Physics and modelling of cryogenic sprays

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Speaker: M. Jaya Vignesh
Supervisors: Prof. Robert Morgan, Dr. Konstantina Vogiatzaki and Dr. Guillaume De Sercey

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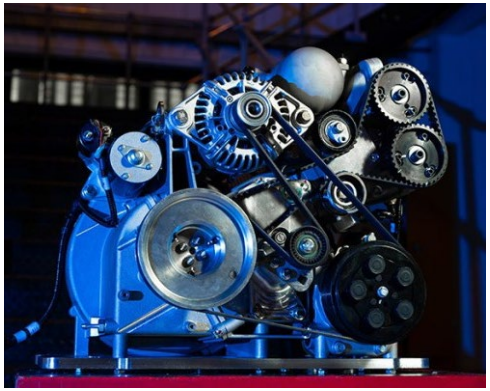
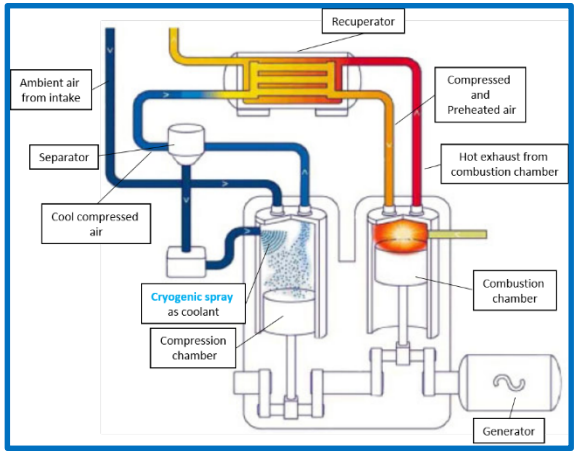
Contents of the presentation

1. Introduction and motivation
2. State of experimental research
3. Thermophysical properties of cryogenic fluids
4. Modelling thermophysical properties
5. Modelling cryogenic jet breakup
6. Current progress and Conclusion

A cryogen is a gas which exists as liquid at below 122 K.



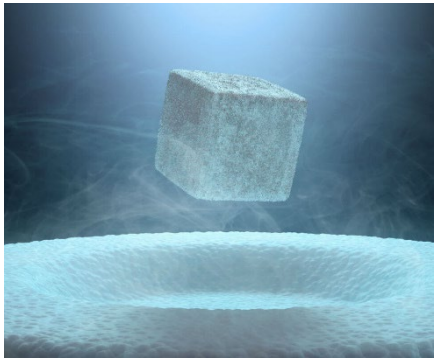
Zero emission engines (Dearman engine)



Cryopower (Split cycle engine)
University of Brighton +Ricardo

Cryogenic rocket engines

Refrigeration and food preparation



Superconductors

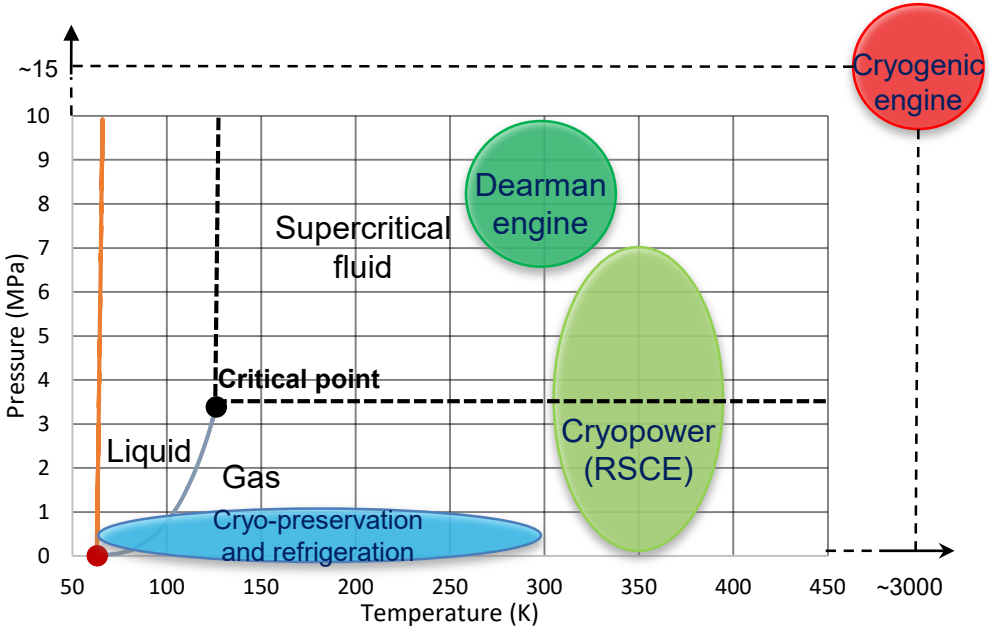
Cryopreservation and medical applications

Cryogenic sprays are coupled with application of cryogenic fluids. Most of these applications use sprays to inject cryogenic fluid into the working environment.

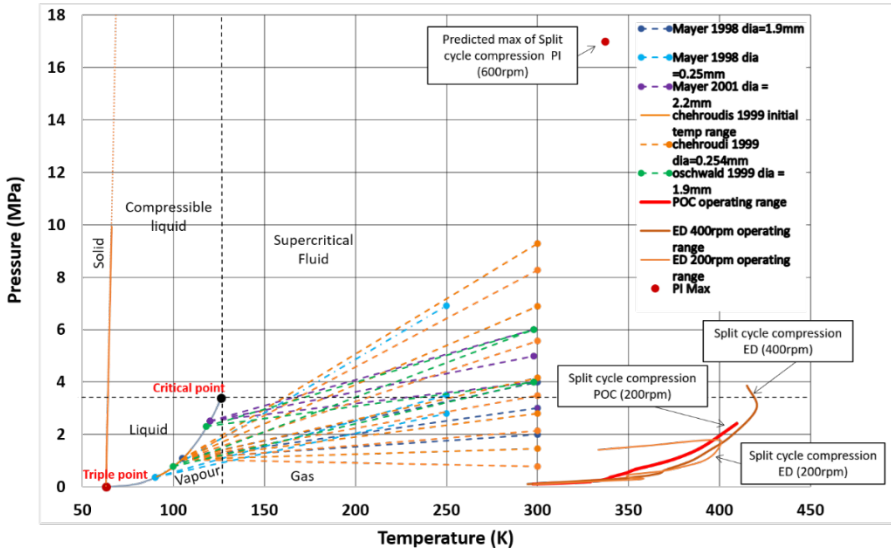
Motivation for research

- Operate in uncommon thermo-fluid regions which exhibit thermodynamic non-idealities

- Lack of adequate experimental data
- Lack of application oriented experiments
- Lack of accurate thermophysical property database



Phase diagram of nitrogen with regions of application of cryogenic fluids



Existing experimental data on cryogenic nitrogen. (The dashed lines are lines connecting injection condition to chamber condition)

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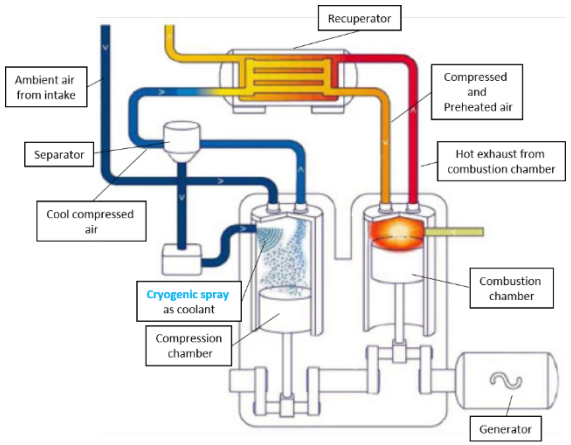
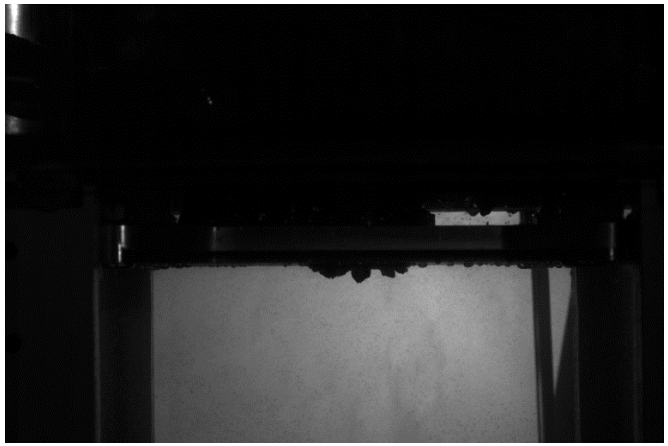
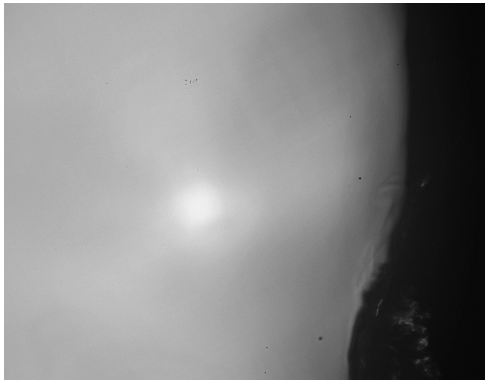
Cryogenic Research at University of Brighton



(RSCE - Recuperated Split Cycle Engine in picture) (Görsmann, 2015)



Injection of LN2 into H2O



Injection of LN2 into atmospheric environment

Simulations using OpenFOAM

Research output

- **The Ultra Low Emissions Potential of the Recuperated Split Cycle Combustion System** (Morgan, 2019)
- **Use of cryogenic fluids for zero toxic emission hybrid engines** (Jaya Vignesh, Harvey, A. Atkins, P. Atkins, Sercey, Heikal, Morgan, K. Vogiatzaki, 2019) (Discussion about the thermodynamic behavior of cryogenics)
- ***Thermodynamic analysis and system design of a novel split cycle engine concept***. (Dong, Morgan, & Heikal, n.d.)
- ***The 60% efficiency reciprocating engine: A modular alternative to large scale combined cycle power***. (Gurr, Atkins, Rawlins, & Morgan, 2016)
- ***Liquid air energy storage – from theory to demonstration***. (Morgan, 2016)

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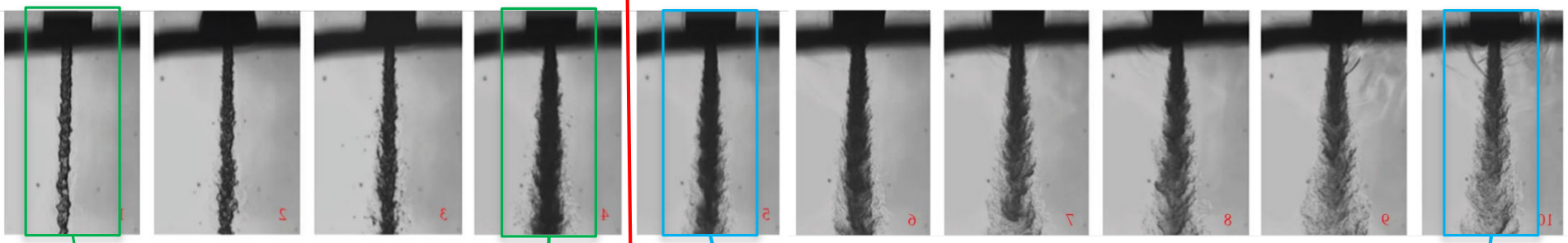
Experimental observation of Cryogenic Sprays

Pcrit = 3.39 MPa

Subcritical

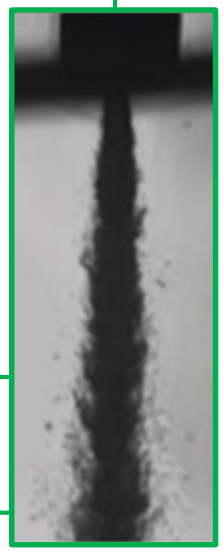
Supercritical



0.78 MPa | 1.46 MPa | 2.14 MPa | 2.81 MPa | 3.49 MPa | 4.17 MPa | 5.56 MPa | 6.88 MPa | 8.27 MPa | 9.29 MPa

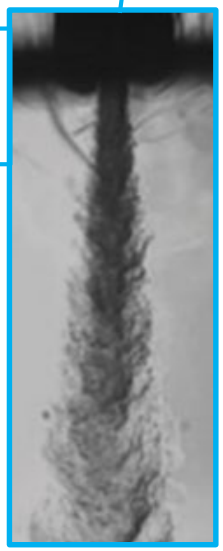
Image sequence of flow evolution of cryogenic LN2 injected into gaseous N2 at 298 K at chamber pressures ranging from subcritical 0.78 Mpa to Supercritical 9.29 Mpa. The chamber pressures are given below the respective flow images.
(Chehroudi et al., 1999)

Appears entirely laminar liquid like



Appears like a evaporating liquid spray

Appears like a dense gas jet



Appears like a rapidly dissipating turbulent gas jet

Visual flow characteristics change from liquid like to gas like at the critical point

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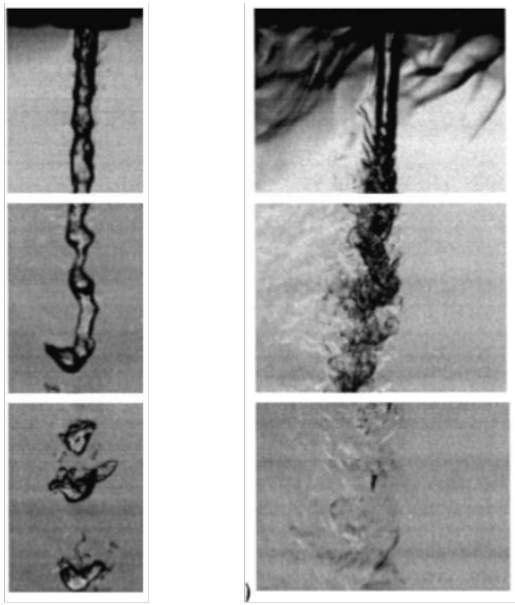
Understanding Cryogenic Sprays

Apart from the chamber fluid composition, the chamber and injection conditions for both cases are exactly the same

Fully liquid like appearance



Fully gas like appearance

Chamber = GN2/GHe

$P_{chamber}$ = 6.9 Mpa
$T_{chamber}$ = 298 K

Chamber = GN2

$P_{chamber}$ = 6.9 Mpa
$T_{chamber}$ = 298 K

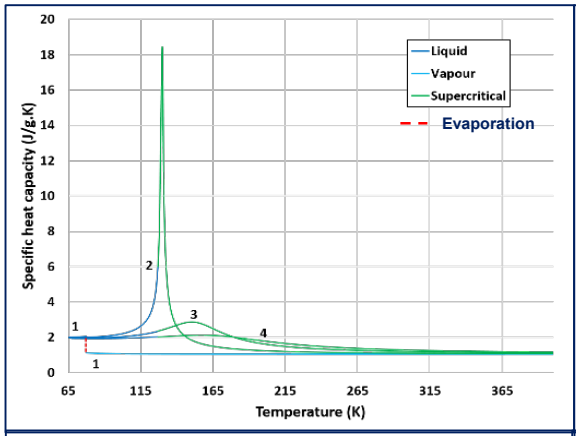
Injection of cryogenic LN2 into gaseous N2/He mixture (left) and N2 (right) both at chamber temperature and pressure of 250 K and 6.9 Mpa. (H. Mayer et al., 1998)

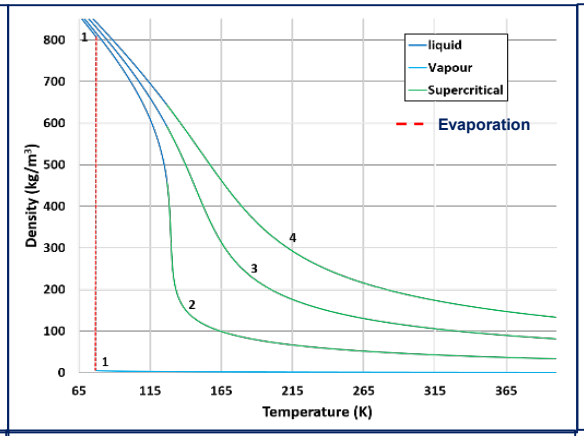
Is critical pressure the decisive factor for the flow characteristic of cryogenic sprays?
Not so simple…..

The pressure at which the flow characteristics change does not depend only on the critical pressure and temperature of the injected liquid**. It also depends on the ambient fluid composition.** This shows the complexity in understanding and modelling cryogenic flows in practical environment.

Current focus on understanding and modelling single fluid cryogenic sprays. i.e. cryogenic fluid injected into ambient gaseous form of the same fluid

Thermophysical Properties of Cryogenic Fluids



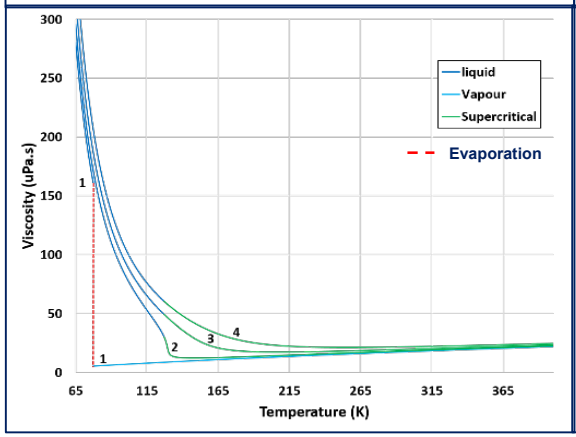


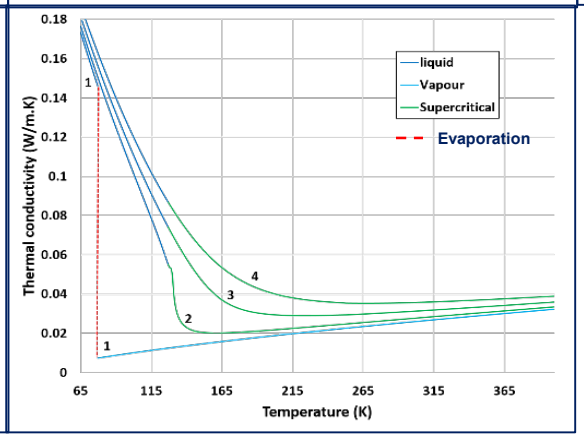
1 = 0.1 Mpa (Atmospheric pressure, Refrigeration and cryo preservation)

2 = 4 Mpa (Just above critical pressure)

3 = 10 Mpa (Maximum pressure in the compression chamber of RSCE, upper stage cryogenic rocket engine combustion chamber)

4 = 17 Mpa (1st stage cryogenic rocket engine combustion chamber pressure)



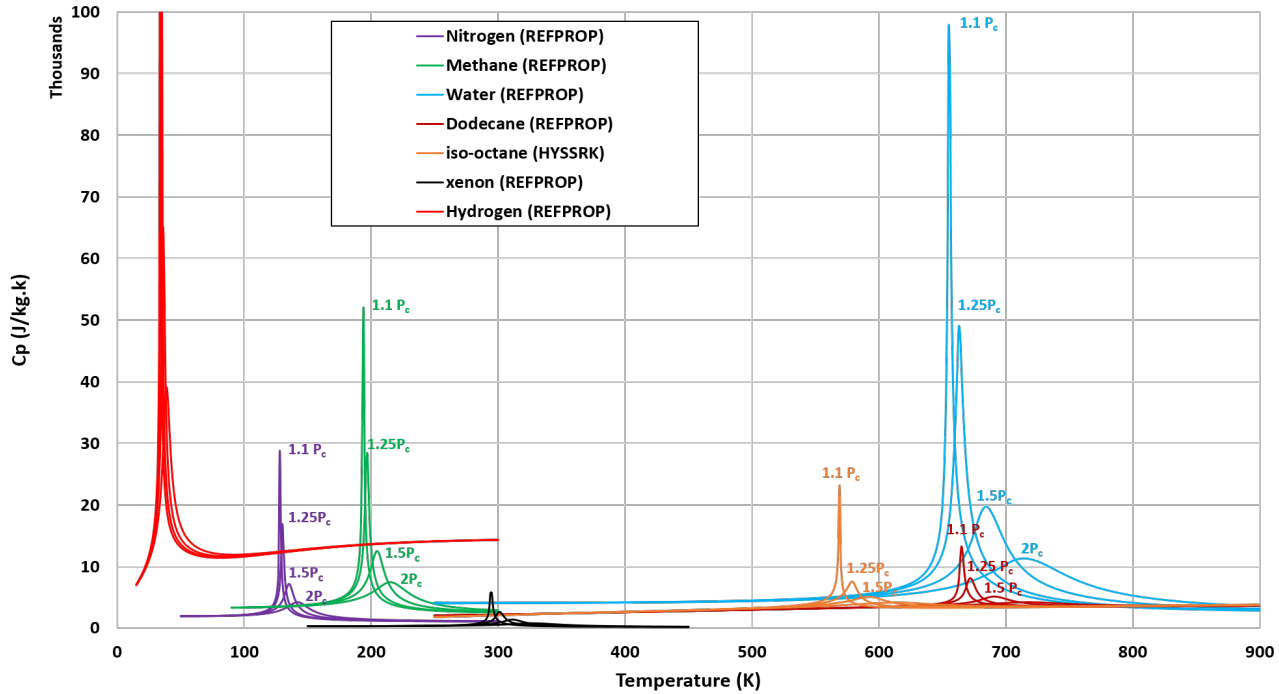


Cryopower (RSCE) compression chamber
0.4 MPa – Start of compression cycle
8 MPa – End of compression cycle

Subcritical – boiling point - evaporation(sudden discontinuity) at boiling point, phase change from liquid to gas

Supercritical – pseudoboiling point - No discontinuity, gradual phase transformation from liquid to gas. Maximum of heat capacity and most rapid change in other thermophysical properties at pseudoboiling point.

Are supercritical cryogenic fluids unique?



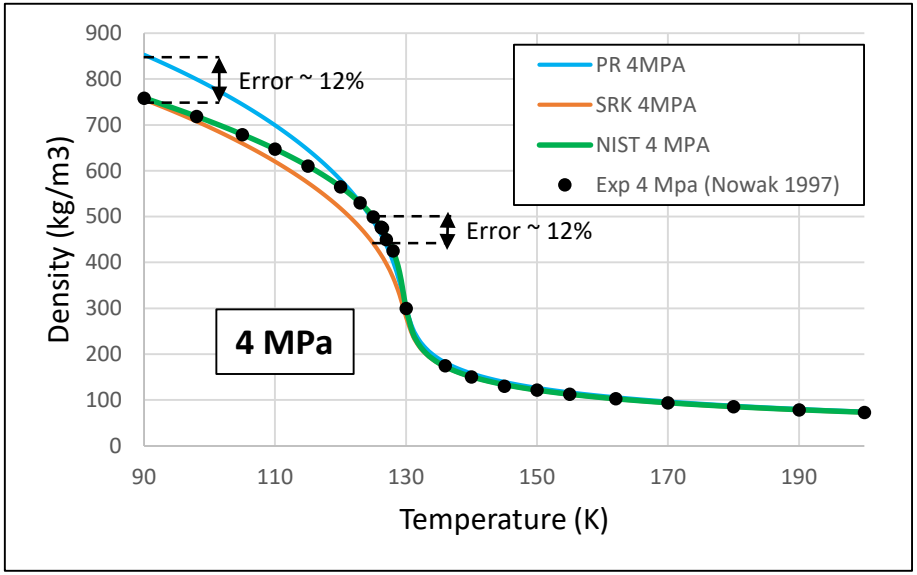
Pc is critical pressure. The plots are 1.1, 1.25, 1.5 and 2 times the critical pressure of the respective fluids

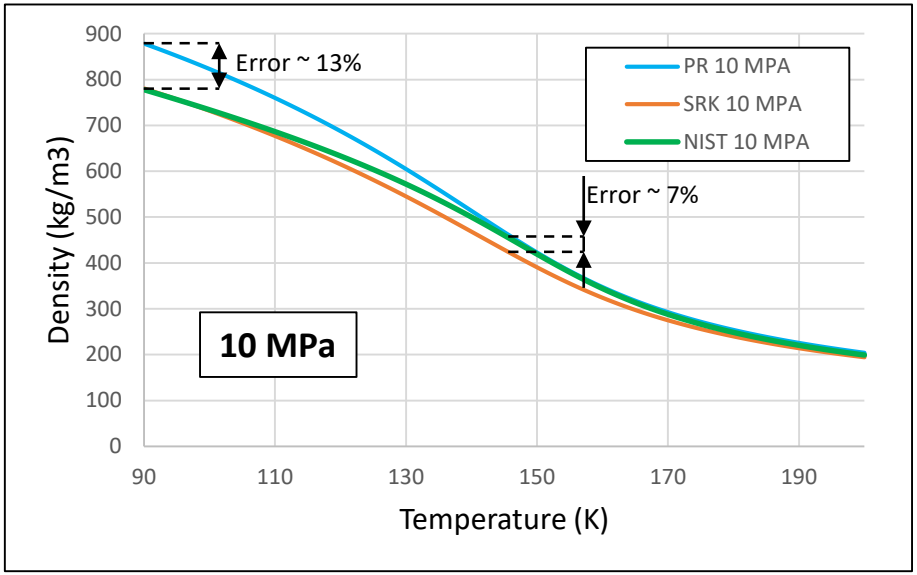
Comparing with other supercritical liquids (like supercritical fuels), at the pseudo boiling point rise in heat capacity is significantly higher for cryogenic fluids. This is also accompanied by steeper change in enthalpy with temperature.

Fundamentally, other supercritical liquids and supercritical cryogenic fluids have the same thermophysics governing them.

But cryogenic supercritical experiments (analysing fundamental thermophysics) are single fluid (like LN2 into N2), which is never the case with other supercritical liquid (including supercritical fuel spray) experiments.

Modelling the properties of a cryogenic fluid using EOS



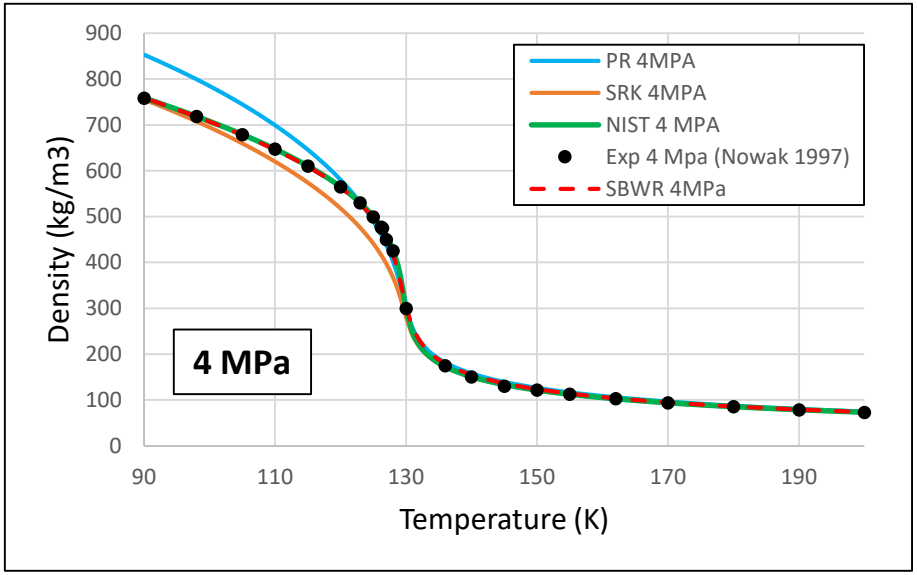


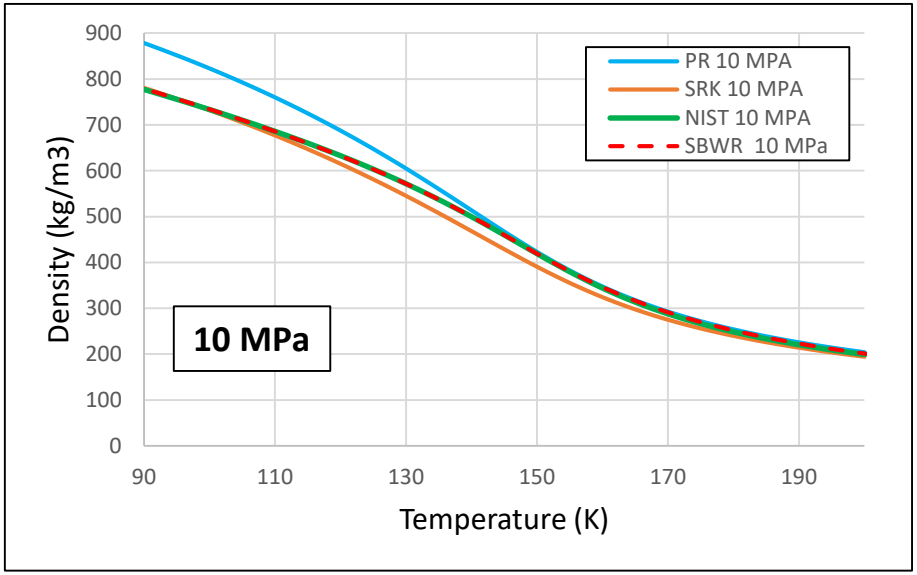
NIST is the most accurate for thermophysical properties. Made up of several EOS and validated by experimental data.

PR (Peng Robinson) EOS and SRK (Soave Redlich Kwong) EOS – Cubic EOS. Widely used.

PR and SRK results in significant deviations.

Modelling the properties of a cryogenic fluid using EOS





NIST is the most accurate for thermophysical properties. Made up of several EOS and validated by experimental data.

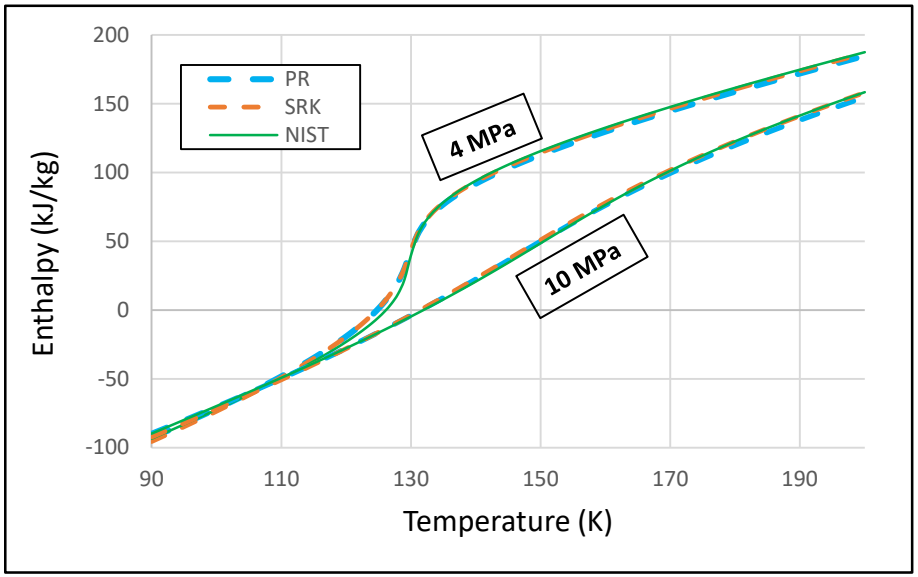
PR (Peng Robinson) EOS and SRK (Soave Redlich Kwong) EOS – Cubic EOS. Widely used.

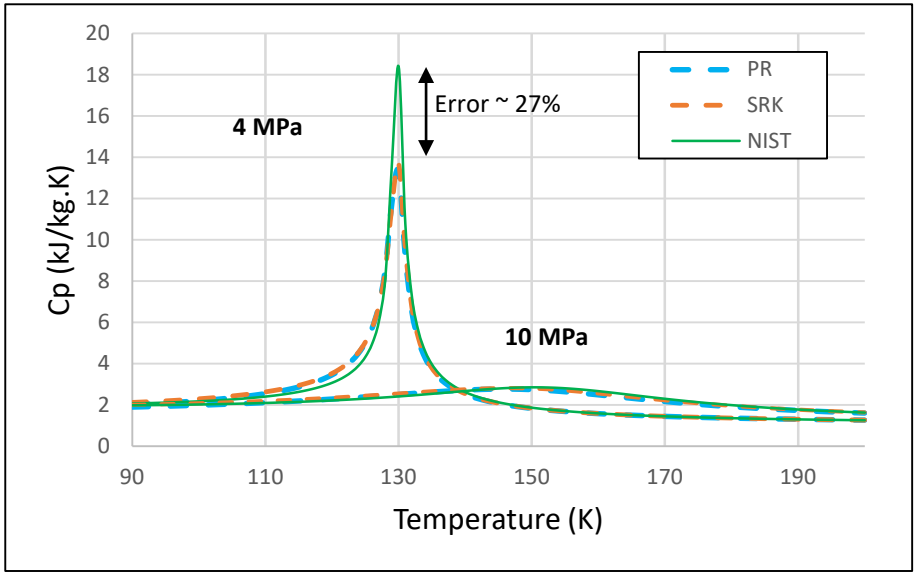
PR and SRK results in significant deviations.

SBWR (Soave modification of Benedict Webb Rubin) non-cubic EOS.

Analysis of SBWR resulted in very accurate density predictions for a wide range of supercritical pressures. Very promising

Thermodynamic properties from EOS





The EOS returns the volume occupied (in turn returns density) for a particular pressure (P), Temperature (T) and other unique properties of the fluid such as critical pressure, critical temperature and acentric factor.

Thermodynamic properties of the fluid are derived using departure functions implemented on the EOS.

Enthalpies are predicted with good accuracy by PR and SRK EOS.

Significant errors in heat capacity prediction especially near critical pressure.

What about the very accurate SBWR EOS?

Can the accurate SBWR be used to calculate thermodynamic properties?

$$H_{dep} = H_{real} - H_{ideal} = RT(Z-1) + \int_{\infty}^{v}\left[T\left(\frac{\partial P}{\partial T}\right) - P\right]dv$$

Departure function for enthalpy. (Peng & Robinson, 1976)

$$C_P = \frac{\partial H}{\partial T} \qquad C_{Pdep} = C_{Preal} - C_{Pideal} = \frac{\partial}{\partial T}\left(RT(Z-1) + \int_{\infty}^{v}\left[T\left(\frac{\partial P}{\partial T}\right) - P\right]dv\right)$$

Soave Redlich Kwong (SRK) (G. Soave, 1972)

$$P = \frac{RT}{V_m - b} - \frac{a(T)}{V_m(V_m + b)}$$

$$Z^3 - Z^2 + Z(A - B - B^2) - AB = 0$$

Only $a(T)$ is a function of temperature and H_{dep} can be simplified to

$$H_{dep} = RT(Z-1) + \frac{T\,{da}/{dT} - a}{b}.\ln\left(\frac{Z+B}{Z}\right)$$

And C_{Pdep} can be subsequently derived

Peng Robinson (PR) (Peng & Robinson, 1976)

$$P = \frac{RT}{V_m - b} - \frac{a(T)}{V_m^2 + 2bV_m - b^2}$$

$$Z^3 - Z^2 + Z(A - B - B^2) - AB = 0$$

Again only $a(T)$ is a function of temperature and H_{dep} can be simplified to

$$H_{dep} = RT(Z-1) + \frac{T\,{da}/{dT} - a}{2\sqrt{2}b}.\ln\left(\frac{Z+\sqrt{2}B}{Z-\sqrt{2}B}\right)$$

And C_{Pdep} can be subsequently derived

A brief explanation of thermodynamic properties calculated using departure functions for PR and SRK.

Can the accurate SBWR be used to calculate thermodynamic properties?

$$H_{dep} = H_{real} - H_{ideal} = RT(Z-1) + \int_{\infty}^{v}\left[T\left(\frac{\partial P}{\partial T}\right) - P\right]dv$$

Departure function for enthalpy. (Peng & Robinson, 1976)

$$C_P = \frac{\partial H}{\partial T} \qquad C_{Pdep} = C_{Preal} - C_{Pideal} = \frac{\partial}{\partial T}\left(RT(Z-1) + \int_{\infty}^{v}\left[T\left(\frac{\partial P}{\partial T}\right) - P\right]dv\right)$$

Soave modification of Benedict Webb Rubin (SBWR) (G. S. Soave, 1999)

$$Z = \frac{P}{RT\rho} = 1 + B\rho + D\rho^4 + E\rho^2(1 + F\rho^2).e^{-F\rho^2}$$

B,D and E are a function of temperature.

$$H_{dep} = ???$$
$$C_{Pdep} = ???$$

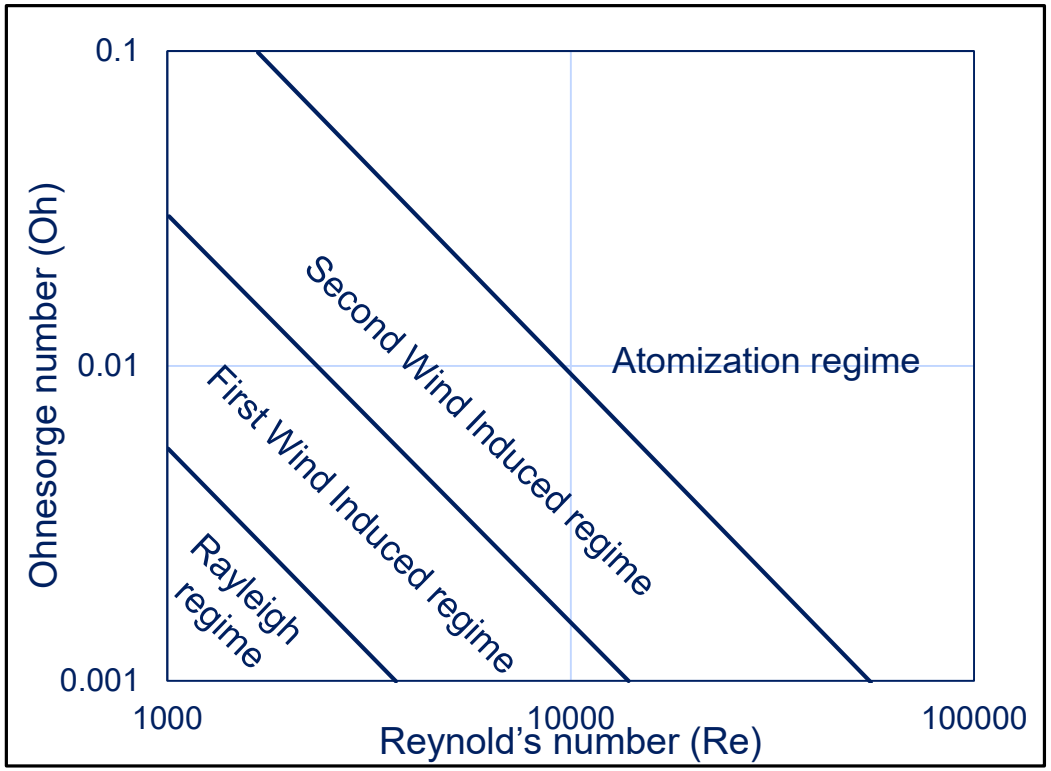
Here calculating H_{dep} and the subsequent thermodynamic properties becomes too complex.

The complexity of using SBWR can be understood when trying to substitute the EOS in the departure functions above.

SBWR which gave accurate density cannot be used to model the thermodynamic properties of fluid due to its complexity

So the problems in accurately modelling cryogenic fluids still exist

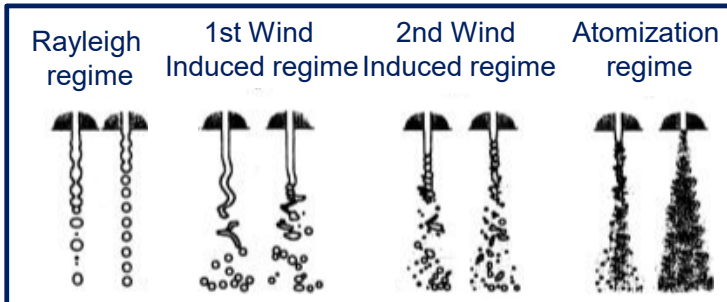
Cryogenic Jet Breakup - Subcritical



Classification of primary jet breakup regimes
Based on Reynold's no and Ohnesorge no

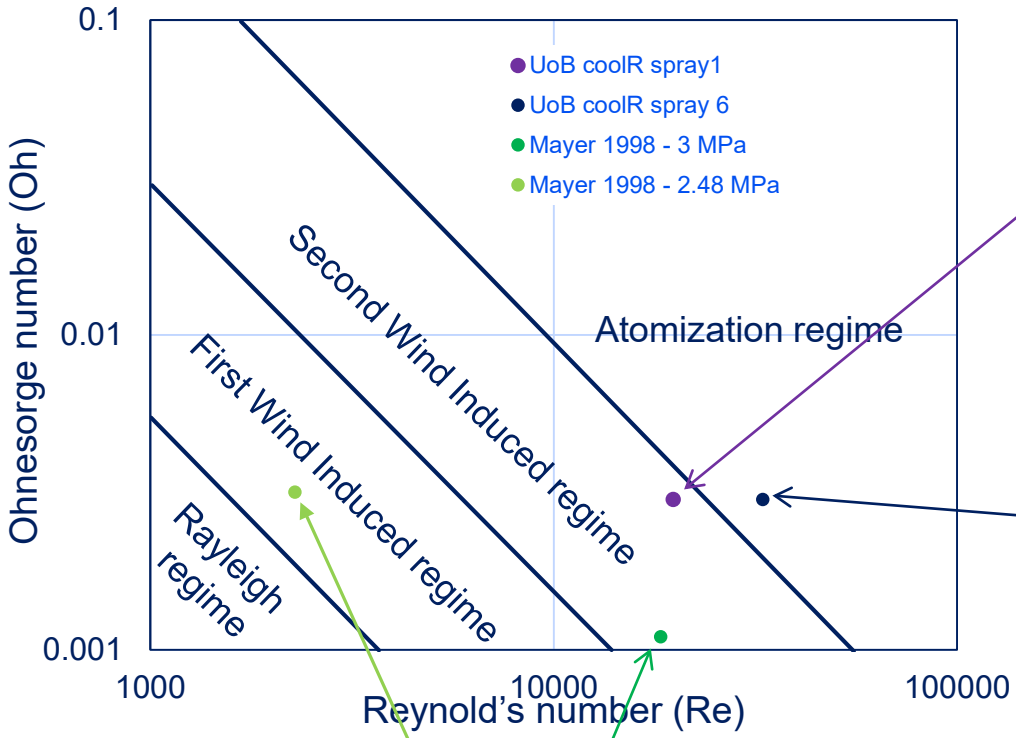
Spray/jet breakup models are important part of Euler-Lagrangian simulations.

The primary and secondary breakup models calculate the droplet parameters from injection/previous droplet parameters.

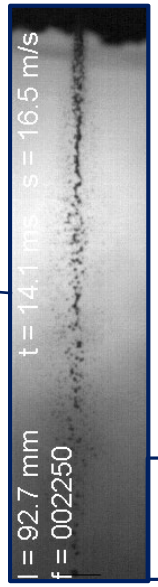


Appearance of primary breakup in various regimes.
(Liu, 2000)

Cryogenic Jet Breakup - Subcritical



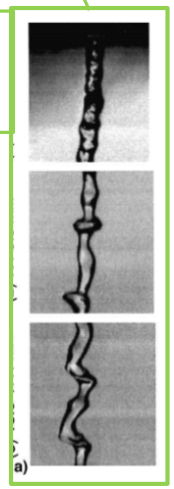
University of Brighton coolR experiment (0.1 MPa ambient pressure)

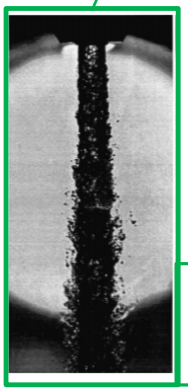


University of Brighton coolR experiment (0.1 MPa ambient pressure)

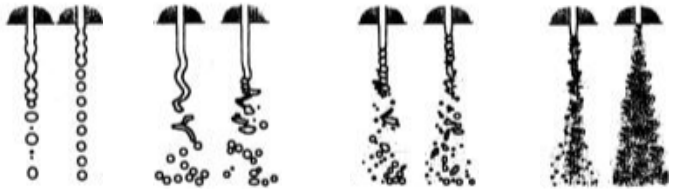
Experimental observations are in good agreement with the theory

Mayer's experiment, 2.48 MPa chamber pressure. (H. Mayer et al., 1998)





Mayer's experiment, 3 MPa chamber pressure. (H. Mayer et al., 1998)



Appearance of primary breakup in various regimes.
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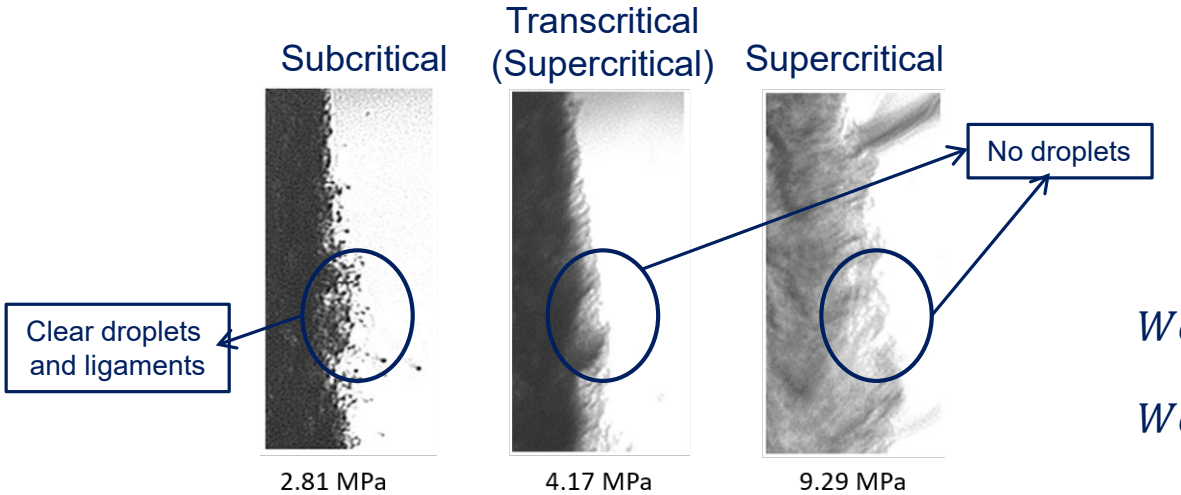
Cryogenic Jet Breakup- Supercritical



Magnified images of flow boundaries of cryogenic LN2 injected into supercritical, transcritical and supercritical chamber pressures. (Chehroudi et al., 1999)

Supercritical – near zero surface tension

$$We = \frac{\rho v^2 l}{\sigma} \approx \infty \text{ (Weber's no for liquid)}$$

$$WeG = \frac{\rho_G v^2 l}{\sigma} \approx \infty \text{ (Gas Weber's no)}$$

$$Oh = \frac{\sqrt{We}}{Re} \approx \infty \text{ (Ohnesorge no)}$$

The breakup of cryogenic liquid jets at supercritical pressures cannot be fit into existing classifications.

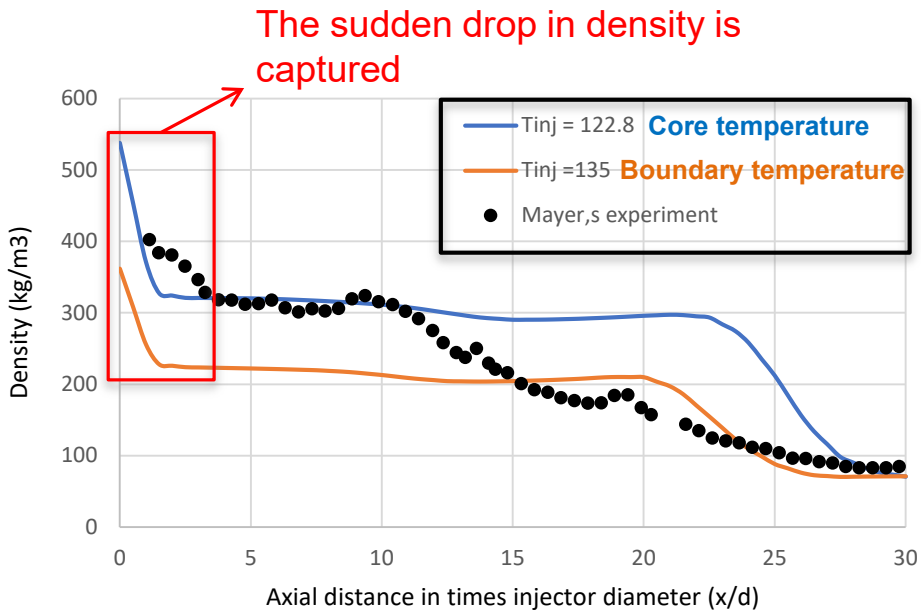
Lack of any droplets results in failure of breakup models.

Euler-Eulerian simulation is the best approach for supercritical cryogenic fluids.

Past, Current and Future work

- Literature review of cryogenic injection experiments – Completed
- Numerical modelling of PR, SRK and SBWR EOS – Completed
- Numerical modelling of thermodynamic properties from PR and SRK EOS - Completed
- Simulating Mayer's (2003) experiments in OpenFOAM with polynomial fitting of NIST's thermophysical properties – In progress
- Numerical modelling of transport properties from PR and SRK EOS – Planned
- Building SRK and extended PR EOS for density, and corresponding thermodynamic and transport models derived from the EOS into OpenFOAM – Planned
- The ultimate objective of my PhD is to create a numerical simulation tool which can accurately simulate cryogenic liquids and sprays

Preliminary simulation results



OpenFOAM simulation of centreline density values of using core temperature (122.8 K) and boundary temperature (135 K) of the jet against experimental measurements of case 9.

Preliminary simulation of Mayer's case 9 (Mayer 2003) results is promising with the simulation capturing the sudden decrease in density qround pseudo boiling point.

	Target Pressure (Mpa)	Target temperature (K)	Target Velocity (m/s)	Chamber Pressure (Mpa)	Average Velocity (m/s)	Tainj (K) (boundary temp)	Tbinj (K) (axial temp)
Mayer Case9	6	120	2	5.85	2	135	122.8

Conclusions

1. For single fluid cryogenic cases critical pressure is the sole criteria determining the flow characteristic.

2. NIST estimates the thermophysical properties of cryogenic fluid accurately but is too complex for modelling.

3. SBWR estimates the density of the cryogenic fluid accurately, but significant hurdles exist in deriving thermophysical properties from it and using it for simulations.

4. Currently we are limited to PR and SRK or a hybrid combination of both.

5. Subcritical cryogenic sprays fit in existing jet breakup regimes and models. Supercritical cryogenic sprays don't.

6. Euler-Lagrangian simulation is not suitable for supercritical cryogenic fluids unless new breakup models are developed –Currently active area of research in our group.

Acknowledgements

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