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NUMERICAL AND EXPERIMENTAL STUDY OF SUPERSONIC NOZZLE FOR ORGANIC RANKINE CYCLE TURBINE

Omnia Elbaz[1, *], Tala El Samad[1], Martin T. White[2], Abdulnaser Sayma[3]

[1] *City St George's, University of London, Northampton Square, London, EC1V 0HB, United Kingdom*
[2] *University of Sussex, Sussex House, Falmer Brighton, BN1 9RH, United Kingdom*
[3]*Brunel University London, Kingston Lane, Uxbridge, Middlesex, UB8 3PH, United Kingdom*

*Corresponding Author: omnia-ahmed.elbaz@citystgeorges.ac.uk

ABSTRACT

Organic Rankine cycles utilise organic fluids characterised by high molecular complexity, while expansion typically occurs near the critical point and the saturation vapour line. This leads to non-ideal compressible fluid dynamic effects. In such instances, the behaviour of the fluid can diverge significantly from that of an ideal gas. The experimental research on non-ideal compressible fluid dynamics, which is crucial for comprehending flow behaviour, assessing system performance, and validating both theoretical and numerical models, remains limited. In this study, a one-dimensional nozzle model, along with two-dimensional inviscid steady-state computational fluid dynamics simulations of the expansion of R245fa through a converging-diverging nozzle, are employed to analyse the flow within the test section installed in the NextORC test facility, which has recently been commissioned at City, St George's, University of London. These numerical investigations aim to enhance the understanding of flow behaviour through the test section and help to plan the subsequent stage of experiments. In both models, real gas properties derived from lookup tables generated with NIST REFPROP utilising Helmholtz energy equations of state are incorporated. The numerical results characterise the flow through the nozzle in terms of pressure and velocity distributions under both design and off-design working conditions, which are then compared with experimental findings obtained during the initial commissioning phase.

1 INTRODUCTION

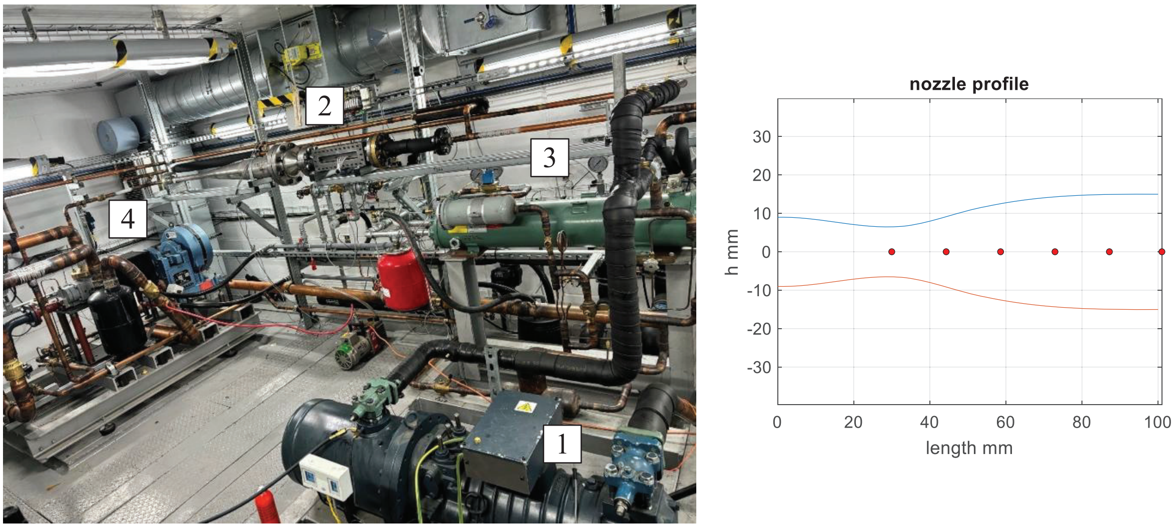
As the expander is a key component of the organic Rankine cycle, research efforts have been dedicated to improving its performance. The design and simulation of ORC turbines can be challenging due to non-ideal compressible fluid dynamic (NICFD) behaviour that stems from using organic fluids as working fluids. These issues arise due to deviations from ideal gas behaviour, which can significantly impact turbine performance and efficiency. Such effects can lead to complicated shock systems and interactions with boundary layers, influencing turbine loss mechanisms as well as efficiency (Hoarau et al., 2021). The potential deviation from ideal gas behaviour, particularly near the vapour saturation line and the critical point, necessitates a detailed study of the flow behaviour to minimise losses such as trailing edge and shock losses to enhance ORC turbine design and efficiency. Over the past decades, numerical methods for simulating NICFD flows have become well established, and initial findings of higher-order simulations, automated turbomachinery design optimisation, and uncertainty quantification methodologies have been reported (Guardone et al., 2024). However, despite significant recent experimental research, there remains a pressing need for further experimental studies to validate and improve the accuracy of numerical simulations (Guardone et al., 2024). This particularly importance since current turbine design methods often rely on empirical models, necessitating intensive numerical simulations to enhance turbine geometry and performance (De Servi et al., 2019).
Although experimental work in the NICFD field is challenging due to the operating conditions (high pressure and temperature) and use of unconventional fluids, several test facilities have been developed

to study the expansion of non-ideal fluids, as detailed in a recent review article (aus der Wiesche, 2023). Examples include the test rig for organic vapours (TROVA) (Spinelli et al., 2017), the flexible asymmetric shock tube (di Paliano et al., 2007), and a facility at Imperial College London (Robertson et al., 2019), all of which are blowdown (batch-operation) facilities. The ORCHID facility (Head et al., 2015) can continually operate and test rotating machinery as well as static cascade geometries, while the closed-loop organic wind tunnel (CLOWT) (Reinker et al., 2017) operates continuously to evaluate flow in both a cascade test section. These facilities have made significant contributions to the study of NICFD flows, including the experimental capture of non- ideal flow behaviour, high-resolution observation of Mach waves and condensation processes, and the development of new measuring techniques. However, there is still a need for further experimental investigation to support in the generation of repeatable datasets across a wide range of operating conditions.

To contribute to the field by providing additional experimental datasets, the NextORC test facility has been recently commissioned. The test rig is a continuous test facility that can be used to investigate the flow field in converging-diverging nozzles under working conditions similar to those found inside the stator guide vane of supersonic ORC turbines. Compared to previous test facilities, the NextORC test rig operates with a different working fluid, namely the refrigerant R245fa, which has been extensively employed in subcritical ORC systems. Although this fluid possesses a relatively high global warming potential, a substantial amount of research related to the design, analysis, and experimental testing of components and ORC systems utilising this fluid have been conducted; thus, the enhanced an understanding of the NICFD effects with help in the development of enhanced design and modelling tools. Moreover, the dimensions and configuration of the converging-diverging nozzle employed in the NextORC test rig differ from those of nozzles used in othe rigs. The geometry of the nozzle directly affects the development of the flow field, including factors such as viscous potential and the intensity, structure, and location of shock waves (Restrepo & Simões-Moreira, 2022). Additionally, possessing experimental data for varying geometries assists in the advancement of numerical models and the validation of developed software for nozzle design (M. Zocca, et al., 2023). Finally, being a continuous facility, the test rig allows multiple measurements to be obtained at steady state, providing stable conditions for the calibration of sensors and helping to ensure repeatability, facilitating a comprehensive assessment of experimental accuracy and uncertainty. In this paper, the results of the initial tests carried out during the commissioning period of the NextORC rig are analysed utilizing numerical simulations. During the expansion of the flow in the converging-diverging nozzle, the flow is characterised using a one-dimensional model and CFD simulations to analyse its behaviour under various working conditions. The 1-D and inviscid CFD simulations are compared to the initial results obtained from the commissioning phase of the facility. The results are helpful to prepare for the next stage of experiments.

2 EXPERIMENTAL SETUP AND TEST CONDITIONS

NextORC is compressor-driven test facility where the working fluid is R245fa passes through four main components which are twin screw compressor, test section and shell and tube condenser and expander (was not included in this set of experiments). The test section is custom-made and consists of the upstream diffuser, a settling chamber, a contraction zone and a converging-diverging nozzle. Figure 1(a) shows a photo of the test rig, and the detailed description of the rig components, measurement techniques and operating procedure is presented in Elbaz et al. (2024). The flow enters the twin-screw compressor, and all the flow discharged from the compressor is then routed through the test section. After the test section, a fraction of the flow is diverted through the condenser and condensed before being mixed with the rest of the fluid leaving the test section outlet. The flow then passes through a series of valves, which can be used to throttle the flow, if necessary, before the flow is returned to the compressor suction. The complete test section incorporates a planar converging-diverging nozzle to investigate expansion.



(a) (b)

Figure 1: a) Photo for NextORC test facility with main components: 1) compressor; 2) test section; 3) condenser; and 4) expander. b) Profile of the converging diverging nozzle.

The test section comprises a rectangular steel channel that accommodates various geometries. The planar nozzle is manufactured from stainless steel and is 100 mm long with throat dimensions of 12.5 mm by 12.5 mm. Both the test section and its components are designed according to the methodology described in White and Sayma (2018). Pressure and temperature measurements along the nozzle are used to understand the expansion from very low velocity to supersonic velocity, with a target outlet Mach number of 2. The pressure field is measured along the nozzle's axis, with pressure measured in the flow direction starting at the throat and extending along the diverging section of the nozzle. This is accomplished using six Kulite pressure transducers, labelled 1-6 in the flow direction, which have a diameter of 0.8 mm in the nozzle's sidewall and an expanded uncertainty of ±2.0% of the full-scale range. Total temperature and pressure are measured at the centreline of the flow in the settling chamber just upstream of the test section. The temperature is measured using a resistance temperature detector (RTD) with expanded uncertainty ranging from ±0.6 to ±3°C. Pressures within the rig, but outside of the test section, are measured with Honeywell transducers, which have an expanded uncertainty of ±2.0% of the Full-Scale Span (FSS) assuming 95% confidence level. Figure 1(b) shows the converging diverging nozzle profile with the locations of the pressure transducers along the nozzle axis.

2.1 Test methodology

During the commissioning phase, a test run was conducted to expand R245fa with a converging-diverging nozzle. The converging-diverging nozzle was tested under various total inflow conditions. Seven intake set points were utilised, with total inlet pressures ranging from 7 bar to 13 bar in 1 bar increments. The compressor operated at a constant speed of 3,500 rpm. The nozzle inlet set points were controlled manually by adjusting the condenser pressure with a pressure regulator. The test period lasted between 8 and 10 minutes for low-pressure instances, and 5 minutes for high-pressure cases to prevent compressor overheating, which could affect steady-state conditions. Table 1 summarises the total inlet conditions, and the corresponding compressibility factor Z value for all tests. The compressibility range of the input conditions for the completed tests ranges between 0.84 to 0.75, indicating a range from nearly dilute to non-ideal conditions. To ensure accurate measurements, pressure data was averaged during the final 100 seconds of each transducer measurement in each test. While efforts were made to maintain constant total pressure by adjusting the condenser regulation valve, no method was applied to control the total inlet temperature. In these trials, the test section was uninsulated, and the rig wasn't heated for an extended period prior to the experimental runs.

Table 1: Test conditions

Test name	**1**	**2**	**3**	**4**	**5**	**6**	**7**
Total pressure (bar)	7	8	9	10	11	12	13
Total temperature (°C)	76.7	83	87.8	92.9	96.1	99.5	102.3
Total compressibility factor (Z)	0.842	0.829	0.815	0.802	0.786	0.77	0.754

3 NUMERICAL METHODS

3.1 Flow regime investigation using a one-dimensional model

From the experimental pressure measurements gathered, it was unclear whether the flow regime inside the nozzle is subsonic or supersonic flow, especially considering the fairly low spatial resolution of the measurements. Hence a quasi-one-dimensional (1-D) approach is used to study the expected expansion within the nozzle, which helps to provide insight into the flow regime by estimating the variation in the flow parameters along the nozzle including pressure, velocity and temperature in the flow direction. The model is based on mass, momentum, and energy conservation equations coupled with real gas model, assuming minimal body forces and adiabatic flow. A direct analytical solution is not possible due to the nonlinear relationship between pressure, velocity, and density in compressible, supersonic flow. As a result, an iterative numerical method is used to determine the static pressure while maintaining mass conservation. The 1-D model is solved using MATLAB, which is integrated with REFPROP version 10 (Lemmon et al., 2010) to predict the thermodynamic properties of the working fluid. The boundary conditions for the 1-D model are the inlet total conditions and outlet static pressure of the nozzle from experiment runs alongside the nozzle geometry installed in the test section.

As a first step, the nozzle critical pressure ratio (PR_{cr}) is determined and compared with the measured nozzle pressure ratio (PR) from the experimental run to assess whether the nozzle is choked. If the flow is choked, then the nozzle outlet pressure following an isentropic expansion, $P_{\mathrm{ex,isen}}$ is then computed through an iterative mass balance using the choked mass flow rate, the nozzle outlet area, and the upstream total conditions with the assumption of constant entropy. To ensure the solution converges on the supersonic solution, rather than the subsonic solution a bounded iterative secant scheme is used. Once $P_{\mathrm{ex,isen}}$ is computed it is then compared to the outlet pressure of the nozzle measured during experimental runs, $P_{\mathrm{ex,exp}}$, to ascertain whether the flow is entirely supersonic along the nozzle or if a normal shock or oblique wave occurs. The static pressure following a normal shock at the nozzle outlet, $P_{\mathrm{ex,shock}}$, is then calculated by using the shock upstream conditions that correspond to the isentropic supersonic pressure, i.e, $P_{\mathrm{ex,isen}}$, along with the corresponding velocity, and density. To do this, an iterative solution is performed that solves mass, momentum, and energy conservation across the shock wave to determine the flow conditions after the shock wave. The pressure, density, and velocity calculated after the shock wave are then used to calculate the total conditions after the shock wave. The calcualted $P_{\mathrm{ex,shock}}$, is then compared to the $P_{\mathrm{ex,exp}}$, to determine whether a shockwave occurs within the nozzle, or if a normal or oblique shock occurs at the nozzle outlet. Table 2 presents the throat's calculated critical pressure that results in choked flow (Ma=1) in the nozzle for each case.
If the flow is choked and $P_{\mathrm{ex,exp}}$ is greater than $P_{\mathrm{ex,shock}}$, then a normal shock wave occurs in the nozzle. To determine the location of the shockwave, it is assumed that a normal shock occurs at a known location x. The supersonic condition just upstream of point x, as well as the subsonic condition immediately after the shock can be determined through the same iterative processes mentioned previously. Once the downstream stagnation conditions are known, the corresponding static pressure at the nozzle outlet can be found through a final iterative mass balance. This series of calculations are iterated to identify the location of the shock that corresponds to the defined static outlet pressure $P_{\mathrm{ex,exp}}$. This is done by defining an objective function which is the difference between the predicted and target outlet pressure and the solution is found through a numerical root-finding algorithm.

3.2 CFD simulations

The performance of the nozzle is also investigated using real-gas computational fluid dynamics (CFD) simulations to determine the flow regime and enhance the understanding of the pressure fields. The total inlet pressure and temperature measured at the settling chamber upstream of the nozzle inlet and the static outlet pressure at the end of the diverging section of the nozzle serve as the boundary conditions derived from the experiment. The geometry of the computational domain replicates the geometry of the nozzle used in the experimental work. The results from the experimental work within the NextORC test section nozzle are compared with numerical CFD simulations conducted using ANSYS Fluent, which integrates with the NIST REFPROP library to account for real fluid properties via lookup tables. In this initial modelling, a 2D inviscid steady-state simulation has been setup. Due to the symmetry of the nozzle, only half the nozzle was simulated, and a symmetry boundary condition was applied at the nozzle centreline. Pressure-velocity coupling was managed using the coupled method, which enhances convergence for compressible flows. The Rhie-Chow momentum-based flux type was employed for flux reconstruction, ensuring numerical consistency. For spatial discretisation, the least squares cell-based approach was utilised to evaluate gradients, while second-order upwind schemes were applied to density, momentum, and energy equations, as well as for pressure discretisation. A structured mesh was generated with refinement near the wall, and mesh independence was confirmed through a grid sensitivity study. The centerline pressure was compared for different three different meshes using the boundary conditions from experiments 4 and 6. The coarse mesh consisted of approximately 21,000 cells, the medium mesh had 57,000 cells, and the fine mesh comprised 82,000 cells. The results obtained with the medium showed less than 0.5% variation in pressure distribution compared to the finer mesh. As such, the medium mesh was selected for subsequent simulations to balance computational time and accuracy. Figure 2 shows an image of the medium mesh to show size distribution and refinement relative to the nozzle size. The solution was deemed converged when scaled residuals for continuity and energy dropped below 10^{-6}, and imbalances have been verified at both the inlet and outlet, as well as through the addition of monitoring points along the nozzle.

Table 2: Throat critical pressure for each case.

Test name	**1**	**2**	**3**	**4**	**5**	**6**	**7**
Critical pressure (bar)	4.25	4.8	5.5	6.13	6.76	7.41	8.06

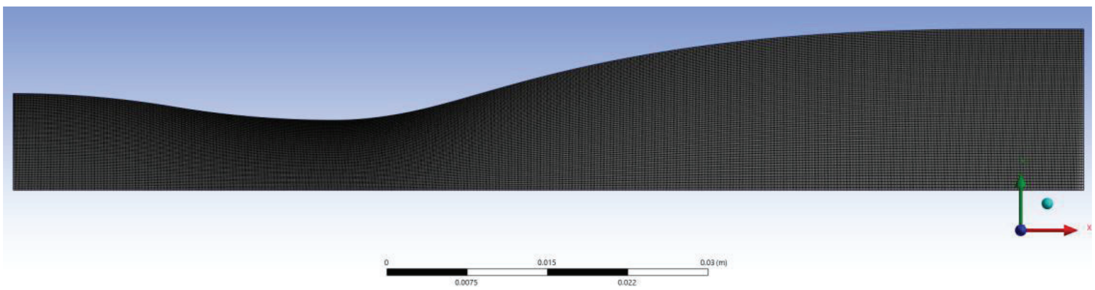


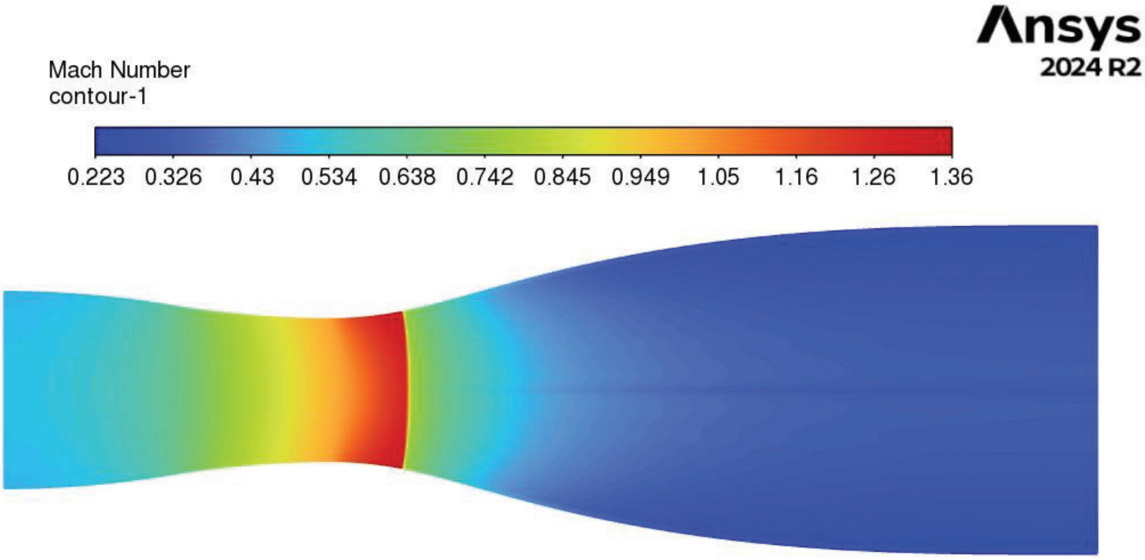
Figure 2: Medium mesh used for the inviscid 2D CFD simulations.

4 RESULTS

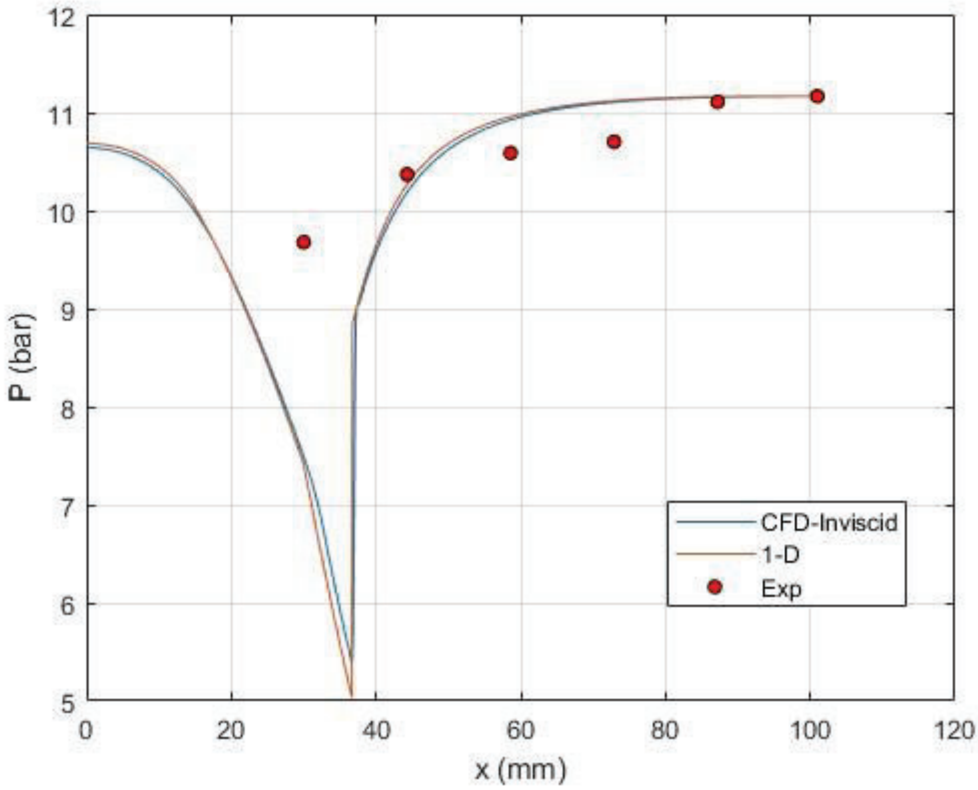
As noted, from the data collected during the commissioning phase, it was difficult to determine whether the flow regime was subsonic or supersonic based solely on the available pressure measurements, necessitating further numerical investigation to understand the pressure field and flow regime inside the converging-diverging nozzle. Figure 1(b) shows the nozzle profile with the position of the six transducers distributed along the diverging part of the nozzle, while Figure 3(a) displays the Mach number contours as predicted from the CFD simulation for experiment 6, where the total inlet pressure and temperature are 12 bar and 99.5°C respectively, and the outlet pressure is 11.16 bar. Figure 3(b) presents a comparison between the 1-D simulation, inviscid CFD simulations and the experimental results. The predicted pressure profile from the 1-D model reveals the presence of a shockwave in the diverging region of the nozzle, which was found to lie between the first transducer at the nozzle throat and the second transducer, which is 6.58mm downstream of the throat. The predicted flow field obtained from the CFD simulation agrees with the 1-D model, and inspection of Mach number contours indicates a choked nozzle with a maximum Mach number of 1.34 and a shock wave in the diverging region of the nozzle. The pressure predicted by the 1-D model exhibits high agreement with the inviscid CFD simulations, with an error of 0.7%. When comparing the numerical results to the experimental results a fairly close match in pressure values is observed downstream of the predicted shock location, although there is a discrepancy between the pressure predicted at the throat position compared to the observed pressure from the experiment. This could be due to viscous effects, boundary layer growth, and thermal conductivity that are not accounted for in the 1-D or the inviscid simulations.

Figure 4 shows a comparison between the pressure profile obtained from the experimental test run, and the 1-D and CFD simulations for experiments 4 and 5. The same behaviour was observed in experiments 5, with supersonic flow in the diverging region of the nozzle and a normal shock wave occurring at 6.08 mm from the throat position. Again, there is a good agreement between the experimental and numerical results, with the exception of the results for the throat pressure. Regarding experiment 4, which corresponds to a total inlet pressure and temperature of 10 bar and 93 °C, respectively, and an outlet pressure of 9.66 bar, both the 1-D model and CFD simulation indicate subsonic flow remains along the entire length of the nozzle. However, again, the experimental flow field deviates from the numerical results where the most significant error is at throat position.

The one-dimensional model and CFD inviscid simulations are useful to understand the behaviour of single-phase fluid dynamics under different situations, such as pressure and velocity changes in converging-diverging nozzles. However, the experimental results do not match either of these models. As noted this could be due to limitations of the 1-D and inviscid approach. However, it also worth noting that this could be due to the extremely small degree of superheat at the nozzle inlet, which ranged between 1 and 3 °C for the test runs reported. Moreover, due to the fairly short operational times which were necessary during the initial commissioning runs, as well the lack of insulation around the test section and any form of trace heating, it is possible that two-phase flow conditions may have been present in the converging-diverging nozzle during the experimental runs, which is not accounted for in the 1-D model or CFD simulations; it is also worth noting that condensation has been a common issue in other ORC test facilities (aus der Wiesche, 2023). Another observation is that there is a small reduction in the pressure as measured by the fourth transducer, which could indicate either separation or condensation in this part of the nozzle. These aspects need further investigation.



(a)



(b)

Figure 3: a) CFD Mach number contour for experiment 6, and b) Comparison of experimental, 1-D and CFD for pressure distribution along the nozzle for experiment 6.

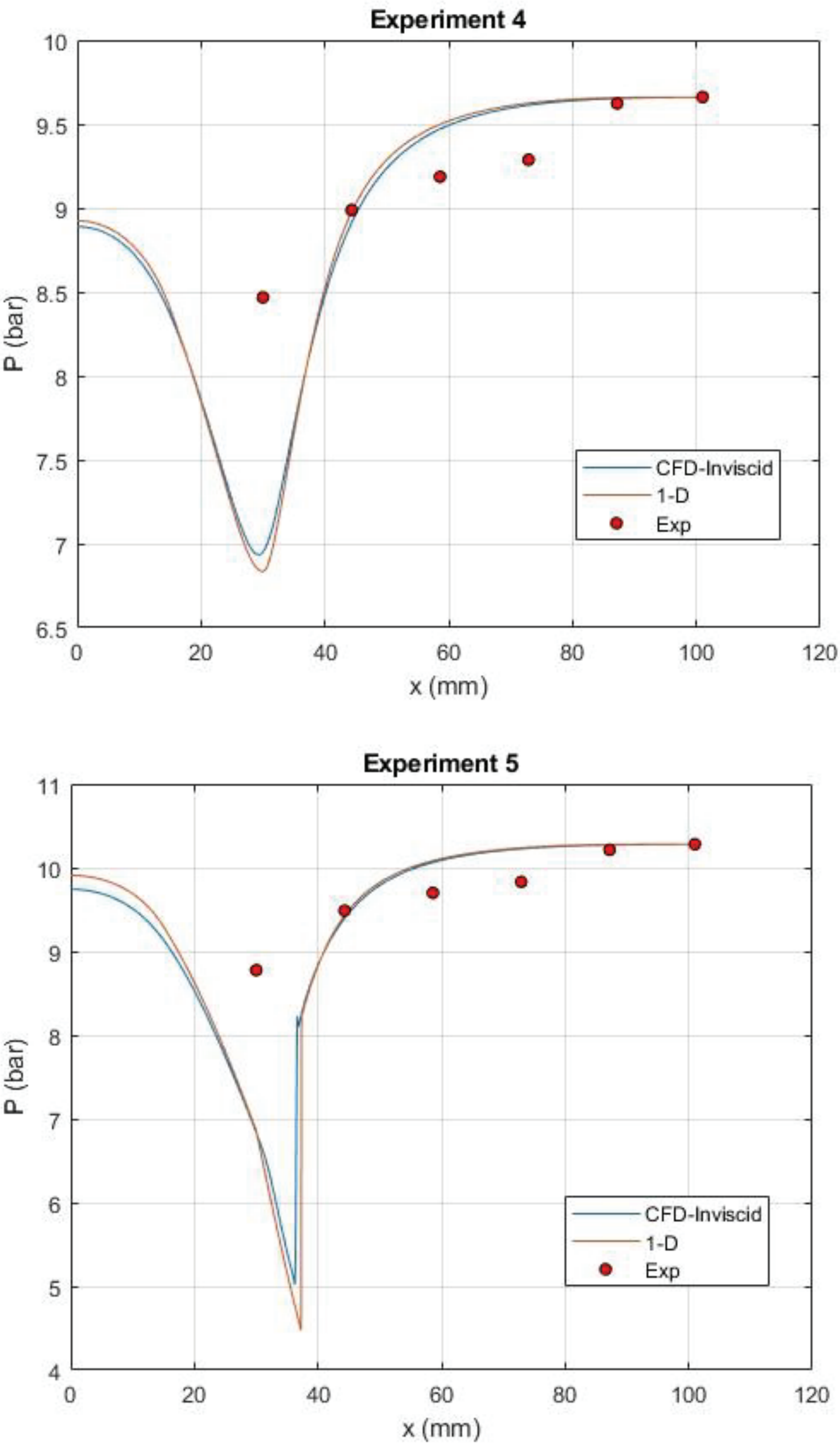


Figure 4: Comparison of experimental, 1-D and CFD for pressure distribution along the nozzle for experiments 4 and 5.

5 CONCLUSIONS AND FUTURE WORK

One-dimensional and inviscid 2D CFD simulations are performed and compared to experimental results to understand the behaviour of the flow field within the NextORC test facility test section, which includes a converging-diverging nozzle, designed to expand the working fluid to a Mach number of 2. These investigations are necessary since, based on the experimental results alone, it was difficult to ascertain whether supersonic flow conditions were achieved. The 1-D and CFD inviscid models indicate that supersonic flow in the diverging region of the nozzle is achieved, although a shock wave is predicted to occur between the pressure transducer installed at the nozzle throat and the first transducer placed within the diverging portion of the nozzle. However, while the 1-D and CFD inviscid simulations showed good agreement between each other, they did not align completely with experimental results, especially for the pressure measurement taken at the nozzle throat position, which demonstrated disagreement with both numerical models. Although this deviation could partly be due to viscous effects which are not considered in the numerical models, factors such as heat transfer and possible two-phase effects could be responsible, especially since these initial tests did not include insulation or enough preheating to the test section before conducting the experiments, while the tests were run with a small degree of superheat. To better understand the flow field, additional numerical CFD 3-D viscous simulations are needed to evaluate whether the disagreement could be caused by viscous and boundary layer effects, as well as possible 3D effects. To avoid condensation, insulation will be applied to the test section alongside the use of an electric heater, and sufficient time will be allowed for preheating the test section before conducting the upcoming experimental runs. For future investigations, numerical modelling will be employed to enhance understanding of the flow behaviour inside the nozzle, while evaluating viscous effects for both 2D and 3D configurations. Additionally, following model validation, the study will extend beyond the facility's limits and encompass a broader spectrum of working conditions utilising the NextORC nozzle geometry.

NOMENCLATURE

1−D	one dimensional (-)
CFD	computational fluid dynamics (-)
NICFD	non-ideal compressible fluid dynamics (-)
P	pressure (bar)
T	temperature (°C)
h	height (mm)
x	distance (m)
PR	pressure ratio (-)

Subscript

cr	critical
ex	exit
exp	experiment
isen	isentropic
shock	shock

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