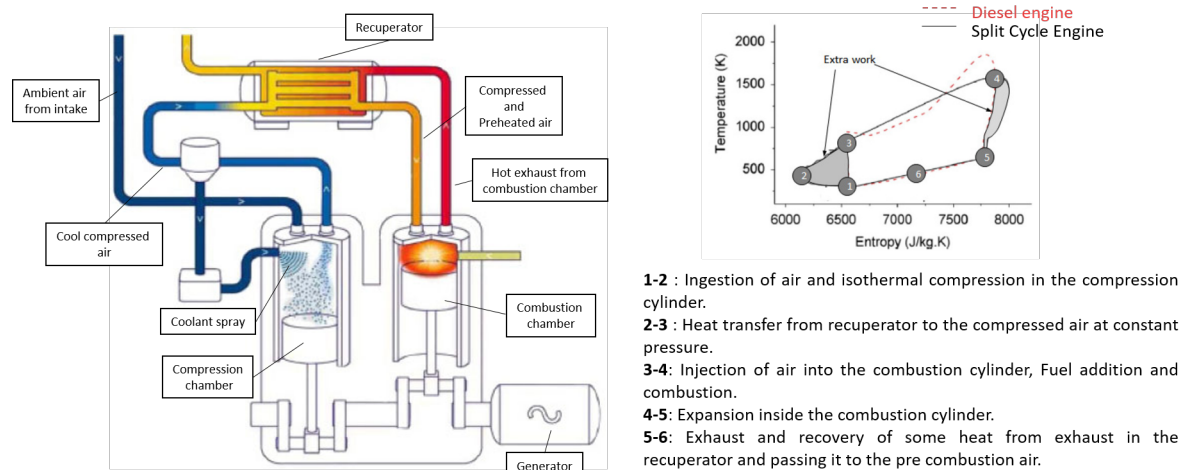


Figure 2. Schematic diagram of recuperated split cycle engine (RSCE) [16] (left) Temperature(T)–Entropy (S) diagram of the RSCE against that of a diesel engine by Morgan [14] (right).

3. Overview of the Thermophysical Properties of Cryogenic Fluids at Conditions Relevant to RSCE

The first step in understanding the behaviour of LN_2 jets is to understand LN_2 thermophysical properties in conditions relevant to RSCE compression. Thermophysical properties of N_2 at pressures from 0.1 MPa to 10 MPa from NIST are shown in Figure 3. This pressure range is relevant to the conditions in the compression chamber of RSCE where the compression chamber pressure starts right from the atmospheric pressure and increases up to a high pressure of 17 MPa. Beyond 10 MPa, the trend in the thermophysical properties with increase in pressure is similar to the trend in increasing supercritical pressures up to 10 MPa depicted in Figure 3. The curves of thermophysical properties against temperature become smoother.

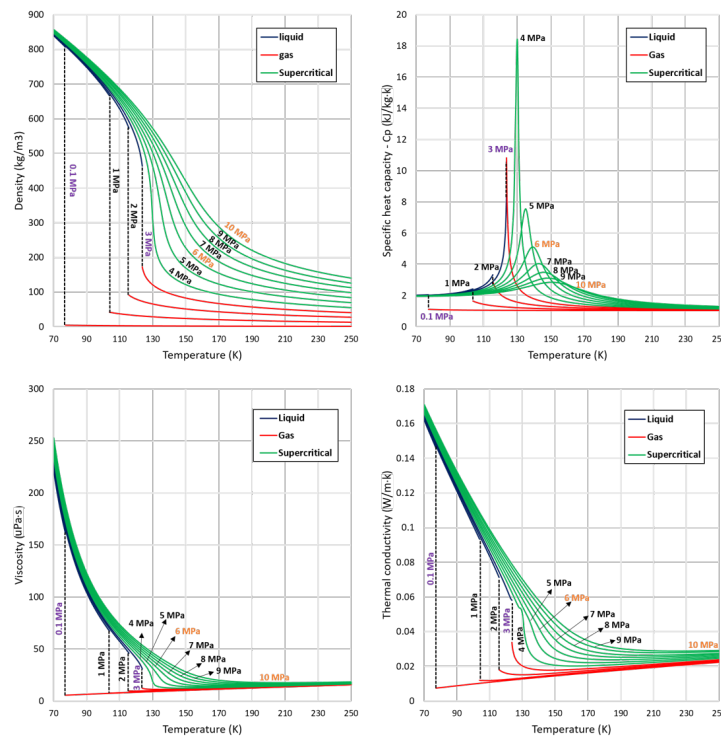


Figure 3. Plots of density (**top-left**), isobaric specific heat capacity (**top-right**), viscosity (**bottom-left**) and thermal conductivity (**bottom-right**) at pressures from 0.1 MPa to 10 MPa using NIST [17] data. The subcritical pressures at which the cryogenic jet has been analysed in this paper are shown with a purple label and the supercritical pressures at which the cryogenic jet has been simulated in this paper are shown with an orange label.

At atmospheric pressure (0.1 MPa), which can be considered as very low subcritical pressure, the LN₂ behaves as any other fluid which vaporises at the boiling point. Correspondingly, the thermodynamic and transport properties instantly change from that of the liquid phase to that of the gaseous phase. The same behaviour prevails at all pressures below the critical pressure of nitrogen (N₂), which is 3.39 MPa. At transcritical (but subcritical) pressure of 3 MPa, significant gradients in the thermophysical properties can be observed just before and after the boiling temperature. A significant rise in heat capacity can also be observed at temperatures just before and after the boiling temperature.

At supercritical pressures, boiling does not take place and hence there is no single boiling temperature for LN₂ at these pressures. The transition from liquid to gaseous phase occurs at a range of temperatures around what is known as the “pseudoboiling” temperature. Beyond the critical temperature, the pseudoboiling temperature for a particular supercritical pressure divides the supercritical fluid into liquid-like and gas-like phases. In a Pressure–Temperature (PT) diagram, the pseudoboiling temperature and the corresponding supercritical pressure always fall on the Widom line [18]. The thermophysical properties of LN₂ (except heat capacity) continuously transform from liquid to that of the gas around this pseudoboiling temperature. This transformation is rapid (but continuous) at supercritical pressures (4 and 5 MPa) near the critical pressure of 3.39 MPa. With increase in supercritical pressure this transformation becomes gradual (still continuous). The absence of the discontinuity which was seen earlier at subcritical pressures in the boiling temperature, denotes the inseparability of liquid and gas phase at supercritical pressures and temperatures. Unlike other thermophysical properties, the heat capacity at supercritical pressures shows a sudden rise as pseudoboiling temperature is approached with a peak exactly at the pseudoboiling temperature. This peak is maximum for the critical pressure and decreases as pressure is further increased.

3.1. Enthalpy and Heat Absorption

Since the main aim of using cryogenic fluids in the compression chamber is to keep the temperature of the working fluid (air) constant during the compression process, another important thermodynamic property to quantify the heat absorption process is enthalpy. From a design point of view it is important to understand at which pressure and temperature conditions the heat absorption potential of the cryogenic fluid is sufficient to absorb the heat generated due to compression and how the injection can be tuned to optimise the process.

The two well known types of heat absorption are latent heat and sensible heat absorption. Latent heat is also known as enthalpy of vaporisation (ΔH_{latent}), which is the enthalpy required to change the phase from liquid to gas at the boiling temperature and is quantified by the enthalpy difference between the liquid and gas phase ($\Delta H_{latent} = H_{gas} - H_{liq}$) at the boiling temperature. Sensible heat is the heat/enthalpy required to raise the temperature of the fluid and depends on the fluid's heat capacity. The sensible heat absorption ($\Delta H_{sensible}$) is quantified as ($\Delta H_{sensible} = C_p \Delta T$). While sensible heat absorption takes place at both subcritical and supercritical pressures, latent heat absorption exists only at the fluid's boiling temperature at subcritical pressures. Figure 4 shows the heat absorption mechanisms (latent heat, distributed latent heat and sensible heat) for cryogenic nitrogen as the temperature increases for a range of subcritical and supercritical pressures. The redistribution of latent heat as distributed latent heat can be understood from the continuous but non-linear rise in enthalpy at temperatures around the pseudo-boiling point for supercritical pressures. This non-linear rise in enthalpy includes both the sensible and the distributed latent heat, and hence is more rapid than sensible heat absorption alone. It should also be noted that at very high supercritical pressures the rise in enthalpy around the pseudoboiling temperature becomes linear again which means that the heat absorption due to distributed latent heat is negligible and sensible heat absorption is dominant.

In previous experiments on a split-cycle prototype, Proof of Concept (POC) isothermal compressor [19] and Engineering Demonstrator (ED) split cycle engine [20,21], water was used as a coolant and the maximum pressure in the compression chamber was less than the critical pressure of water [19,21], therefore the cooling was achieved without significant vaporisation taking place in the compression chamber. Thus, only sensible heat absorption was utilised which resulted in quasi-isothermal compression. To achieve a near-ideal isothermal compression, the heat generated due to compression should be absorbed more rapidly.

If cryogenic nitrogen is used as coolant instead and is injected into the compression chamber at subcritical pressures, it absorbs heat slowly and continuously in the form of sensible heat absorption up to the boiling temperature where it suddenly absorbs a large amount of heat as latent heat absorption and vaporises into gas. The gaseous phase of the injected coolant will then continue to absorb heat slowly as sensible heat absorption until its temperature reaches the chamber temperature. This might result in more cooling at some localised position corresponding to the point where the liquid phase reaches the boiling temperature and transitions to gas phase. Also, as most of the heat due to compression is produced at higher pressures corresponding to supercritical pressures, this abrupt cooling might be counter productive to achieve uniform cooling in the compression chamber. On the other hand, if the cryogenic nitrogen is injected into the compression chamber at supercritical pressures, the coolant absorbs heat slowly and continuously in the form of sensible heat at temperatures much lower and much higher than the pseudoboiling temperature. But at temperatures around the pseudoboiling temperature, the coolant absorbs heat continuously but much more rapidly than at other temperatures, due to the combined sensible and distributed latent heat absorption. This can be leveraged to achieve uniform cooling throughout the chamber. This will also be demonstrated by our numerical simulation in the following sections.

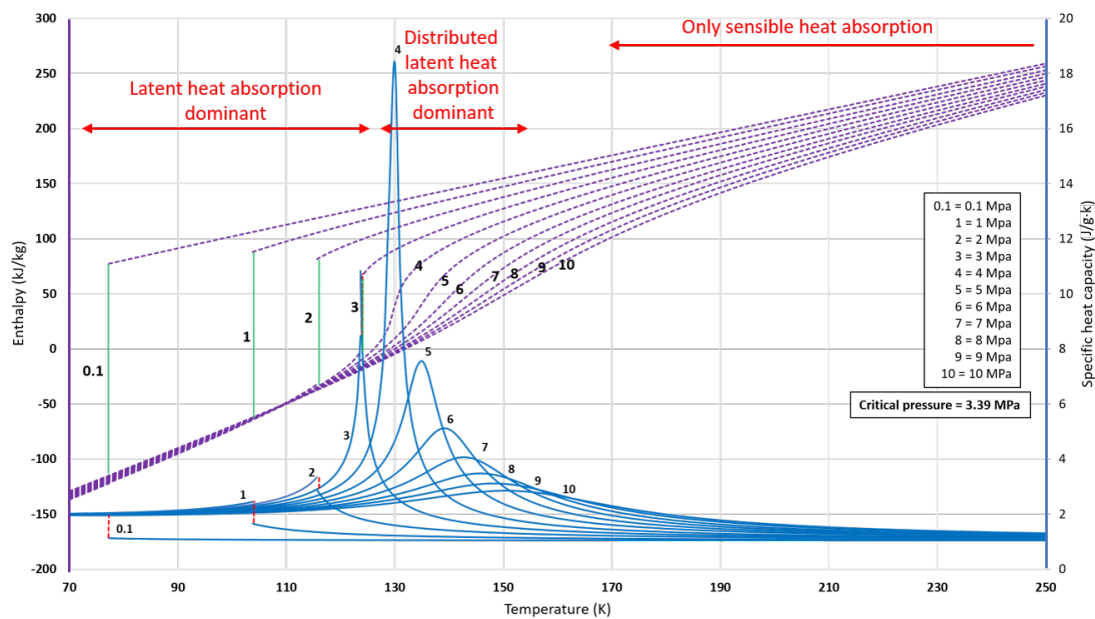


Figure 4. Enthalpy vs. temperature and isobaric heat capacity (C_p) vs. temperature of nitrogen from NIST [17] values for pressures 0.1 to 10 MPa.

3.2. Surface Tension

One important property relevant to atomisation dynamics of any fluid (including cryogenics) is the surface tension. The physics behind the surface tension are the same for any liquid. However, cryogenic liquids used at atmospheric temperature and any pressure conditions quickly reach low or zero surface tension as they rapidly transition into a gas or supercritical fluid. To our knowledge, the surface tension of cryogenic liquids has not been properly discussed in the literature. Surface tension predominantly arises from imbalance in the inter-molecular forces acting on an interface. It is strongly affected by temperature, whereas the influence of pressure is negligible as demonstrated by recent experiments on surface tension by Leonard [22]. The dependence of surface tension on temperature is linear as it can be seen in Figure 5 for nitrogen. With increasing temperature the surface tension reduces, ultimately reaching a value of zero at the critical temperature. Beyond this temperature surface tension no longer exists. Thus, cryogenic jets usually have a short potential core and outside of this core they present a gas-like behaviour, as we will see in the next sections.

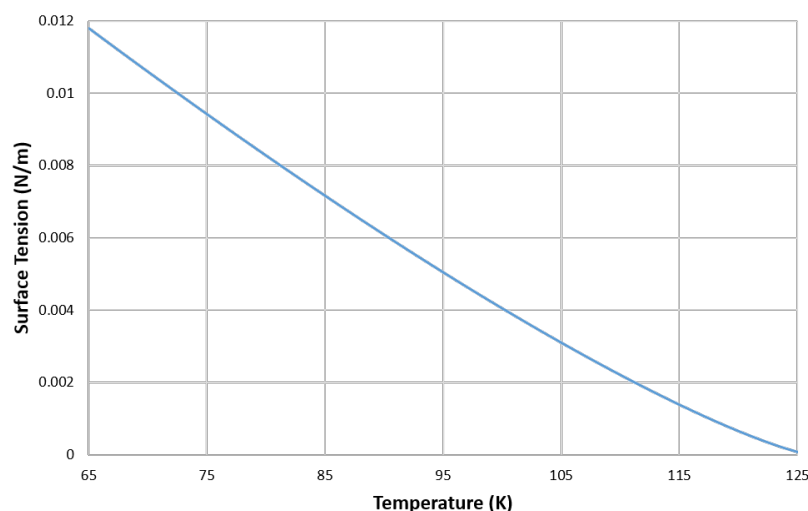


Figure 5. Surface tension plot of nitrogen against temperature from NIST [17].

4. Results and Discussion

4.1. Overview of the Dynamics of Cryogenic Jets

Following the description of the thermophysical properties of cryogenic fluids in the previous section, it is important to also understand how these properties link with the evolution of the cryogenic jet dynamics. In this section we look into the impact of various thermophysical properties on the transport of the different phases which exist in a cryogenic jet. At subcritical pressures, as mentioned at the introduction, there are experimental evidences that the cryogenic jet consists of a liquid phase which as the jet penetrates breaks up into droplets that vaporise upon reaching the boiling temperature, similar to other liquid jets. At supercritical pressures though, the cryogenic jets behave significantly different. Unlike other liquid or gas jets where the jet domain is comprised mostly of a single fluid phase, in a cryogenic jet that comes in contact with a hot supercritical environment, the fluid in the jet possesses properties corresponding to three different phases, namely liquid-like, transitional and gas-like. These phases can be classified based on their temperature with respect to the fluid's pseudo-boiling temperature, liquid-like ($T < T_{pb}$), transitional ($T \approx T_{pb}$) and gas-like ($T > T_{pb}$) as suggested by Banuti [23]. The existence of these separate phases is due to the fact that the fluid experiences the supercritical pressure almost immediately on entering the chamber, whereas it takes some time for the liquid to heat from liquid-like to gas-like via a transition phase. The time needed to heat up depends on the thermal conductivity and heat capacity of the fluid which in turn depend on the pressure and temperature experienced by the fluid. To illustrate the separation of the phases, we include some representative black illuminated images of cryogenic LN₂ jets injected into gaseous nitrogen at 300 K (see Figure 6) from Chehroudi's [24] experiment. A theoretical analysis of the mechanical forces and thermodynamics involved in each of these distinct phases is summarised in Table 1 and will be used to guide the jet description at sub and supercritical conditions in the next two sub-sections.

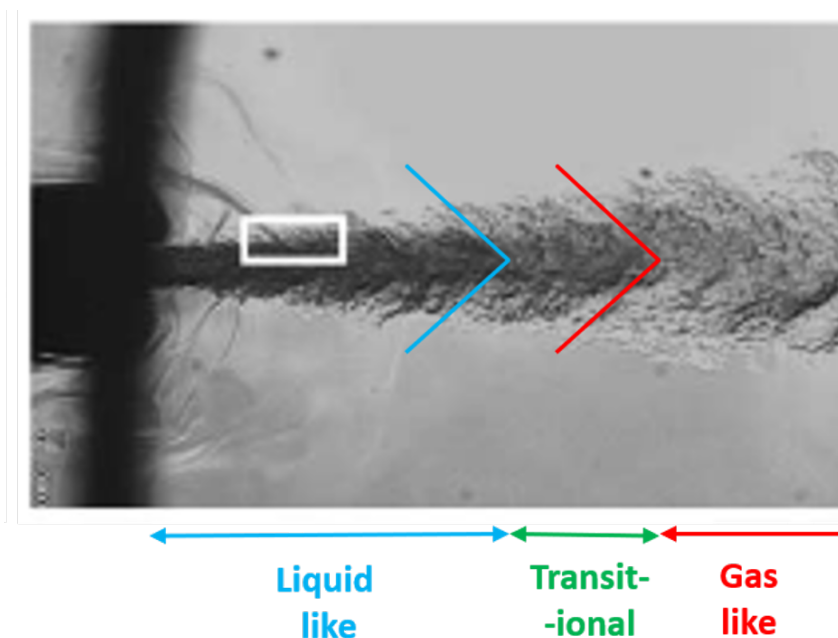


Figure 6. Visualisation of cryogenic N₂ injected into a chamber maintained at a supercritical pressure of 9 MPa and supercritical temperature of 298 K by Chehroudi [24]. The extent of the different phase domains is located approximately.

Table 1. Table of thermodynamic and mechanical forces and mechanism in action for various phases of fluid at supercritical pressures.

	Liquid-Like ($T < T_{pb}$)	Transitional ($T \approx T_{pb}$)	Gas-Like ($T > T_{pb}$)
Mechanical disintegration (Forces in action)	• Inertia • Viscous forces • Aerodynamic forces • Surface tension	• Inertia • Viscous forces • Aerodynamic forces	• Inertia • Viscous forces • Aerodynamic forces
Thermal disintegration (Thermodynamics in action)	• Heat transfer	• Heat transfer • Low molecular diffusion	• High molecular diffusion
Thermophysical properties involved	• Density • Heat capacity (thermodynamic) • Viscosity and Thermal conductivity (transport) • Surface tension	• Density • Heat capacity (thermodynamic) • Viscosity and Thermal conductivity (transport) • Diffusion coefficient	• Density • Viscosity and Thermal conductivity (transport) • Diffusion coefficient

4.2. Categorisation of Subcritical Cryogenic Jets Based on Breakup Regimes

In this section we focus on the dynamics of droplet formation at subcritical conditions. Existing experiments from the literature along with new preliminary in house data presented for the first time are included in order to provide a comprehensive categorisation of cryogenic jet break up dynamics. As demonstrated in Section 3 the cryogenic fluid properties under subcritical conditions are similar to that of other fluids. At these conditions the fluids possess surface tension and vaporise upon reaching the boiling point. The experiments by Mayer [7,8] and Chehrouzhi [9] have clearly shown the presence of droplets and ligaments, however no extensive research has been carried out to determine if the breakup regimes follow the same pattern as existing classification for other fluids. Here, in order to determine if the cryogenic jet appearance coincides with existing theory, the classification of primary atomisation regime of cryogenic jets is presented.

The dynamics of the cryogenic liquid jet breakup at subcritical pressures are dictated primarily by the interaction between the mechanical forces, surface tension, viscosity, aerodynamic forces and inertia. This is the reason the Weber number, Reynolds number and Ohnesorge number are used here to compare the dominant forces dictating the breakup and thus predict the breakup regime. The NIST [17] online database was initially used to accurately estimate the thermophysical properties corresponding to injection conditions. These thermophysical properties were then used to calculate the corresponding dimensionless Weber, Reynolds and Ohnesorge numbers.

- The Weber number is used to measure the relative dominance of inertia over surface tension and is calculated as:

$$We = \frac{\rho u^2 l}{\sigma} \quad (1)$$

where ρ is the density of the fluid, u is the velocity of the fluid, l is the characteristic length and σ is the surface tension.

- The Reynolds number quantifies the ratio of inertial forces to viscous forces and is calculated as:

$$Re = \frac{\rho u l}{\mu} \quad (2)$$

where μ is the viscosity of the fluid.

- The Ohnesorge number which derives from the Weber number and the Reynolds number is used to relate the viscous forces to inertial and surface tension forces. Ohnesorge number is calculated as:

$$Oh = \frac{\sqrt{We}}{Re} \quad (3)$$

Figure 7 presents the predicted primary breakup regime based on the above numbers for subcritical Mayer's experiments [7] and new in-house UoB's cryogenic experiments at atmospheric pressure. It can be seen that the appearance of the cryogenic jets for all the experimental cases corresponds well with the expected primary atomisation regimes (following the description of Liu [25]) that are predicted by the We, Re and Oh numbers. More specifically, the regimes identified are:

- Rayleigh regime: In the Rayleigh regime, surface tension induced instabilities are the primary reason for the liquid jet breakup. The diameter of the droplets produced during the primary breakup in the Rayleigh regime is equal to the jet and plain orifice injector diameter.
- First wind induced regime: In the first wind induced regime both surface tension and aerodynamic forces play a significant role in the liquid jet breakup. The diameter of the droplets produced during the primary breakup in this regime are smaller than the jet and plain orifice injector diameter.
- Second wind induced regime: In the second wind induced regime, the role of surface tension in the breakup reduces significantly and is predominantly influenced by the aerodynamic forces. The diameter of droplets produced during the primary breakup in this regime are also smaller than the jet and the plain orifice injector diameter.
- Atomisation regime: In the atomisation regime the small irregularities induced by several factors such as turbulence, cavitation, etc. grow rapidly leading to catastrophic breakup into droplets and ligaments. The diameter of the droplets produced during the breakup in the atomisation regime are much much smaller than the jet and plain orifice injector diameter.

In all the above four regimes viscosity has a damping effect on the developing instabilities which lead to breakup.

The categorisation provided in Figure 7 can be considered as an evidence that the existing jet breakup and droplet formation theories can be applied to subcritical cryogenic jets as well. In terms of modelling, this categorisation also implies that there is no need for developing new models and conventional models such as the well tested Eulerian–Lagrangian approaches used in other IC related studies can be used [26].

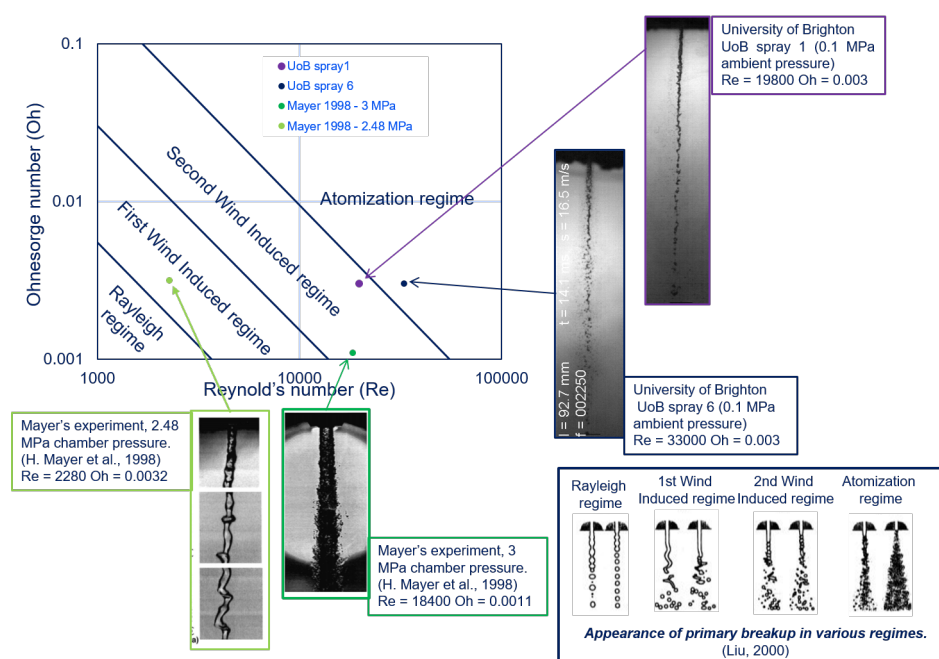


Figure 7. Primary atomisation regime classification of subcritical cryogenic jets from Mayer's experiments [7] and in-house University of Brighton experiments. The appearance of primary fluid jet breakup at various breakup regimes by Liu [25] is also depicted at the bottom-right.

4.3. Numerical Simulations of Cryogenic LN₂ at Supercritical Conditions

In this section we suggest an one-fluid modelling framework within OpenFoam based on a novel approach of specifying the thermophysical properties as polynomials. This framework will be used to extract conclusions for cryogenic jet behaviour during injection at high pressure that promote the supercritical behaviour. We use the geometry from the Mayer experiments [8] and we will present six simulations (see Table 2) for conditions relevant to the RSCE. The temperatures of the injected nitrogen are 120 K and 135 K. At 120 K nitrogen is a liquid below the pseudoboiling temperature, whereas at 135 K nitrogen is supercritical and much closer to the pseudoboiling point. As a consequence, the cold nitrogen is injected either as a liquid or in a supercritical state, while the nitrogen in the chamber is always supercritical. Regardless of pressure, the temperature of 120 K will always correspond to liquid state and the temperature of 135 K will correspond to supercritical state. The analysis will allow us to provide insight into the effect of the injection temperature and chamber pressure on the cryogenic jet dynamics.

Table 2. Table of cases of LN₂ injection at 2 m/s through a 2.2 mm diameter orifice into a chamber filled with gaseous N₂ for simulating various compression chamber conditions.

Case	Simulation	Injection Temp (K)	Chamber Pressure (MPa)	Chamber Temp (K)
1	RSCE T _{inj} = 120 (chamber-Low)	120	6	300
2	RSCE T _{inj} = 135 (chamber-Low)	135	6	300
3	RSCE T _{inj} = 120 (chamber-Intermediate)	120	10	300
4	RSCE T _{inj} = 135 (chamber-Intermediate)	135	10	300
5	RSCE T _{inj} = 120 (chamber-Max)	120	17	300
6	RSCE T _{inj} = 135 (chamber-Max)	135	17	300

4.3.1. Thermophysical Model Setup

As highlighted by Section 3, for numerical simulations to be accurate there is a need for an accurate thermophysical model that predicts the rapid changes in the fluid specific heat capacity, density, viscosity, thermal conductivity and enthalpy near the critical point and the pseudo boiling point in order to lead to accurate prediction of the heat absorbed by the LN₂. Real fluid Equations of State (EOS) have been used in previous studies (Soave–Redlich–Kwong (SRK), Peng–Robinson (PR), Benedict–Webb–Rubin (BWR) and modified BWR (MBWR)) [27–29]. In our previous work [30] we have analysed in detail the behaviour of these equations of state for conditions relevant to RSCE. Our analysis of cubic EOS'es SRK and PR for N₂ resulted in the observation that SRK is more suitable for our simulations as it estimates the density, thermodynamic properties and transport properties (using Chung's model) with better accuracy for a broad temperature range. On the other hand, PR is slightly more accurate around the pseudoboiling point for supercritical pressures, however it deviates significantly for temperatures lower than the pseudoboiling point.

In this work we use an alternative novel approach of specifying the thermophysical properties from polynomials. Since polynomials are fast to compute and easy to implement, the NIST data [17] were fitted with polynomials of various degree for a temperature range of 70 K to 400 K. The NIST database is based on a model by Span et al. [31]. The polynomial fitting for all the cases is presented in Figure 8 and compared against NIST. For all the cases, the polynomial fits of density, viscosity and

thermal conductivity were equal or more accurate than PR or SRK predictions. Due to the large gradient in isobaric heat capacity at 6 MPa, the polynomial fit was not able to capture the NIST data as accurately as for other thermophysical properties. The accuracy of the polynomial fit functions in estimating the heat capacity increases with increase in pressure. This can be seen in the Figure 8, at the highest supercritical pressure (17 MPa) simulated. No noticeable difference between heat capacity (C_p) estimates of NIST and polynomial fit can be observed.

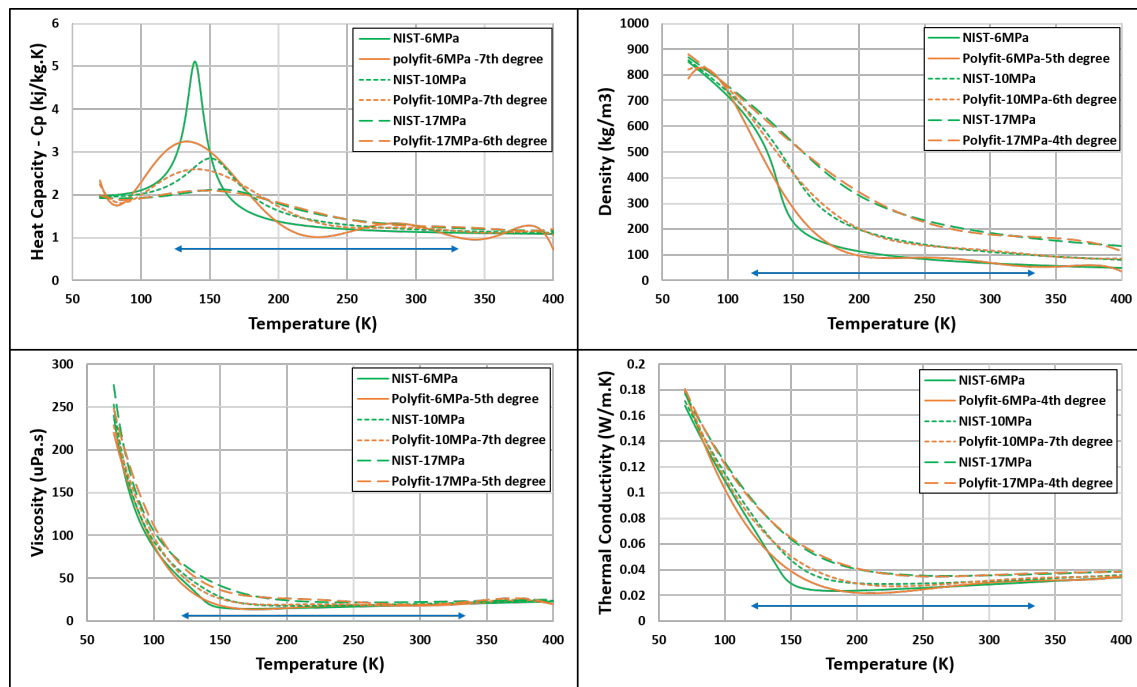


Figure 8. Plots of polynomial functions of thermophysical property (heat capacity, **top-left**; density **top-right**; viscosity, **bottom-left**; thermal conductivity, **bottom-right**) obtained from polynomial fitting of NIST data, against temperature. The range of temperatures encountered in the simulation is within the double arrow headed blue line.

4.3.2. Solver

Since there are no droplets observed at supercritical pressures the existing primary and secondary breakup models within the Eulerian–Lagrangian frameworks commonly used for engine simulations cannot be used. These breakup models estimate the resulting droplet parameters from existing droplet or injection parameters based on the We , Re and/or Oh numbers. At supercritical conditions though, due to zero surface tension the We number and Oh number tend to infinity resulting in the failure of these breakup models. Thus, it is more suitable to use Euler–Euler simulations to predict the evolution of the injected LN_2 . We use as basis a compressible approach within OpenFoam [32] and modifications have been made to account for real fluid thermodynamic properties. We use a Volume of Fluid (VoF) inspired method where the governing equations are solved for a single effective fluid. The two constituent fluids (LN_2 and N_2) are treated as one fluid, and their properties are calculated as averages of the individual fluids which are weighted by local volume fraction. The volume fraction of the fluids are represented as α and $1 - \alpha$. In previous VoF approaches α represented the volume fraction of fluid 1 ($\alpha = \alpha_1$), $1 - \alpha$ represented the volume fraction of fluid 2 ($1 - \alpha = \alpha_2$) and an interface between these two fluids was numerically reconstructed. In our case since surface tension for most of the jet is negligible, α can be considered as representative of the volume fraction of the N_2 in the domain resulting from LN_2 transitioning to supercritical state and becoming gaseous (fluid 1). The remaining ($1 - \alpha = \alpha_2$) represents the N_2 that preexisted in the chamber (fluid 2).

The properties of the single effective fluid are calculated as a weighted mean of each constituent property:

- Density:

$$\rho = \rho_1\alpha + \rho_2(1 - \alpha) \quad (4)$$

- Viscosity:

$$\mu = \mu_1\alpha + \mu_2(1 - \alpha) \quad (5)$$

- Velocity:

$$\mathbf{U} = \mathbf{U}_1\alpha + \mathbf{U}_2(1 - \alpha) \quad (6)$$

where 1 and 2 refers to the two constituent fluids respectively.

The governing equations solved by the solver for the single effective fluid are

- Continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0 \quad (7)$$

- Momentum equation:

$$\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \cdot (\rho \mathbf{U} \mathbf{U}) - \nabla \cdot (\mu \nabla \mathbf{U}) = \sigma k_c \nabla \alpha - \mathbf{g} \cdot \mathbf{x} \nabla \rho - \nabla p_d \quad (8)$$

where σ is the surface tension coefficient specified by the user (in our case is set to zero since the LN_2 will quickly vaporise), k_c is the curvature of the interface between fluids calculated by the solver as $k_c = \nabla \cdot (\nabla \alpha / |\nabla \alpha|)$, p_d is the dynamic pressure calculated as $p_d = p - \rho \mathbf{g} \cdot \mathbf{x}$, where $\mathbf{g}$ is the gravity and $\mathbf{x}$ is the position vector.

- Temperature equation (energy):

$$\frac{\partial \rho T}{\partial t} + \nabla \cdot (\rho \mathbf{U} T) - \nabla \cdot (\mu \nabla T) = - \left(\frac{\partial \rho K}{\partial t} + \nabla \cdot (\rho \mathbf{U} K) + \nabla \cdot (\mathbf{U} p) \right) \left(\frac{\alpha}{C_{v,1}} + \frac{1 - \alpha}{C_{v,2}} \right) \quad (9)$$

where T is the temperature, K is the kinetic energy calculated by the solver as $K = (|\mathbf{U}|^2/2)$, $C_{v,1}$ and $C_{v,2}$ are the specific heat capacity at constant volume for fluid 1 and fluid 2 respectively.

- VoF equation:

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\mathbf{U} \alpha) + \nabla \cdot [\mathbf{U}_c \alpha (1 - \alpha)] = 0 \quad (10)$$

where $\nabla \cdot [\mathbf{U}_c \alpha (1 - \alpha)]$ is a compression term commonly introduced to achieve a sharper interface where $\mathbf{U}_c$ is the artificial compression velocity. Since we do not require compression of the interface due to the expected diffusive nature of cryogenic jet at supercritical pressures, the $\mathbf{U}_c$ is set to zero. Thus, the VoF equation effectively solved by the solver is simplified to

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\mathbf{U} \alpha) = 0 \quad (11)$$

The isobaric thermophysical properties of each of these fluids are calculated by polynomials (described in Section 4.3.1) where temperature is the input.

4.3.3. Computational Domain

Two meshes mesh 1 and mesh 2 are used in this simulation. The 3D computational domain of mesh 1 consists of a cylindrical chamber of 500 mm length (half the length of the full chamber) and

122 mm diameter, along with a cylindrical injector of length 90 mm and 2.2 mm diameter (Figure 9). The 3D computational domain of mesh 2 consists of the full chamber of the Mayer experiment of 1000 mm length and 122 mm diameter, along with a patch inlet instead of a full injector (Figure 10). Mesh 1 is used to get a fully developed velocity profile for injection at the inlet in mesh 2.

Both mesh 1 and mesh 2 are axi-symmetric. The injector in mesh 1 is discretised uniformly in the axial direction and graded in the radial direction, as presented in Figure 11. The chamber in both mesh 1 and mesh 2 are discretised such that the mesh is finer near the axis in the radial direction and near the injector in the axial direction. A cut section of mesh 2 is presented in Figure 12 to display this chamber discretisation. The radial discretisation of the inlet plane of mesh 2 is the same as that of the injector in mesh 1. The minimum and maximum cell volume in mesh 1 are $1.861 \times 10^{-12} \text{ m}^3$ and $9.611 \times 10^{-8} \text{ m}^3$ respectively, whereas the minimum and maximum cell volume in mesh 2 is $1.995 \times 10^{-1} \text{ m}^3$ and $2.606 \times 10^{-7} \text{ m}^3$ respectively. Regarding the time step size, an adaptive time step was used which is based on a maximum Courant number of 0.5.

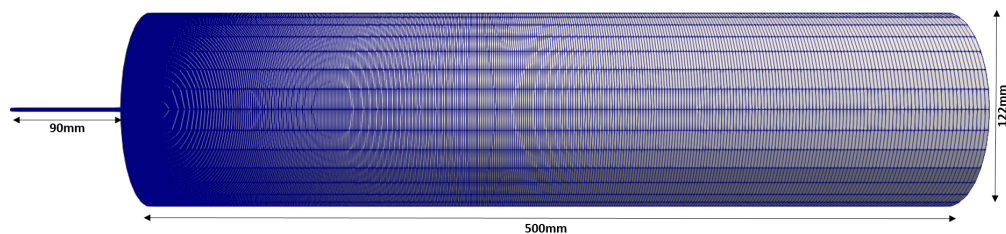


Figure 9. Dimensions of the computational domain of mesh 1 consisting of the injector and half-length chamber.

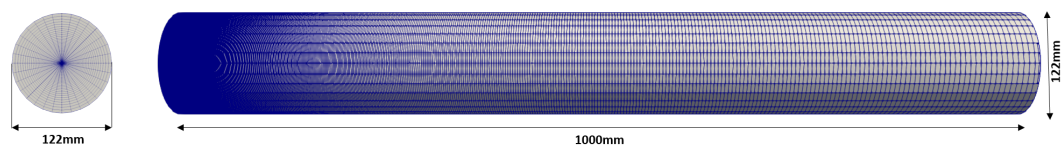


Figure 10. Dimension of the computational domain of mesh 2 consisting of the chamber alone.

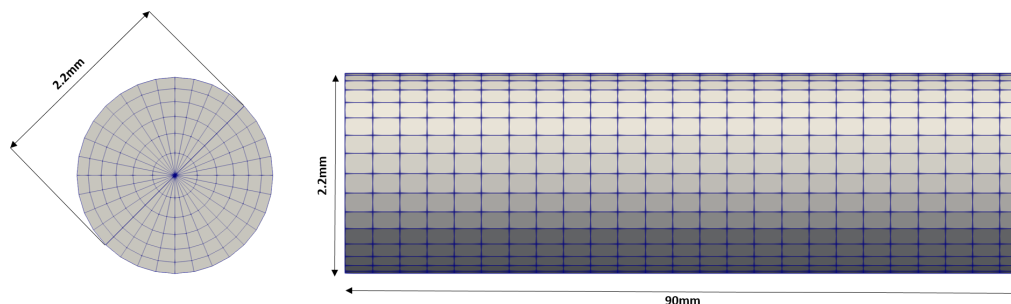


Figure 11. Discretisation of the injector in mesh 1. Please note that the figure only represents a small portion of the injector in the axial direction.

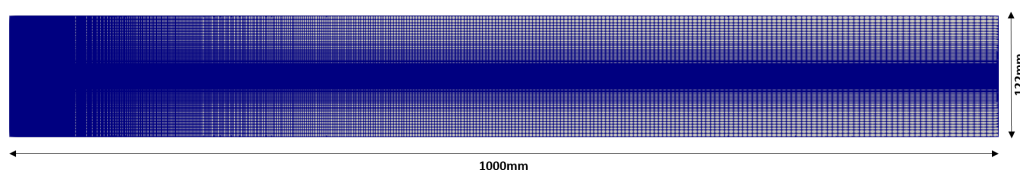


Figure 12. Section along the axis of mesh 2 showing mesh discretisation along the axis and near the inlet.

4.3.4. Boundary Conditions

The boundary conditions implemented in mesh 1 are given in Figure 13 and the boundary conditions implemented in mesh 2 are given in Figure 14. In both meshes the chamber is closed and Dirichlet boundary condition (isothermal and no-slip) is implemented at the walls. Though the heat transfer in the injector is expected to play a significant role in the evolution of a cryogenic jet, lack of available data quantifying this effect forces us to use isothermal walls. For all cases, the simulation is run for $t = 0.25$ s from injection (at the start of the injector) on mesh1 and the fully developed velocity profile at the end of the injector is extracted from mesh 1 simulation and utilised at the inlet of mesh 2 with 5% turbulent intensity (TI). Then the simulation is run for $t = 1$ s with mesh 2 to simulate the jet evolution.

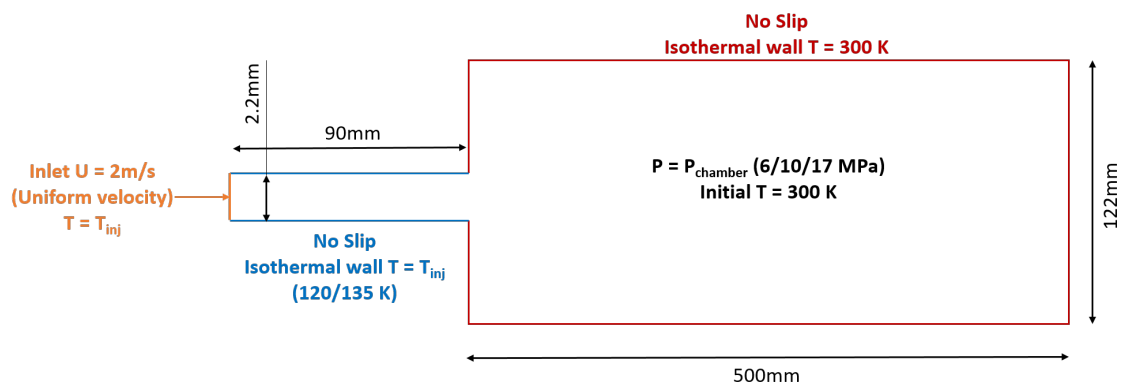


Figure 13. Boundary conditions implemented in mesh 1 to obtain a fully developed velocity profile at the end of the injector.

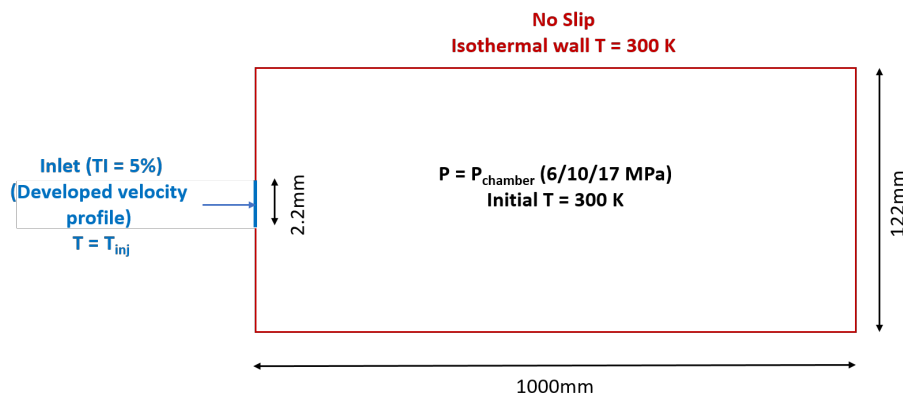


Figure 14. Boundary conditions implemented in mesh 2.

4.3.5. Turbulence Model

The Taylor and Kolmogorov length scale analysis based on the injection and chamber conditions for each of the cases is presented in Table 3. Density and viscosity are obtained from NIST [17] corresponding to the temperature and pressure experienced by the fluid. Comparing these length scales with the mesh scale in Table 4, it can be seen that the maximum cell volume is fine enough to capture the Taylor scale, and the minimum cell volume is of the order of the Kolmogorov scale. Since the mesh scale corresponding to the maximum cell volume are encountered only out of the simulation's domain of analysis, the mesh scale in the simulation's domain of interest is fine enough to capture Kolmogorov scales. Thus, no turbulence model was utilised.

Table 3. Table of turbulence length scales associated with all the cases in Table 2.

Case	Temperature (K)	Pressure (MPa)	Velocity (m/s)	Diameter (m)	Density (kg/m ³)	Viscosity (Pa·s)	Reynolds No	Taylor Scale (m)	Kolmogorov Scale (m)
1	120	6	2	2×10^{-3}	595.14	50.058×10^6	5.23×10^4	1.383×10^{-2}	2.892×10^{-4}
2	135	6	2	2×10^{-3}	430.05	28.132×10^6	6.73×10^4	1.219×10^{-2}	2.393×10^{-4}
1 and 2	300	6	2	2×10^{-3}	68.075	18.897×10^6	1.58×10^4	2.516×10^{-2}	7.096×10^{-4}
3	120	10	2	2×10^{-3}	632.90	58.104×10^6	4.79×10^4	1.445×10^{-2}	3.089×10^{-4}
4	135	10	2	2×10^{-3}	537.19	40.731×10^6	5.80×10^4	1.313×10^{-2}	2.676×10^{-4}
3 and 4	300	10	2	2×10^{-3}	111.73	19.920×10^6	2.47×10^4	2.012×10^{-2}	5.076×10^{-4}
5	120	17	2	2×10^{-3}	674.35	68.924×10^6	4.30×10^4	1.525×10^{-2}	3.349×10^{-4}
6	135	17	2	2×10^{-3}	606.74	52.561×10^6	5.08×10^4	1.403×10^{-2}	2.955×10^{-4}
5 and 6	300	17	2	2×10^{-3}	184.11	21.957×10^6	3.69×10^4	1.646×10^{-2}	3.756×10^{-4}

Table 4. Mesh scale analysis of mesh 1 and mesh 2.

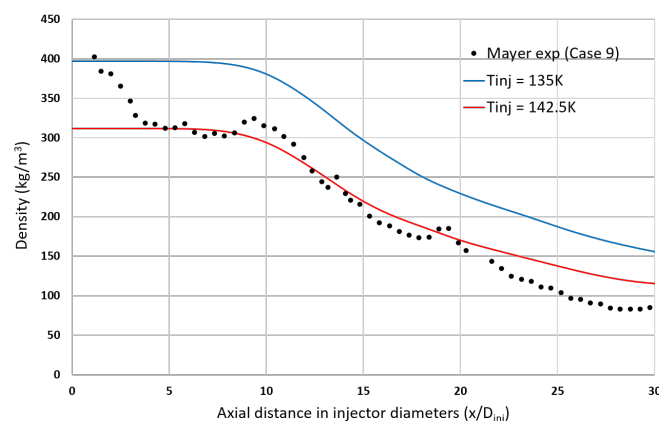
Mesh	Min Cell Vol (m ³)	Max Cell Vol (m ³)	$\sqrt[3]{(Min\ Cell\ Vol)}$ (m)	$\sqrt[3]{Max\ Cell\ Vol}$ (m)
Mesh 1	1.861×10^{-12}	9.611×10^{-8}	1.230×10^{-4}	4.581×10^{-3}
Mesh 2	1.953×10^{-12}	2.606×10^{-7}	1.250×10^{-4}	6.388×10^{-3}

4.3.6. Solver Validation

The solver was validated against the Mayer’s experimental “case 9” where liquid nitrogen is injected at 2 m/s into a pressurised (5.85 MPa) chamber filled with gaseous nitrogen. The details of the case are given in Table 5. A 2D computational domain of the injector and chamber with the same level of discretisation and boundary conditions as in Sections 4.3.3 and 4.3.4 was utilised. The jet is allowed to develop for 0.25 s in the 2D mesh 2 and then time averaged for a duration of 0.5 s to compare against Mayer’s experimental values. Though the injection temperature is reported to be in the experiments as 135 K in this case, Muller [33] suggested that the injection temperature could be higher than the measured one due to heat transfer in the injector. Following this, we perform two sets of simulations with varying inlet temperatures (135 K and 142.5 K). Comparison with experimental data for the axial density (see Figure 15) shows a very agreement for $x/d = 5$ and further downstream for 142.5 K. The accurate prediction of the density transition from liquid like to gas-like confirms that the code is capable of reproducing accurately the phase change processes taking place. Small discrepancies before the $x/d = 5$ are attributed to the uncertainties of the measurements of the injection temperature.

Table 5. Table of injection and chamber conditions associated with Mayer’s case 9 [8].

Experiment	Injection			Chamber		
	Fluid	Velocity (m/s)	Temp (K)	Fluid	Pressure (MPa)	Temp (K)
Mayer case 9 [8]	N ₂	2	135	N ₂	5.85	298

**Figure 15.** Comparison of solver results with two injection temperatures ($T_{inj} = 135$ K and $T_{inj} = 142.5$ K) against Mayer’s experimental [8] axial density measurements for case 9.

4.3.7. RSCE Chamber Simulation Results

The temperature distribution in the chamber at 1 s from the start of injection for all the cases of Table 2 is presented in Figure 16. The injection here represents the fluid leaving the injector and entering into the chamber while the different pressure and temperature chamber conditions represent the conditions that would occur in the compression chamber of RSCE engine at different piston positions.

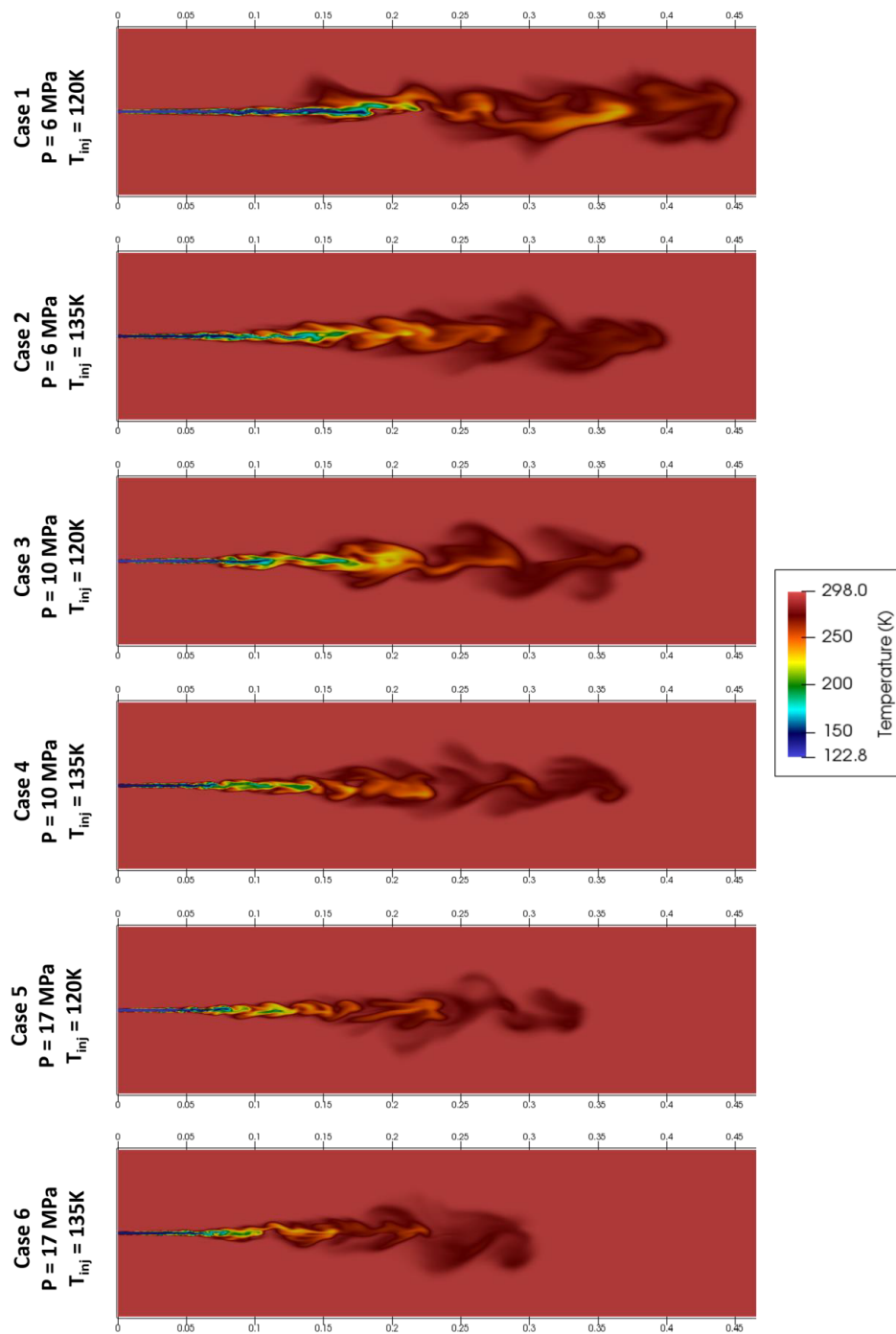


Figure 16. Temperature distribution for all the cases at cut section plane passing through the axis of cylindrical mesh (chamber) at $t = 1$ s from injection.

For a chamber pressure of 6 MPa, the injection temperature of the LN₂ for case 1 (120 K) is significantly lower than the pseudoboiling point (140 K) for the same pressure. This results in the colder core (dark blue) of the jet injected at 120 K penetrating farther (almost twice as far) into the chamber than the jet injected at 135 K (case 2, closer to the pseudoboiling point), as the fluid needs to overcome the significant rise in heat capacity which peaks at the pseudo-boiling point. Also due to the drastic increase in heat capacity, the outer fluid absorbs a significant amount of heat and keeps the inner core protected from heat transfer. This in turn also results in the injected fluid penetrating deeper into the chamber, which corresponds to a more rapid cooling than the 135 K injection. As the pressure increases to 10 MPa, the heat capacity peaks diminish which results in a reduction in the difference between the colder core lengths of injection at 120 K and 135 K. At 17 MPa there is not much difference in the heat capacity values of nitrogen for 120 K and 135 K. The very small difference in the colder core is due to the difference in injection temperature alone, unlike the cases of the lower supercritical pressures where the difference is also due to the heat capacity spike experienced by the fluid as it heats up after injection in Case 1.

A complementary analysis in terms of heat absorption by the cryogenic fluid in the compression chamber is presented based on the enthalpy of the fluid. Figure 17 presents the difference between the instantaneous enthalpy of the cryogenic nitrogen in the jet at $t = 1$ s from the start of injection and the enthalpy of the nitrogen at the chamber temperature and pressure corresponding to the case. This difference in enthalpy (ΔH) is used in order to visualise the distribution of the heat absorption potential of a cryogenic jet at various pressures, in line with the explanation given in Section 3.1. The isosurface of $\Delta H = 250$ kJ/kg for case 1 and 2 at 6 MPa approximately encloses the LN₂ which has the potential to absorb heat through distributed latent heat in addition to the sensible heat. For cases 3 to 6 the distributed latent heat disappears and there is only sensible heat for the entire temperature range as already explained in the Section 3.1. For all three pressure conditions the advantage of injecting the cryogenic nitrogen at a lower temperature (120 K) is clearly visible as the fluid with available enthalpy difference penetrates further into the chamber and occupies more volume than injecting it at a higher temperature (135 K). This is only due to the injected nitrogen starting at a lower enthalpy at lower temperatures. But interestingly when injecting at a lower temperature and lower supercritical pressure, there is a significant enhancement in the heat absorption potential of the cryogenic fluid, when compared to injecting at a lower temperature and higher supercritical pressures. This can be observed by comparing injections at 6 MPa with injections at higher supercritical pressures in Figure 17. The fluid with available enthalpy difference for the 120 K injection at 6 MPa penetrates almost 50% longer and occupies more volume than the 135 K injection.

Overall, injecting the fluid at temperatures well below the pseudoboiling temperature at low supercritical pressures provides the best performance in terms of deeper penetration and greater heat absorption (due to the distributed latent heat), while also avoiding a large instantaneous heat absorption which exists at subcritical temperatures.

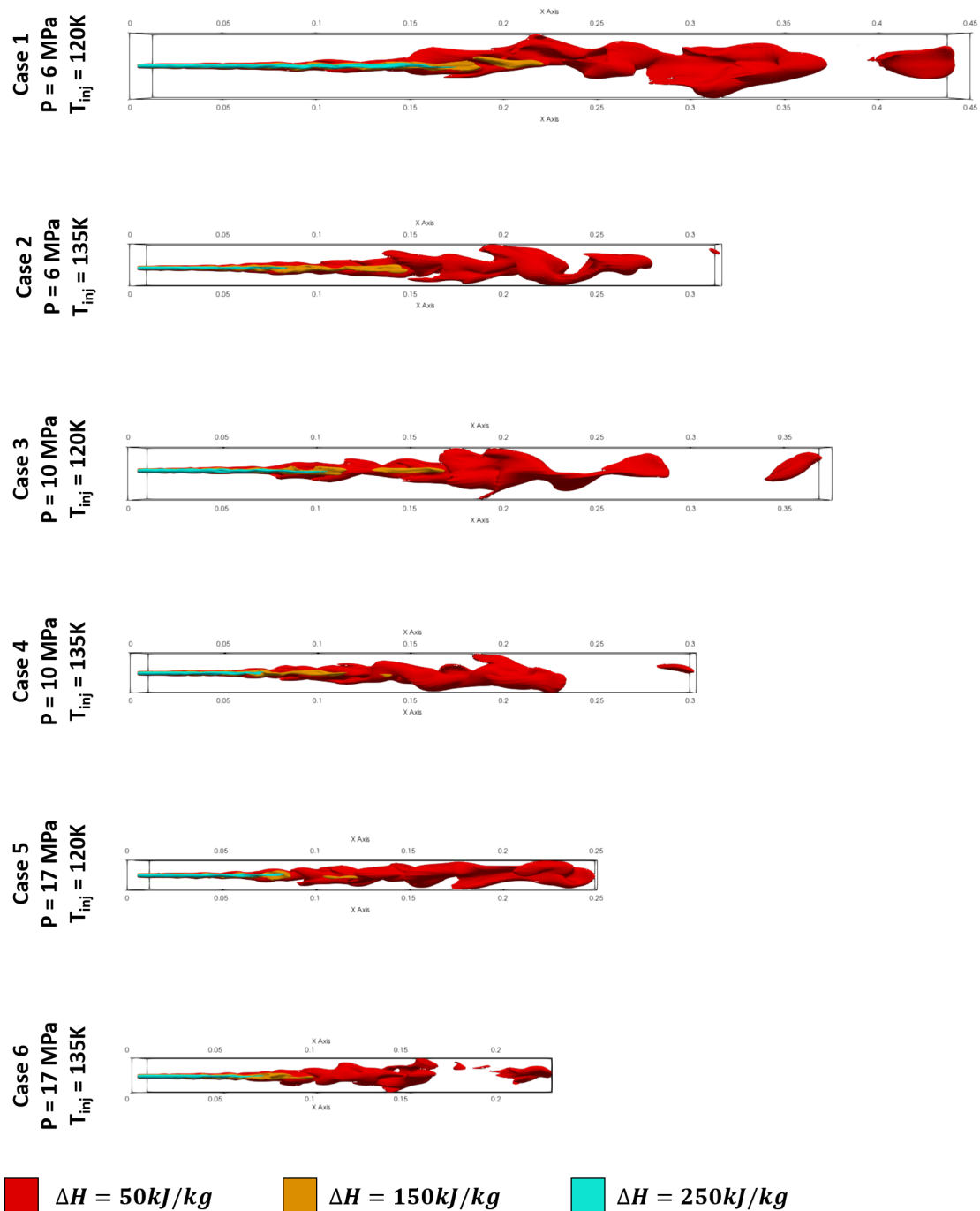


Figure 17. Isosurfaces corresponding to three different enthalpy differences, between the enthalpy of the injected nitrogen and the enthalpy of the nitrogen at chamber temperature for all the cases at $t = 1$ s from injection.

4.3.8. Influence of Turbulence Fluctuations at Inlet

In order to examine the influence of turbulence fluctuations at the inlet, case 1, which penetrates the most into the chamber, is additionally run without any turbulence fluctuations. This case is named as case Extra1 and compared with case 1 in Figure 18. The reason for simulating this additional case is twofold. From a modelling point of view, correctly capturing the primary jet breakup involves correctly reproducing the inlet fluctuations. Moreover since this is a study to better control injection

this case serves as a “virtual” experiment to assess if turbulence is an important parameter that should be tuned when the RSCE system is optimised.

The cold dense core in the case Extra1 (without turbulent fluctuations at inlet) penetrates almost three times longer than case 1 (with turbulent fluctuations at inlet). Even the disintegration of the jet after the cold core, where the fluid transforms from liquid like to gas like is spread out over a longer span than the case without any turbulent fluctuations. To better observe this, the location where the liquid like to gas like transformation occurs in case Extra1 is isolated and compared against case 1. Though at first the deeper penetration in the case Extra 1 seems advantageous to achieve heat absorption axially throughout the compression chamber, it can be seen in the figure that the disintegration in the radial direction is very limited which could be counter productive in achieving uniform heat absorption. The reason for the rapid disintegration with turbulent fluctuations at the inlet is quite clear, as these fluctuations grow rapidly. Overall, the cryogenic jet evolution and disintegration is extremely sensitive to the turbulent fluctuations at the inlet which should be carefully taken into account, but it also provides a way to control the jet penetration and disintegration inside the compression chamber.

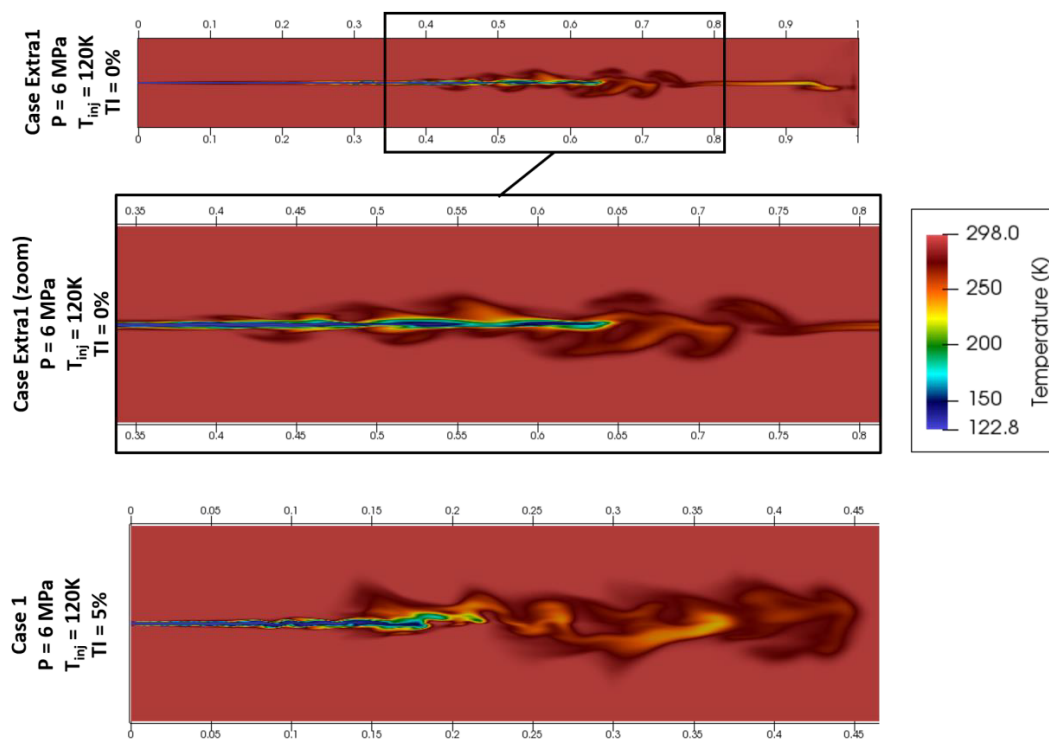


Figure 18. Temperature distribution comparison at cut section plane passing through the axis of the cylindrical mesh (chamber) for case 1 with and without turbulent fluctuations at the inlet.

5. Conclusions

The objective of this work is to contribute to the better understanding of the dynamics of cryogenic fluid injection in an engine compression chamber. Following a comprehensive overview of thermodynamics properties of LN_2 at various pressures and temperatures representative of a compression chamber, a combination of experimental analysis and numerical simulations was presented providing insight into the jet behavior at both sub and supercritical conditions in order to cover the full spectrum of conditions in the compression chamber. For the subcritical regime, following an extensive literature review as well as using new in house experimental data presented here for the first time, we performed a categorisation of the primary break-up atomisation regimes. We compared the atomisation regimes based on the appearance of the cryogenic jets under various

operating conditions against the expected regime from the We, Re and Oh numbers of the jets as they are described in the literature for other liquids. We found that the two maps coincided providing a strong evidence that at subcritical conditions the cryogenic jets behave as other fluids in terms of primary atomisation. For the numerical simulations of supercritical conditions of the cryogenic jets we developed a new methodology within OpenFoam to account for the Real Fluid Thermodynamics based on polynomial fits which we then implemented to explore the behaviour of the jet in three different chamber pressures and two temperatures. One major conclusion is that injecting at low temperatures (temperatures well below pseudoboiling temperature) and low supercritical pressures results in deeper penetration and better heat absorption due to the distributed latent heat, while also avoiding a large instantaneous heat absorption. In addition, a large enthalpy difference exists between the injection state and chamber state at lower pressures which supports the conclusion above as more heat can be absorbed. An additional conclusion is that the cryogenic jet evolution and disintegration is significantly affected by turbulent fluctuations at inlet.

Author Contributions: Conceptualisation, all authors; operating conditions A.A. and R.M.; numerical methodology, J.M.G. and K.V.; simulations, J.M.G. and G.T.; visualisation, J.M.G.; analysis J.M.G., K.V. and G.T.; validation, J.M.G., K.V. and G.d.S.; writing—original draft preparation, J.M.G. and K.V.; writing—review and editing, all authors; project administration, K.V.; funding acquisition, K.V.; supervision, K.V., R.M. and G.d.S. All authors have read and agreed to the published version of the manuscript.

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