The 4th International Symposium - Supercritical CO2 Power Cycles
September 9-10, 2014, Pittsburgh, Pennsylvania (Style 'Event Detail')

An Investigation of Condensation Effects in Supercritical Carbon Dioxide Compressors

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ABSTRACT

Supercritical CO_2 (S-CO_2) power cycles have demonstrated significant performance improvements in concentrated solar and nuclear applications. These cycles promise an increase in thermal-to-electric conversion efficiency of up to 50% over conventional gas turbines [1] and have become a priority for research, development and deployment. In these applications the CO_2 is compressed to pressures above the critical value using radial compressors. The thermodynamic state change of the working fluid is close to the critical point and near the vapor-liquid equilibrium region where phase change effects are important.

This paper presents a systematic assessment of condensation on the performance and stability of centrifugal compressors operating in S-CO_2. The approach combines numerical simulations with experimental tests to assess the relative importance of two-phase effects on the internal flow behavior

and to define the implications for radial turbomachinery design. The condensation onset is assessed in a systematic analysis approaching the critical point. A non-dimensional criterion is established that determines whether condensation might occur. This criterion relates the time required for stable liquid droplets to form, which depends on the expansion through the vapor-pressure curve, and the residence time of the flow under saturated conditions. Two-phase flow effects can be considered negligible when the ratio of the two time scales is much smaller than unity.

It is found that condensation is not a concern away from the critical point. Two-phase numerical calculations supported by experimental findings suggest that the timescale associated with nucleation is much longer than the residence time of the flow in the condensing region, meaning that the fluid cannot condense. Pressure measurements in a converging diverging nozzle show that condensation cannot occur at the level of subcooling characteristic of radial compressors away from the critical point. The implications are not limited to S-CO_2 power cycles but extend to applications of radial machines for dense, saturated gases.

In the immediate vicinity of the critical point, two-phase effects are expected to become more prominent due to larger residence times. However, the singular behavior of thermodynamic properties at the critical point prevents the numerical schemes from capturing important gas dynamic effects. These limitations require experimental assessment, which is the focus of ongoing and future research.

Introduction

Phase change in turbomachinery has been studied extensively for steam turbines, where a significant amount of the flow condenses as it expands through the last turbine stages. This phenomenon, however, is uncommon in compressors where the compression process occurs away from the two-phase region. Nevertheless, condensation can occur due to local flow acceleration such as for example near the leading edge of an impeller [2][3], as shown schematically in Figure 1.

There is a lack of literature on the impact of condensation on compressor performance and stability, let alone in compression systems operating with S-CO_2. Gyarmathy [4] identified three different loss mechanisms associated with phase change in turbomachinery: kinematic relaxation loss, breaking losses and thermodynamic wetness loss. The kinematic relaxation loss is associated with the friction between the liquid and gas phases, which can lead to flow separation near the leading edge and increased aerodynamic loss. The breaking loss is generated by the impact of liquid droplets against rotating components and dissipates part of the work input of the rotor. Due to the small amount of condensed fluid in compressors the impact on the overall performance of this loss mechanism is expected to be negligible. Finally, the thermodynamic wetness loss is associated with the entropy generation due to heat transfer between finite temperature differences at non-equilibrium state. This usually accounts for about 45% of the overall loss due to phase change in steam turbines and could greatly reduce the efficiency of S-CO_2 compressors.

Condensation due to rapid expansion in high-speed flows usually occurs at non-equilibrium conditions [5]. Due to the rapid expansion rate the fluid can reach pressures and temperatures below saturation without condensation. This is illustrated schematically for CO_2 in a temperature-pressure diagram in Figure 2. In an isentropic expansion from an initial state A the flow reaches saturation condition B and dips below saturation pressure and temperature. Phase change proceeds at a finite rate or condensation time and, if the expansion of the gas is rapid enough, the fluid attains a non-equilibrium or metastable state D over a finite period of time [15]. This is often referred to as the Wilson line or the spinodal limit. Schnerr [5] indicates that an expansion rate of $1^{o}C/\mu s$, typical of high speed flows in converging-diverging nozzles, leads to subcooling of up to 30-40K to metastable conditions and onset of condensation at maximum nucleation rates of $\sim 10^{22}$-10^{25} $m^{-3}s^{-1}$. The fluid eventually reverts to a state of equilibrium, reaching condition E. The difference in temperature between states E and C, which is the state the fluid would reach in a quasi-steady expansion under equilibrium condensation, is what leads to the mentioned thermodynamic wetness losses.

A number of researchers have addressed the problem of non-equilibrium condensation in high-speed flows. Gyarmathy [4], Schnerr [5], Guha [6] Duff [7], Ryzhov [15] and Nakawa [8] have used converging diverging nozzles with different fluids, including water vapor, nitrogen and CO_2. In these, the onset of condensation is defined through static pressure measurements. The heat of condensation leads to a pressure drop in the converging section or a pressure rise in the diverging section. Duff [7] demonstrated that the onset of condensation at 0.1% of moisture can be detected with simple static pressure measurements in CO_2. More recently, Yazdani at al. [9] conducted CFD simulations of the two-phase flow of CO_2 in converging diverging nozzles. The study used the data from Nakawa et al. [8] to validate the numerical code and to assess the condensation of CO_2 at high pressure but away from the critical point. The application of interest is the condensation in refrigerant ejectors and the work focuses on the interaction of condensation in supersonic flow and shock waves. The numerical assessment of Batadjiev et al. [2] and Rinaldi et al. [3] found that conditions for condensation are reached in S-CO_2 near the leading edge of the impeller. [2] suggests that this might not be the case away from the critical point, however, the study requires further experimental evidence to support the CFD calculations.

The modeling of the phase transition process requires the definition of (i) the energy required to form a droplet of a critical radius that can grow to stable size and (ii) the rate of formation of these critical droplets. Classical nucleation theory defines the Gibbs free energy [10] and the rate of condensation [11] from the liquid and gas densities, the local gas temperature, the level of super-saturation and the surface tension. The presence of impurities in the gas, such as dust particles or other species, might reduce the Gibbs free energy barrier by ~3-4 orders of magnitude and lead to nearly 10 orders of magnitude larger condensation rates. However, [5] and [7] show that during rapid expansion, homogeneous nucleation is the dominating mechanism even in the presence of foreign contaminants. Spontaneous nucleation, which occurs during rapid expansions in nozzles or near the leading edge of a blade, will produce nuclei many orders of magnitude greater in number than those that could be present in the form of foreign contaminants [7]. Homogeneous nucleation can therefore be safely assumed in these applications.

Near the critical point the surface tension vanishes and the rate of condensation increases, reducing nucleation times. This suggests that two-phase effects are more prominent closer to the critical point. Despite much work in the field, the issue of transcritical phase change is not fully understood. Yet without this fundamental characterization of the underlying phenomena, the design of compressors often remains a costly test-fail-fix endeavor, leading to deleterious instabilities or poor performance.

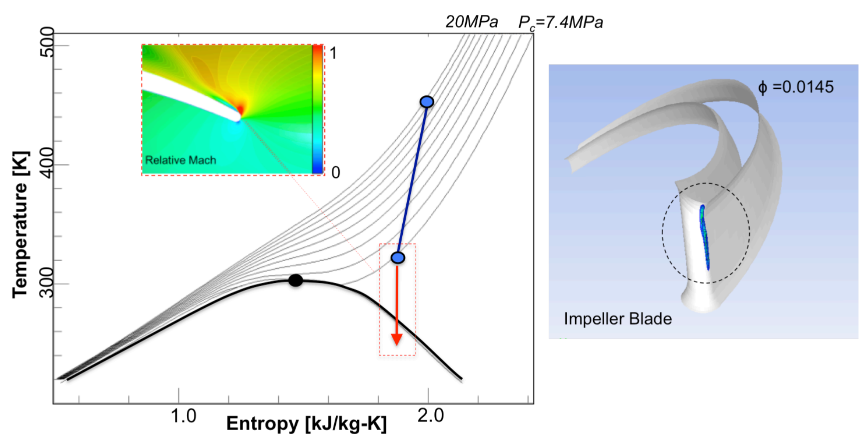

Figure 1. Temperature-Entropy diagram illustrating isentropic expansion to saturation near impeller leading edge

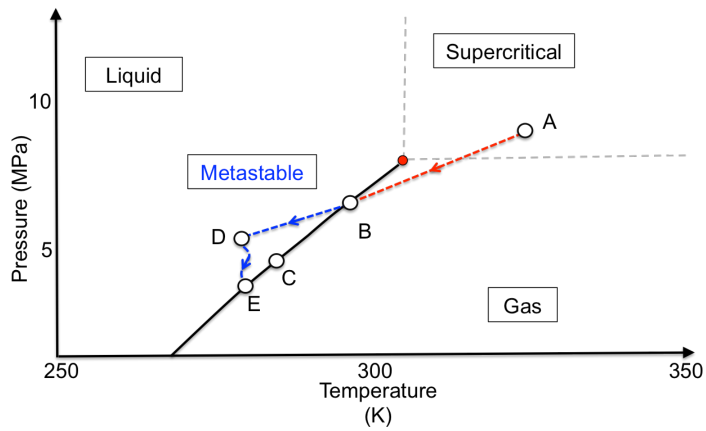

Figure 2. Pressure–temperature diagram illustrating isentropic expansion to metastable conditions

Scope of Paper

While a great deal of work has been carried out on characterizing condensation away from the critical point and at low pressures, very little is known about transcritical condensation and its impact on the internal flow behavior of supercritical CO_2 compressors. The aim of this paper is to rigorously characterize the impact of localized condensation on turbomachinery performance when operating closer and closer to the critical point. More specifically, the objectives of the paper are to: (1) fully characterize the thermodynamic state of CO_2 during the expansion process into the saturated region (2) assess whether condensation can take place in compressors operating away and at the critical point and (3) investigate the impact of condensation on stage performance and stability.

A non-dimensional criterion is defined that determines whether condensation might occur. The criterion relates the time required for stable liquid droplets to form, which depends on the expansion through the vapor-pressure curve, and the residence time of the flow under saturated conditions. Combining two-phase numerical computations with lab-scale experiments, the onset of condensation is assessed in a converging diverging nozzle.

It will be shown that the nucleation time scale ratio is much smaller than unity away from the critical point, indicating that condensation in supercritical CO_2 compressors is not a concern. The pressure measurements in the converging diverging nozzle show that condensation cannot occur at the level of sub-cooling characteristic of the expansion near the impeller leading edge in S-CO_2 compressors. The experimental measurements validate the two-phase computations. The method is then applied to investigate condensation in a candidate compressor. It is shown that condensation has no impact on stage performance and stability away from the critical point. The observed behavior is consistent with that of cavitation in liquid water pumps for which large regions of cavitating flow are required in order to impact machine performance and stability.

Technical Approach

The commercial solver ANSYS CFX 14 [12] was used for all the calculations. A detailed description of the numerical methodology can be found in [2] and [13]. The computational method is based on a finite-volume approach using an implicit, compressible formulation with second order spatial discretization. The Reynolds Averaged Navier-Stokes (RANS) equations are closed through the two-equation k-ω shear stress transport (SST) turbulence model. NIST's formulation of the Span and Wagner Equation of State (EOS) model, called RefProp [14], was adopted and incorporated in the CFD solver in the form of lookup tables as described in [2]. The implementation was tested and validated through a systematic refinement of the lookup tables and compared with experimental data in a converging diverging nozzle.

Two-Phase Model and Timescale Analysis

Two-phase calculations were conducted using a user-defined model for droplet nucleation and growth in ANSYS CFX 14. This is based on classical nucleation theory under the assumptions of non-equilibrium, homogeneous condensation. Further details of the numerical methodology can be found in [2]. Heterogeneous condensation was initially modeled including the droplet contact angle θ, however, the results, which are consistent with the literature [5] [7], suggest that the homogenous condensation assumption is sufficient. To model the metastable phase the lookup table from the NIST-REFPROP EOS are extrapolated into the two-phase region as described in [2].

The nucleation time is defined:

$$t_n = \frac{1}{J_{\max} V} \quad (1)$$

where V is the volume of fluid below saturation, as illustrated in Figure 5 and J_{max} is the maximum normalized rate of nucleation. The nucleation rate is defined as [2]:

$$J = \left[\sqrt{\frac{2\sigma}{\pi m^3}} \frac{\rho_v^2}{\rho_l}\right] e^{\left(-\frac{\Delta G^*}{kT}\right)} \quad (2)$$

with

$$\Delta G^* = \frac{4}{3}\pi r^{*2}\sigma \quad (3)$$

and

$$r^* = \frac{2\sigma}{\rho_l \left[g(p_v,T) - g(p_s,T)\right]} \quad (4)$$

The residence time of fluid in the condensing region is defined as:

$$t_r = \frac{l}{c_{ave}} \quad (5)$$

where l is the length of the condensing volume as shown schematically in Figure 3, and c_{ave} is the average flow velocity. The limit to condensation is defined by the ratio of timescales $\tau_{cl}=t_r/t_n$. Condensation limit ratios below 1 indicate that the nucleation time is larger than the residence time, implying that condensation cannot occur.

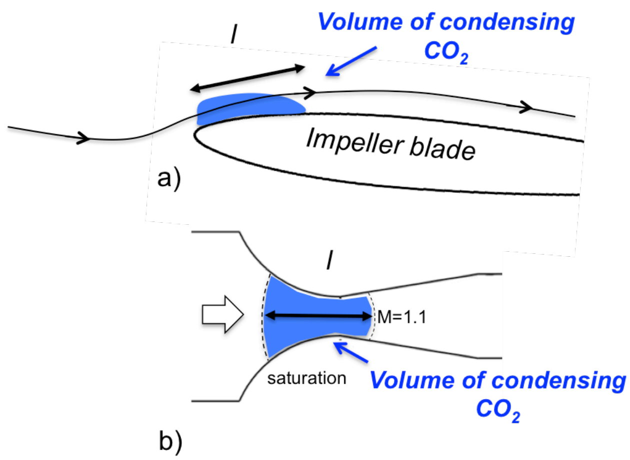

Figure 3. Definition of condensation length scale and condensing volume for compressor blade a) and nozzle test section b) – Mach number in candidate compressor below 1.1 [2].

Experimental Assessment:

A laboratory scale experiment in supercritical CO_2 was conceived, designed, implemented and operated. The experimental assessment was used to explore the space of timescales of interest, to define margins for condensation onset, and to validate the condensation model and the numerical methodology.

The tests are non-rotating, simple blowdown type tests using pressurized CO_2 bottles in an open-loop arrangement as shown schematically in Figure 4. The fluid from commercial available CO_2 bottles is stored in a heated charge tank which is connected to a nozzle test section by a fast acting valve. The CO_2 properties are measured during rapid expansion in a converging-diverging (C-D) nozzle from different inlet flow conditions, as shown schematically on a pressure-temperature diagram in Figure 5. The inlet conditions in the tank are marked as blue circles, red lines represents isentropic expansions, and the blue lines illustrate the expansion into metastable conditions. The nucleation time depends on the expansion through the vapor-pressure curve, the fluid properties, and the concentration of other constituents in the fluid mixture. A reduction of the tank temperature will yield a larger excursion into the two-phase region increasing the residence time and decreasing the nucleation time.

The charge conditions can be set over a wide range of temperatures and pressures within the supercritical region. The maximum temperature and pressure are constrained by the charge tank operating limits. The charge conditions are monitored using a fast response pressure transducer and K-type thermocouple. The modular setup of the nozzle test section allows for a wide variety of test configurations and a relatively quick turnaround time. The dimensions of the nozzle test section are consistent with and representative of the characteristic length scale of the estimated condensing region in the candidate compressor. The details of the compressor geometry are given in [2]. The rate of expansion ,dT/dt, is set to 1C/μs, a typical value at the LE of the impeller. The nozzle throat is R=5mm in diameter, and the length of the condensing region varies from R to 3R..The blowdown experiment is carried out over short time intervals, typically 500 nozzle flow-through times, during which the charge tank pressure drops less than 0.1% and the measurement can be assumed quasi-steady. A dump tank is placed downstream of the nozzle test section to capture the CO_2 before releasing it to the atmosphere. The nozzle back pressure is set by a vacuum pump connected to the dump tank.

The focus of the current assessment is on the converging section as the relative Mach numbers in CO_2 compressors is typically less than 1.1 [2]. Pressure transducers are mounted along the converging nozzle wall and are used to detect the onset of condensation. A unique feature of the experiment is the capability to deduce the speed of sound using Helmholtz resonator based forced response measurements, as described in a later section.

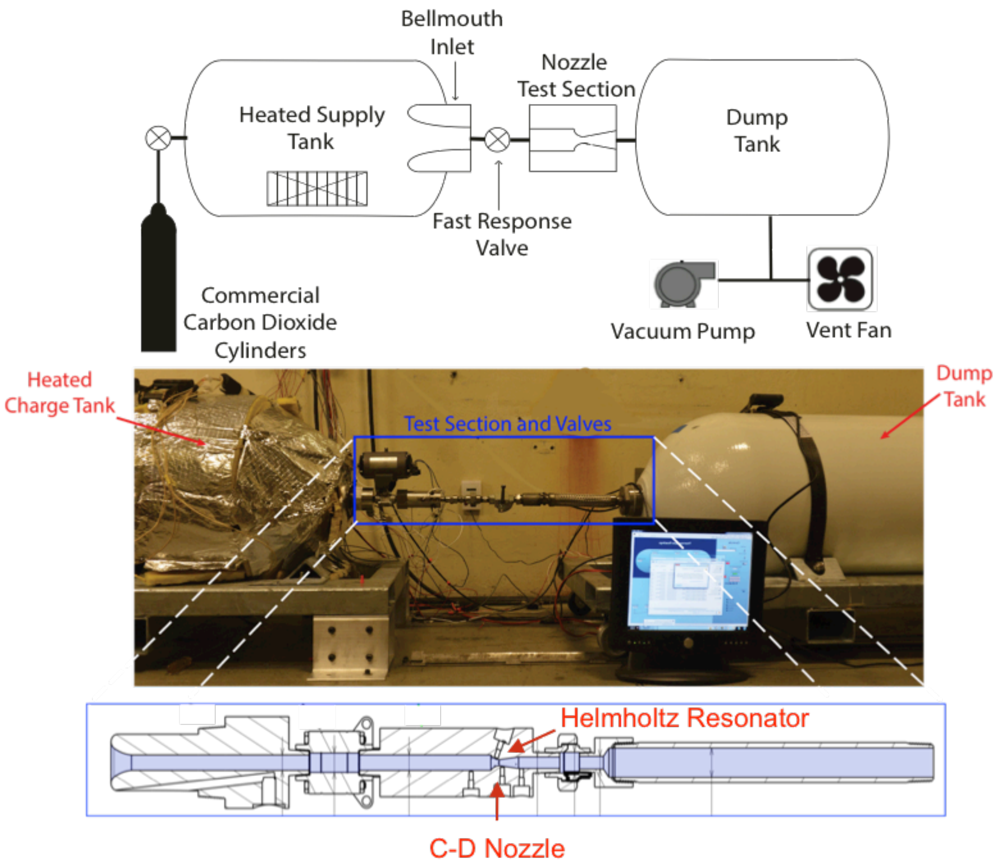

Figure 4. ***Laboratory scale experiment for assessment of supercritical*** CO_2 ***internal*** **flow.**

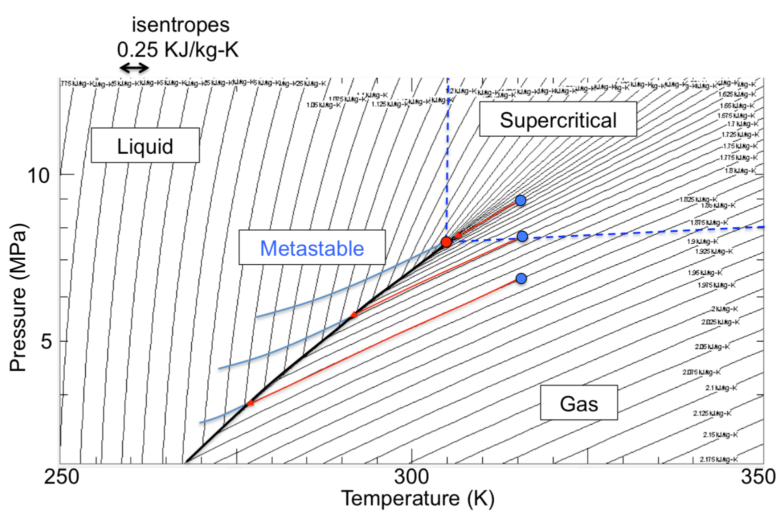

Figure 5. Pressure–temperature diagram illustrating isentropic expansion in experimental nozzle test section at different charge tank conditions.

Condensation Assessment

Blowdown tests were carried out at supercritical inlet conditions and approaching the critical point at initial charge tank pressures of 74.4 bar, 78.6 bar and 89.1 bar respectively, as shown in Figure 6. The test was carried out until the charge tank pressure dropped to 55 bar, 67 bar and 68 bar respectively so as to investigate potential condensation for an extended range of compressor inlet conditions. For all inlet conditions, expansion occurred into the two-phase region in the converging nozzle section.

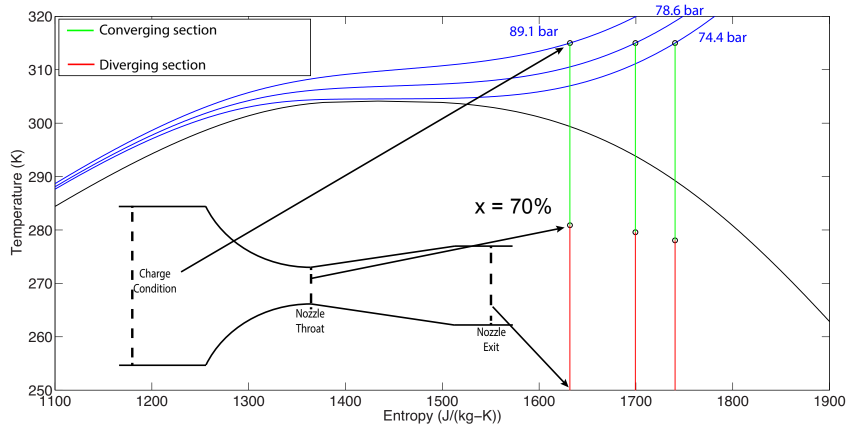

Figure 6. Temperature-Entropy diagram illustrating charge tank conditions and expansion in converging nozzle section below saturation conditions for tests away from critical point.

Assessment Away from the Critical Point:

The results of the numerical simulation for the test closest to saturation (89bar) are shown in Figure 7.Since the nozzle exit pressure was set to atmospheric conditions, the CO_2 temperature drops below the triple point and outside the range of the real gas tables generated with REFPROP. For such values the table extrapolation yields significant challenges and possibly numerical instabilities. Therefore, the nozzle diverging section is intentionally truncated in the simulations to ensure convergence..

Even though the fluid attains super-cooled temperatures, $T\text{-}T_{sat}$ up to 36 K, the two-phase calculations show a negligible fraction of liquid CO_2. This suggests that condensation does not occur. It can therefore be concluded that the computed mass fraction of condensed CO_2 is not sufficient to have an impact on the internal fluid behavior. The implication is that two-phase flow simulations are not required as long as the EOS model is amended with the metastable properties of the fluid. This is further investigated through a time scale analysis. It is found that the timescale ratio, τ_{cl}, becomes ~10^{-4}, implying that the time required for stable liquid droplets to form is significantly larger than the residence time of the flow inside the nucleating region. Figure 8 compares the computational results with the experimental measurements and the theoretical 1-D real gas model reported in [2]. The measured static pressure distribution along the nozzle wall is in good agreement with the computed values, mostly with errors less than 0.5, except for the second pressure measurement where the error is about 3%. This is likely caused by small differences in nozzle geometry due to the manufacturing and CAD tolerances.

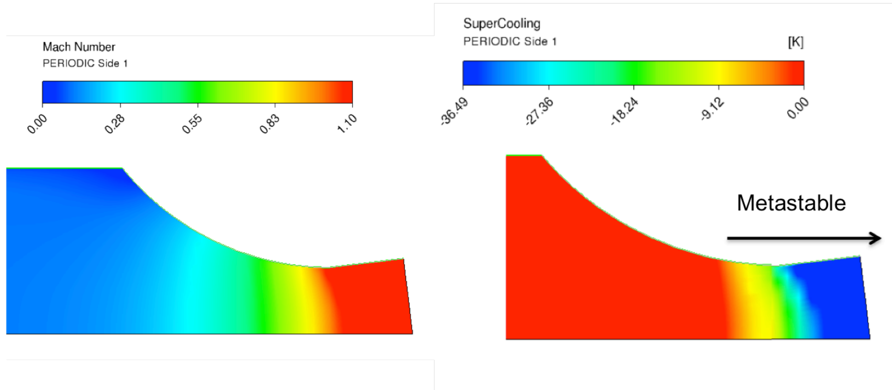

Figure 7. Computed contours of Mach number and Super-cooling ($T-T_{sat}$) in converging-diverging nozzle.

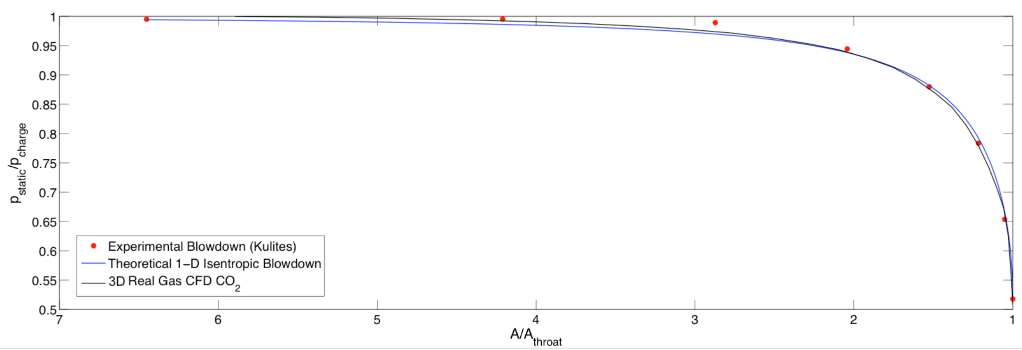

Figure 8. Static pressure along the nozzle wall – Experimental data (red dots) compared with 1D real gas model (blue line) and two-phase, 3D .computation (black line)

The experimental findings, backed by the calculations, suggest that CO_2 compressor with inlet conditions away from the critical point operate without condensation, despite local flow expansion into the two-phase region. Figure 8 shows no drop in static pressure, as expected when condensation is absent. More specifically, the measurements indicate that, away from the critical point, condensation does not occur for Mach numbers up to sonic conditions. This is corroborated by the limited super-cooling in the convergent section per the numerical assessment of non-equilibrium condensation.

To quantify potential changes in static pressure distribution in the case of condensation, a one-dimensional compressible flow analysis with heat addition was carried out [2]. As indicated in Figure 6, the quality near the throat is 70%. It is thus safe to assume condensation onset at 30% moisture in the influence coefficient based approach. The results are plotted on top of the previous findings in Figure 9. Heat addition due to condensation leads to thermal choking before the throat and a 16% drop in static pressure near sonic conditions.

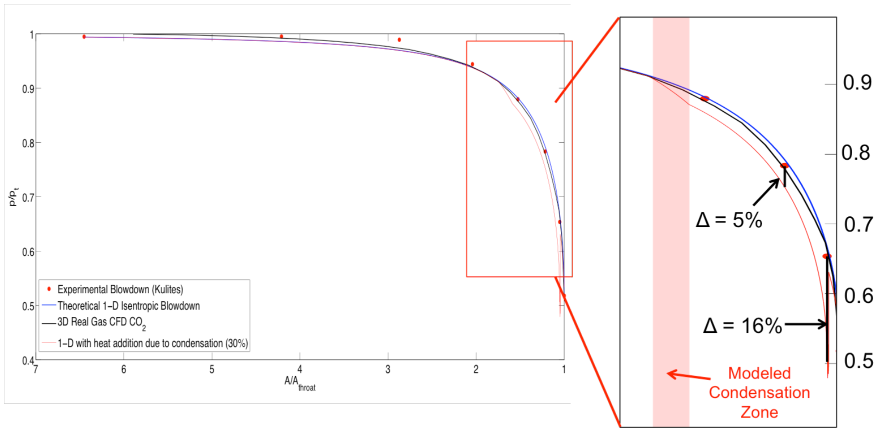

Figure 9. Static pressure along the nozzle wall – Experimental data (red dots) 1D theoretical model for real gas (blue line), two-phase 3D CFD (black line) and 1-D theoretical model with heat addition due to latent heat of condensation (red line)

It is expected that a condensation onset at about 0.1% presence of moisture can be detected through simple static pressure measurements, as demonstrated for CO_2 at low pressure in [4]. A negligible amount of droplet formation could be present, but it is expected to have no impact on performance and stability of compressors stages. Condensation occurs in the diverging section and further testing is ongoing with increased measurement resolution in the diverging section to characterize the dynamics of the flow. Similarly, no noticeable static pressure drop was observed in all experiments away from the critical point (at 89 bar, 74 bar and 70 bar) suggesting that condensation can be ruled out. This is consistent with similar experiments with water steam conducted by Schnerr [5], where the Mach numbers were in the range 1.3-1.5 at condensation onset.

The analysis is extended to a candidate S-CO_2 compressor defined in [2]. The analysis considered different inlet states progressively approaching the critical point, as shown in Figure 10 Doing so, the fluid expands deeper and deeper into the two-phase region while the surface tension of the fluid vanishes asymptotically. This suggests a significant increase in the nucleation rate such that t_r/t_n might become unity. However, the computations show t_r/t_n<<1 for the cases away from the critical point.

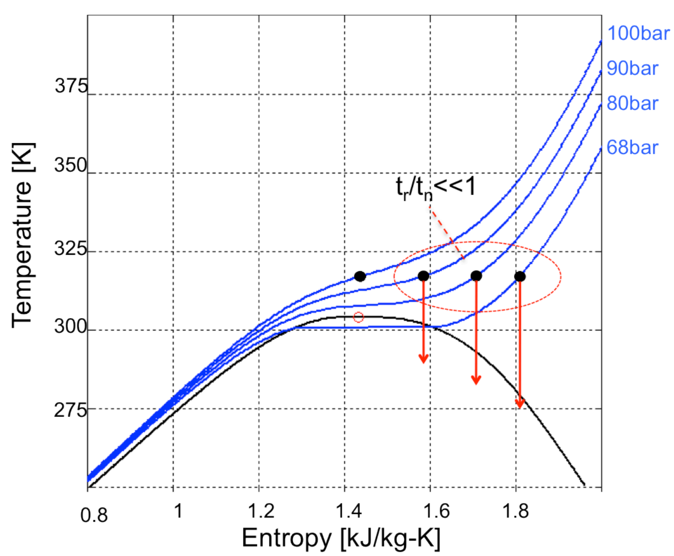

Figure 10. Analysis of condensation in S-CO_2 compressor approaching critical point [2]

Near the critical point a 5% variation in surface tension leads to differences in the rate of condensation J of up to 2 to 3 orders of magnitude and much reduced nucleation times. However, because of the large variations of thermodynamic properties at the critical point it is difficult to separate two-phase effects from real gas effects and increased resolution of the pressure measurements is required. Moreover, the extrapolation of the real gas properties into the metastable region yields increased difficulty due to the sharp gradients of the thermodynamic properties, requiring validation with the experimental data. This is the focus of current and future research.

The fluid properties at metastable conditions are required to define the Gibbs free energy of the vapor in the non- equilibrium condensation computations. As metastable properties have not yet been measured experimentally for CO_2, especially at high pressure and near the critical point, the gas properties were extrapolated into the liquid domain. A similar technique has been used extensively in the past to model non-equilibrium condensation for water vapor in steam turbines, leading to the development of the IAPWS-97 database [12]. However, to the authors' knowledge no such database has been published for CO_2 at high pressures. In this study a cubic extrapolation was used as described in [2].

Although the agreement between the computations and the experimental measurements are encouraging, the metastable phase characterization used in the computations must be more thoroughly validated with experimental data. This is the focus of ongoing and future work. To define the state of the metastable fluid, two thermodynamic properties need to be measured. In the current experimental setup the static pressure and the speed of sound are measured. Optical flow measurements are challenging at high pressure and at small scale so that a novel method was developed to experimentally determine the speed of sound.

Metastable Phase Characterization through Speed of Sound Measurements:

The speed of sound in the fluid is determined through measurements of the Helmholtz resonance frequency and known geometry,

$$f_H = \frac{c}{2\pi}\sqrt{\frac{A}{VL}} \tag{6}$$

where f_H is the Helmholtz frequency in Hz, *c* is the speed of sound of the fluid in the plenum, *A* is the cross-sectional area of the neck, *V* is the plenum volume, and *L* is the length of the neck, as shown in Figure 11. A fast response Kulite pressure transducer forms the plenum endwall. It is assumed that the flow in the plenum is in thermodynamic equilibrium with the flow near the nozzle endwall. The speed of sound is deduced using forced response experiments where the Helmholtz resonators (HR), placed along the nozzle wall, are excited by sound waves emitted from a piezoelectric membrane located upstream of the nozzle bellmouth inlet in the charge tank as shown schematically in Figure 12. Multiple frequency sweeps of the piezoelectric actuator are carried out to determine the dynamic response of the Helmholtz resonator. Transfer functions, from piezoelectric actuator command input to Kulite sensor output are determined via spectral analysis. The resonance frequency is identified in the transfer function via gain peak and phase roll off. The error in speed of sound measurement is mostly set by the manufacturing tolerances of the HR dimensions. Given the geometric tolerances in L, D, and H of 1%, 2% and .14% respectively, a maximum error in the speed of sound of 2% is expected..

The development of this measurement technique is still in progress. The speed of sound measurement via Helmholtz resonators has so far been demonstrated at static conditions using air as working fluid. First results are plotted in Figure 13 where the measured peak response and phase roll-off are at the expected frequency of 3250 Hz, corresponding to the speed of sound for air at room temperature. Assessment of this method in CO_2 during blowdown testing near and at the critical point are currently ongoing.

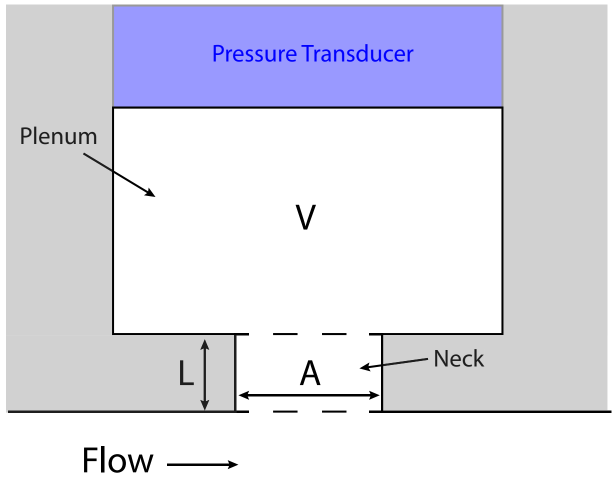

Figure 11. Schematic Representation of Helmholtz Resonator

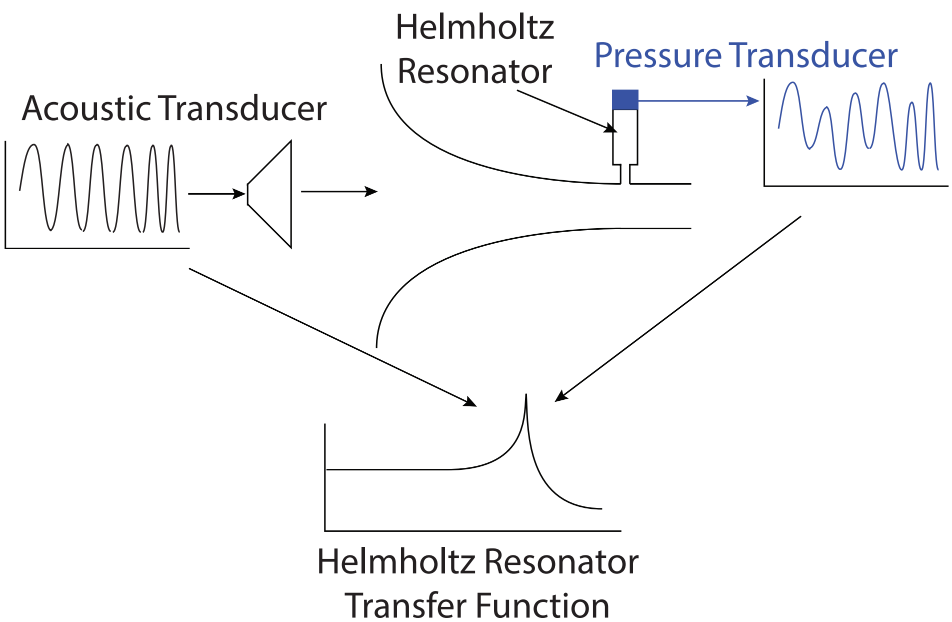

Figure 12. Helmholtz Resonator Excitation Concept

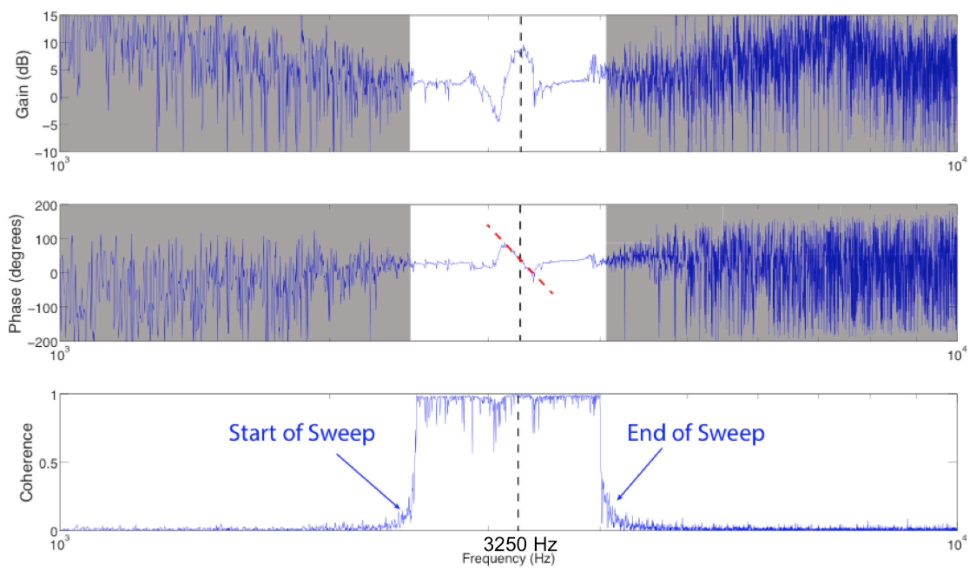

Figure 13. Helmholtz Resonator Excitation at 3250 Hz corresponding to speed of sound in air – Gain [dB] (top), phase (mid) and coherence (bottom)

CONCLUSIONS

This paper presents a systematic assessment of condensation effects in supercritical CO_2 compressors. While the main focus is on investigating the condensation onset in a converging-diverging nozzle when approaching the critical point, the proposed framework serves as a foundation for the definition of the impact of two-phase flows in turbomachinery operating with dense gases and near saturation.

A non-dimensional criterion that determines whether condensation might occur is established. This criterion relates the nucleation time, which depends on the rate of expansion through the vapor-pressure curve, and the residence time of the flow under saturated conditions. Two-phase flow effects can be considered negligible when the ratio of the two time scales is smaller than unity.

Experimental tests, backed by two-phase calculations of a canonical test case reveal that condensation cannot occur at the rate of expansion characteristics of compressors operating away from the critical point. More specifically it is found that, for conditions away from the critical point, the time required for stable droplets to form is by four orders of magnitude longer than the residence time of the flow in the nucleating region.

In the immediate vicinity of the critical point, two-phase effects are expected to become more prominent. The timescale ration increases due to reduced nucleation times and larger residence times. Further investigation is required to assess the behavior near the critical point and at supersonic Mach numbers in the diverging section. This is the focus of ongoing and furture research.

NOMENCLATURE

A	area
c	speed of sound
f_h	Helmholtz resonator frequency
g	specific Gibbs free energy
G	Gibbs free energy
J	nucleation rate

k	Boltzmann's constant
l	condensation length scale
L	Helmholtz resonator length scale
m	molecular mass
n_s	isentropic pressure exponent
p	pressure
r	droplet radius
R	nozzle throat radius
s	entropy
t_n	nucleation time
t_r	residence time
T	temperature
T_{sat}	saturation temperature
v	specific volume
V	volume
θ	contact angle
ρ	density
σ	surface tension
τ_{cl}	condensation limit ratio

subscripts:

$_{ave}$	average
$_{l}$	liquid phase
$_{t}$	total
$_{v}$	vapor phase

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ACKNOWLEDGEMENTS

This research was funded by Mitsubishi Heavy Industries Takasago R&D Center which is gratefully acknowledged. In particular, the authors would like to thank Dr. Eisaku Ito, and Mr. Akihiro Nakaniwa for their support and for providing experimental data.