An Investigation of Condensation Effects in Supercritical Carbon Dioxide Compressors

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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 (Wright, S., 2012, "Overview of S-CO_2 Power Cycles," Mech. Eng., 134(1), pp. 40–43), 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. The objectives are 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 investigated in a systematic manner approaching the critical point. A nondimensional 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. The study shows that condensation is not a concern away from the critical point. Numerical two-phase calculations supported by experimental data indicate that the timescale associated with nucleation is much longer than the residence time of the flow in the saturated region, leaving little opportunity for the fluid to 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 longer 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. [DOI: 10.1115/1.4029577]

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 as reported by Wright [1], Baltadjiev et al. [2] and Rinaldi et al. [3] and as shown schematically in Fig. 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 nonequilibrium state. This usually accounts for about 45% of the overall loss due to phase change in steam turbines and has the potential to greatly reduce the efficiency of S-CO_2 compressors.

Condensation due to rapid expansion in high-speed flows usually occurs at nonequilibrium conditions [5]. Due to the rapid expansion rate, the fluid can reach pressures and temperatures below saturation without condensation. This is illustrated schematically in Fig. 2 for CO_2 in a temperature–pressure diagram. In an isentropic expansion from 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 nonequilibrium or metastable state D over a finite period of time [6]. This is often referred to as the Wilson line or the spinodal limit. Schnerr [5] indicates that an expansion rate of 1 °C/μs, typical of high-speed flows in converging–diverging nozzles, leads to subcooling of up to 30–40 K 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

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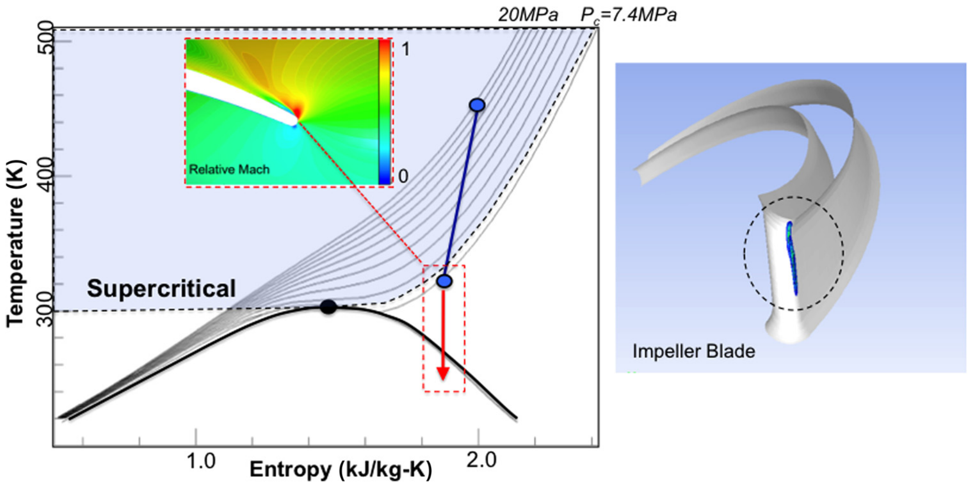

Fig. 1 Temperature-entropy diagram illustrating isentropic expansion to saturation near impeller leading edge

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], Ryzhov [6], Guha [7], Duff [8], and Nakagawa et al. [9] 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 [8] 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. [10] conducted computational fluid dynamics (CFD) simulations of the two-phase flow of CO_2 in converging diverging nozzles. The study used the data from Nakagawa et al. [9] 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 Baltadjiev 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. Baltadjiev et al. [2] suggest that this might not be the case away from the critical point, however, the study requires further experimental evidence to support the numerical calculations.

Modeling the phase transition process requires the definition of (i) the energy required to form a droplet of a critical radius that

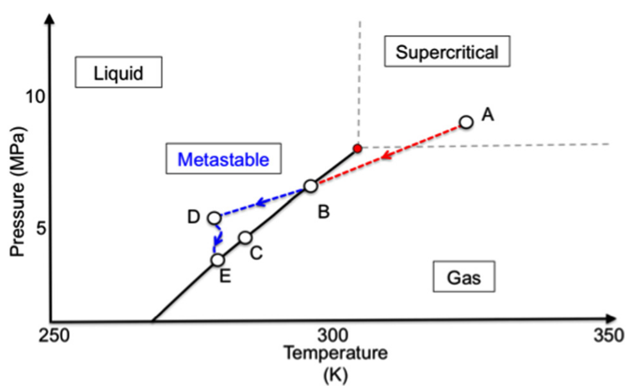

Fig. 2 Pressure–temperature diagram illustrating isentropic expansion to metastable conditions

can grow to stable size and (ii) the rate of formation of these critical droplets. Classical nucleation theory [11,12] defines the Gibbs free energy and the rate of condensation 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 $\sim$4 orders of magnitude and lead to nearly ten orders of magnitude larger condensation rates. However, Schnerr [5] and Duff [8] 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 [8]. 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 can be 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.

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 nondimensional 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 subcooling 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 if the isentropic expansion does not reach 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 14.5 [13] was used for all the calculations. A detailed description of the numerical methodology can be found in Refs. [2] and [14]. 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 equations are closed through the two-equation k-ω shear stress transport turbulence model. NIST's formulation of the Span and Wagner equation of state (EOS) model, RefProp [15], was adopted and incorporated in the CFD solver in the form of lookup tables [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 14.5. This is based on classical nucleation theory under the assumptions of nonequilibrium, homogeneous condensation. Further detail of the numerical methodology can be found in Ref. [2]. Heterogeneous condensation was initially modeled including the droplet contact angle θ, however, the results, which are consistent with the literature [5,8], 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 Ref. [2].

The nucleation time is defined

$$t_n = \frac{1}{J_{max} V} \tag{1}$$

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

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

with

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

and

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

The residence time of fluid in the saturated region is defined as

$$t_r = \frac{l}{c_{ave}} \tag{5}$$

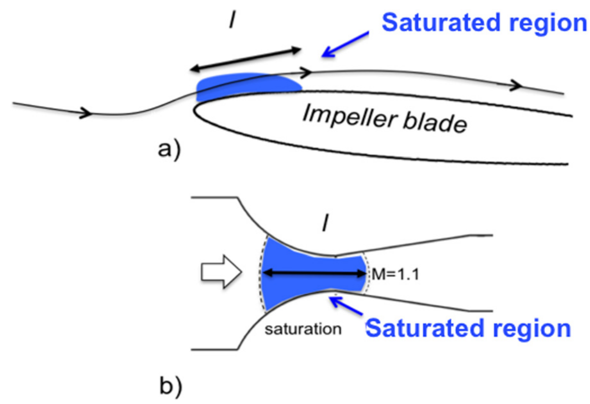

Fig. 3 Definition of condensation length scale and saturated region for compressor blade (*a*) and nozzle test section (*b*)—Mach number in candidate compressor below 1.1 [2]

where l is the length of the saturated region as shown schematically in Fig. 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 longer than the residence time, implying that condensation cannot occur.

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

The experiments are nonrotating, simple blowdown type tests using pressurized CO_2 bottles in an open-loop arrangement as shown schematically in Fig. 4. The fluid from commercially 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 Fig. 5. The inlet conditions in the tank are indicated by the gray circles lined up to the right, the arrows extending from these circles represent isentropic expansions from the gas phase, and the dashed lines illustrate the expansion into the metastable region. The critical point is marked as a white circle. 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 a 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

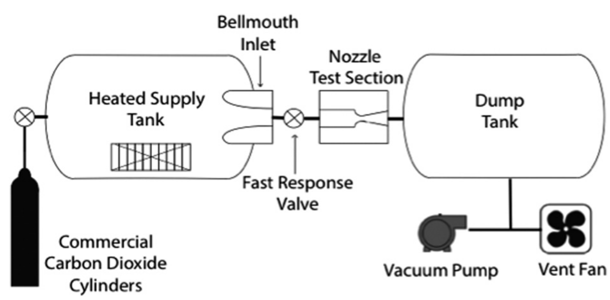

Fig. 4 Laboratory scale experiment for assessment of supercritical CO_2 internal flow

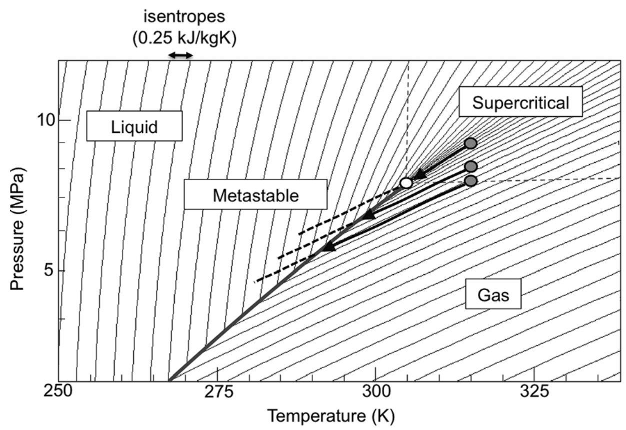

Fig. 5 Pressure–temperature diagram illustrating isentropic expansion in experimental nozzle test section—variation of nozzle inlet conditions leads to increased excursion into metastable region

dimensions of the nozzle test section are consistent with and representative of the characteristic length scale of the saturated region in the candidate compressor. The details of the compressor geometry are given in Ref. [2]. The rate of expansion, dT/dt, is set to $1\,^{\circ}\mathrm{C}/\mu\mathrm{s}$, a typical value at the leading edge of the impeller. The nozzle throat diameter is $D = 5$ mm, and the length of the saturated region varies from D/2 to 3/2D. 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. The 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 later in the Metastable Phase Characterization Through Speed of Sound Measurements section.

Assessment of Condensation

Blowdown tests were carried out at supercritical inlet conditions and approaching the critical point at initial charge tank pressures 74.4, 78.6, and 89.1 corresponding to P/P_c 1.01, 1.06, and 1.2, respectively, as shown in Fig. 6. The isentropic expansion in the nozzle leads to supercritical conditions near the throat with an entropy ratio S/S_c for each test case of 1.16, 1.13, and 1.03, respectively. The test was carried out until the charge tank pressure dropped to $P/P_c \sim 0.9$ 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.

Condensation Assessment Away From the Critical Point. The results of the numerical simulation for the test closest to saturation ($S/S_c = 1.03$) are shown in Fig. 7. Since the nozzle

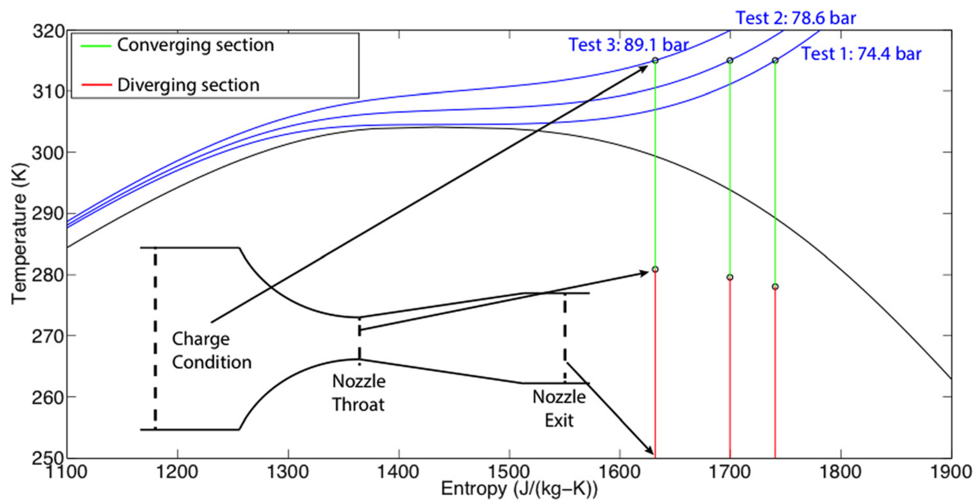

Fig. 6 Temperature-entropy diagram illustrating charge tank conditions and expansion in converging nozzle section below saturation conditions for tests away from critical point

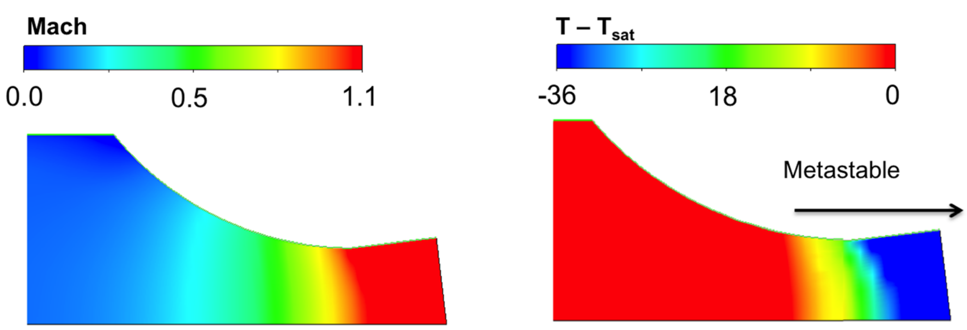

Fig. 7 Computed contours of Mach number and super-cooling (T-T_{sat}) in converging–diverging nozzle

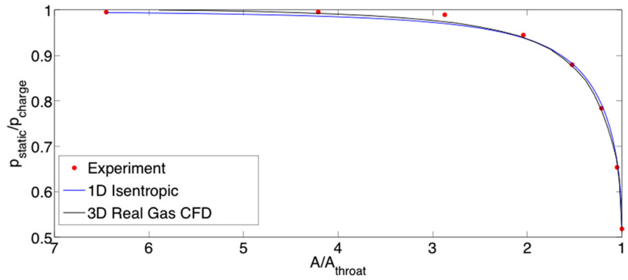

Fig. 8 Static pressure along the nozzle wall—experimental measurements agree with 1D real gas model and two-phase 3D computations, suggesting no condensation can occur in nozzle converging section

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-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 $\sim 10^{-4}$, 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 1D real gas model reported in Ref. [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 flow recirculation in the abrupt transition between the upstream duct and nozzle inlet.

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,

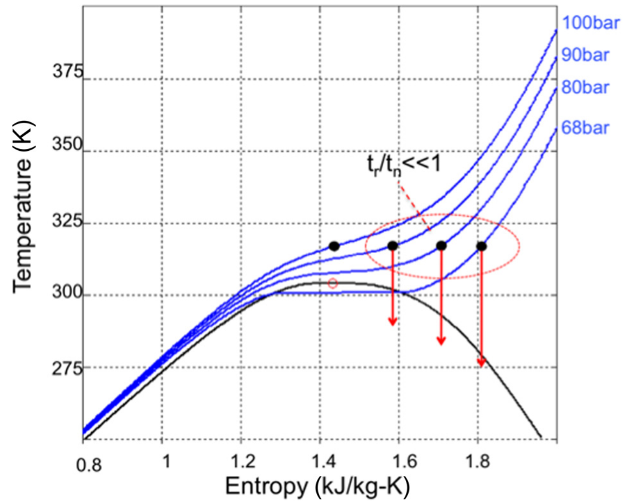

Fig. 10 Analysis of condensation in S-CO_2 compressor approaching critical point [2]—timescale analysis suggests condensation time much smaller than residence time

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 nonequilibrium 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 using influence coefficients for real gases [2]. As indicated in Fig. 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 Fig. 9. Heat addition due to condensation leads to thermal choking before the throat and a 16% drop in static pressure near sonic conditions.

It is expected that condensation onset can be detected through simple static pressure measurements at about 0.1% of moisture, as demonstrated for CO_2 at low pressure [8]. A negligible amount of droplet formation could be present, but it is expected to have no impact on compressor performance and stability. Further analysis confirms that condensation and dry ice formation occurs in the diverging section. Similarly, no noticeable static pressure drop was observed in all experiments away from the critical point (at

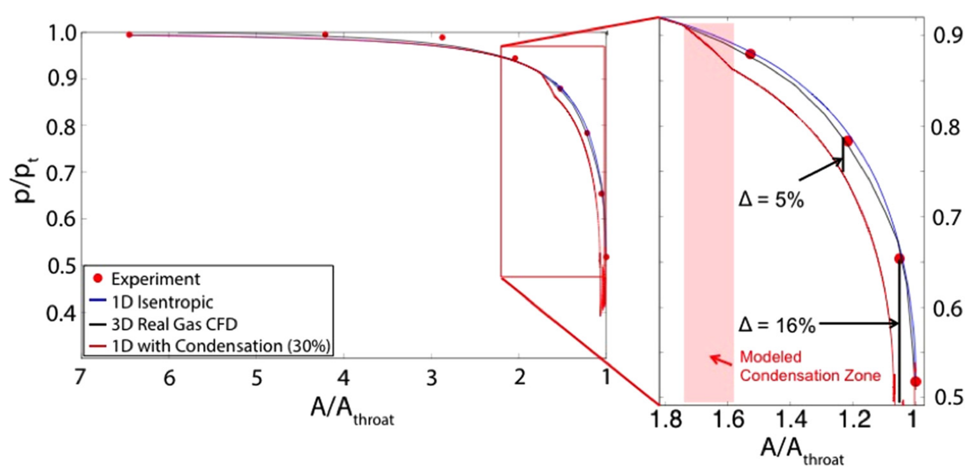

Fig. 9 1D real gas analysis illustrates impact of potential condensation on static pressure in nozzle converging section—latent heat of condensation leads to thermal choking before throat and a 16% drop in static pressure. Experimental measurements show no pressure drop, ruling out condensation.

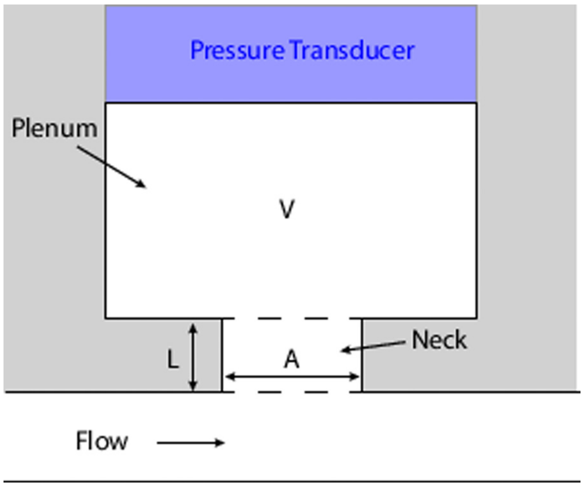

Fig. 11 Schematic representation of Helmholtz resonator

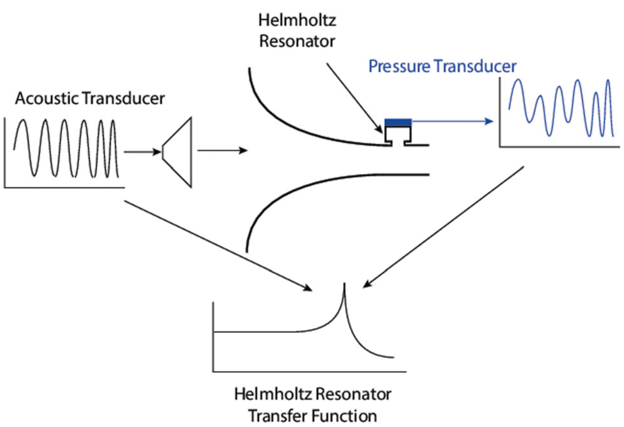

Fig. 12 Helmholtz resonator excitation concept

$S/S_c = 1.13$ and 1.16) 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 Refs. [2] and [14]. The analysis considered different inlet states progressively approaching the critical point, as shown in Fig. 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 $t_r/t_n \ll 1$ for the cases away for $S/S_c > 1.01$.

At the critical point, a 5% variation in surface tension leads to differences in the rate of condensation of up to 2–3 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 becomes more challenging due to the sharp gradients in thermodynamic properties, requiring validation with experimental data.

The fluid properties at metastable conditions are required to define the Gibbs free energy of the vapor in the nonequilibrium 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 nonequilibrium condensation for water vapor in steam turbines, leading to the development of the IAPWS-97 database [13]. 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 Ref. [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

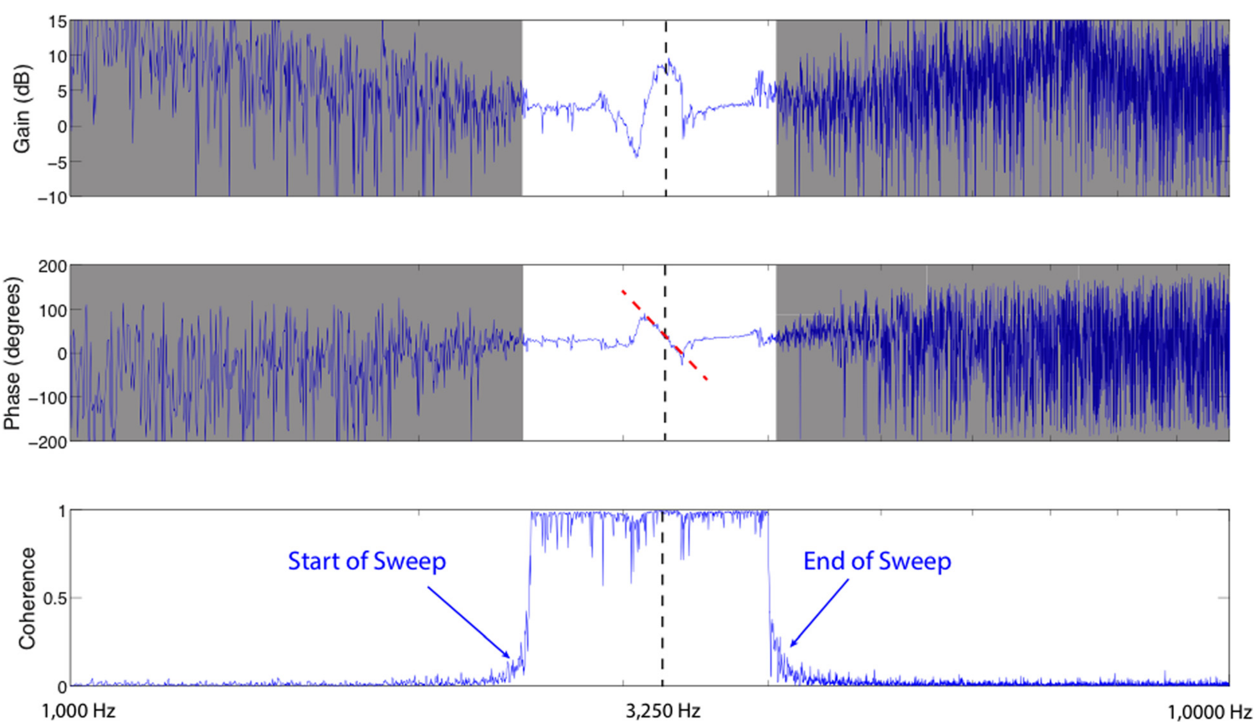

Fig. 13 Speed of sound measurement in air using forced response Helmholtz resonator experiments—gain (dB) (top), phase (center), and coherence (bottom)

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 Fig. 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 Fig. 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 peak gain 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 HR has so far been demonstrated at static conditions using air as working fluid. First results are plotted in Fig. 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 is currently ongoing.

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 near saturation conditions.

A nondimensional 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, supported by two-phase calculations of a canonical test case reveal that condensation cannot occur at the rate of expansion characteristics of compressors operating away ($S/S_c > 1.01$) 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 ratio 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 future research.

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Nomenclature

A = area
c = speed of sound
D = nozzle throat diameter
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
P = pressure
r = droplet radius
s = entropy
S = entropy
T = temperature
t_n = nucleation time
t_r = residence time
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
c = critical
l = liquid phase
t = total
v = vapor phase

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