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# Diffuser performance of centrifugal compressor in supercritical CO<sub>2</sub> power systems

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# Abstract

The paper focuses on understanding the performance of a vaned diffuser in a supercritical  $CO_2$  compressor using real gas assumptions. The rapidly changing properties of  $CO_2$  in the non-ideal thermodynamic region can have a significant impact on the performance of the diffuser. To account for this, the relationship between the flow properties (i.e. fundamental derivative) and the local geometry (i.e. cross-sectional area of the nozzle) has been discussed theoretically. To examine it analytically, the study has considered the influence of real gas properties on the performance of a vaned diffuser using computational fluid dynamics (CFD) modelling. The selected compressor stage geometry is similar to the compressor impeller tested in the Sandia s $CO_2$  compression loop facility. The effect of changes in the number of blades and the corresponding changes in the cross throat area on the flow properties such as density and speed of sound were investigated and discussed. The results illustrate that a diffuser with a higher number of blades (smaller throat area) compared to a diffuser with a wider throat area has a higher probability of creating flow instability in the passage stage.

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| Nomenclature       |   |
|--------------------|---|
| А                  | cross-sectional area                                    |
| с                  | speed of sound  |
| $c_p$              | isobaric specific heat capacity                         |
| Μ                  | Mach number   |
| Р                  | pressure  |
| s                  | entropy   |
| t                  | throat  |
| Т                  | temperature   |
| u                  | velocity  |
| W <sub>shaft</sub> | shaft work  |
| Х                  | coordinate in flow direction                            |
| $\beta_p$          | isobaric compressibility, $1/v (\partial v/\partial T)$ |
| γ                  | ratio of specific heats                                 |
| Γ                  | fundamental derivative                                  |
| v                  | specific volume   |
| ρ                  | density   |

# 1. Introduction

The environmental impact of fossil fuel consumption has brought global attention to the earth's primary sources of energy. There is an estimation that energy and industry-related emissions are predicted to more than double by 2050 compared to 1990 levels [1]. Therefore, there is an urgent need to address fuel switching options and intelligent use of existing resources. One way of reducing the energy demand of industrial processes is to recover high temperature waste heat and convert this to electrical power where there is no need for the direct use of the heat. Waste heat to electrical power conversion can be achieved with different technologies, such as the conventional Steam Rankine Cycle (SRC) and the Organic Rankine Cycle (ORC), amongst others. To increase the overall thermal efficiency of these systems, even at moderate turbine inlet temperatures, carbon dioxide (CO<sub>2</sub>) is being introduced as novel working fluid for waste heat to power systems [2].

CO<sub>2</sub> is a high density working fluid; this enables the design of equipment that is highly compact for the same power output, when compared to SRC and ORC equipment. Additionally, CO<sub>2</sub> is a low-cost, non-flammable and non-toxic working fluid [3]. Supercritical carbon dioxide (sCO<sub>2</sub>) systems were originally conceived for nuclear or concentrated solar power generation applications [4, 5]. However, the availability of high-temperature waste heat in industrial environments and the inability of working fluids employed in ORC systems to operate efficiently at these temperatures, provided the impetus for consideration of the sCO<sub>2</sub> cycle for a broader range of applications, including waste heat for power generation.

To date, most of the interest and development of sCO<sub>2</sub> heat-to-power systems has taken place in the MWe power range, for market and economic reasons, and the availability of sCO<sub>2</sub> components from the petrochemical industry. Very little work has been carried out in the sub MWe power range due to challenges of turbomachinery design and costs. Only two significant empirical studies, by Sandia National Laboratory and Tokyo Institute of Technology, have been carried out to demonstrate the feasibility of sCO<sub>2</sub> Brayton cycle applications and to examine the system performance and characteristic [6-8].

Other researchers have focused on the modelling and defining the real gas thermodynamic effects on blade performance. Among them, Behafaird and Podowski [9] examined supercritical  $CO_2$  flow inside a high-speed compressor using a numerical DNS solver. Their main focus was on validation of the numerical modelling and comparison of the results of the real gas and ideal gas models with the experimental data published by Sandia laboratory. Similarly, in another CFD modelling study, Pecnik et al. [10] used a three-dimensional simulation to investigate the performance of a supercritical  $CO_2$  centrifugal compressor in the thermodynamic region slightly above

the vapour-liquid critical point. Following these investigations, Baltadjiev et al. [11] investigated real gas effects on the performance of centrifugal compressors operating in the supercritical CO<sub>2</sub> region using CFD modelling. They studied chock and compressor stage matching. The problem of condensation has also been considered by Baltadjiev et al. [11] and by Lettieri et al. [12]. These studies combined numerical simulations with experimental tests and considered the possibility of droplet formation while approaching the critical point. The results showed that close to the critical point, two-phase effects are expected to become more prominent due to longer residence times of the flow.

It was also observed that operation in the vicinity of the critical point (which is desired for highest efficiency) causes instabilities in the compressor performance that needs to be addressed through the design process [6]. Up to now, little attention has been paid to the effect of supercritical flow properties on turbomachinery design features. One exception is the work of Colonna and Harinck [13] that investigated the real gas effects on turbine nozzles of Organic Rankine Cycle systems with siloxane MDM as working non-ideal fluid. They concluded that standard design methods are not well suited for design optimization in the strongly non-ideal thermodynamic regions.

### 2. Scope and approach

While most of the previous works have been carried out on the internal flow behavior of  $sCO_2$  in turbomachinery, very little attention was placed on the effect of real gas properties on the the design methods employed. This study focuses on fundamental design aspects to achieve the compressor target operation conditions and to improve the performance in the supercritical region. For this purpose, a vaned diffuser is considered as a case study. The advantages of having a vaned diffuser compared to a vaneless diffuser for  $sCO_2$  compressors have been studied by Lettieri et al. [14]. Consequently, in the present study, only a vaned diffuser has been considered for the investigations.

From the early study on compressors performance, the importance of the vaned diffuser design, specifically the number of vanes, has been emphasised since vaned diffuser stall is relatively severe, and can lead to flow instability and surge [15, 16]. In the presence of real gas, the number of blades becomes a dominant factor due to the change of cross-sectional area and its impact on the compressor performance. Therefore, in this paper, firstly analytical investigations are carried out to determine the relationship between the area change and the flow properties. Secondly, CFD modelling of a designed sCO<sub>2</sub> compressor (operating close to the critical point) was carried out to investigate the flow stability for two different vane numbers (13 and 17). The selected compressor has similar dimensions with the experimental compressor investigated at Sandia National Laboratories [6]. The compressor impeller is a relatively small component, of diameter 37.3 mm with 6+6 vanes.

#### 3. Real gas effect on one-dimensional flow

 $sCO_2$  compressor design features cannot be examined unless there is a clear understanding of the relationship between the real gas thermodynamics and compressor aerodynamics. The real gas effects cause dramatic changes in the flow behaviour that impact the governing equations. The following is the equation of mass conservation for quasione-dimensional flow in a nozzle of variable cross-sectional area A(x), where x is the coordinate in the flow direction:

$$\frac{d}{dx}(\rho uA) = 0\tag{1}$$

The conservation of momentum with the presence of shaft work can be written as following:

$$udu + \frac{1}{\rho}dp = -dw_{shaft} \tag{2}$$

$$\frac{dT}{T} = \left[\frac{M^2}{\left(1 - M^2\right)}\frac{\gamma - 1}{\beta_p T}\right]\frac{dA}{A} - \left[\frac{\beta_p T}{\left(1 - M^2\right)}\right]\frac{dw_{shaft}}{c_p T}$$
(3)

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$$\frac{du}{u} = -\left[\frac{1}{\left(1-M^2\right)}\right]\frac{dA}{A} + \left[\frac{1}{\left(1-M^2\right)}\frac{\left(\beta_p T\right)^2}{\left(\gamma-1\right)}\right]\frac{dw_{shaft}}{c_p T}$$
(4)

More details of equations (3 and 4) can be found in Baltadjiev et al. [11]. The incremental Mach number changes due to the area change are summarised below and represent the general case for flow in a channel with varying area and shaft work:

$$\frac{dM^2}{M^2} = \frac{2du}{u} - \frac{dT}{T}$$
(5)

$$\frac{dM^2}{M^2} = -2\left[\frac{1+(\Gamma-1)M^2}{(1-M^2)}\right]\frac{dA}{A} + \left[\frac{1}{(1-M^2)}\frac{1}{\upsilon}\left(\frac{\partial\upsilon}{\partial T}\right)_p\frac{\Gamma}{(\Gamma-1)}\right]\frac{dw_{shaft}}{c_p}$$
(6)

From the above, the sonic condition can be linked to the local flow geometry. At the condition M=1, the quantity in the square brackets must be zero for continuous variation of the Mach number through the sonic point. For this reason, the area changes must approach the following limitation as the sonic point is approached:

$$\frac{1}{A}\frac{dA}{dx} \rightarrow \frac{1}{2(\Gamma-1)}\frac{1}{\nu}\left(\frac{d\nu}{dT}\right)\frac{dw_{shaft}}{c_{p}dx}, \quad M \rightarrow 1$$
(7)

The above relation determines the stability limit.  $\Gamma$  is the fundamental derivative. The non-dimensional definition of  $\Gamma$  is as follows:

$$\Gamma = 1 + \frac{\rho}{c} \left( \frac{\partial c}{\partial \rho} \right) = \frac{1}{2} \rho^3 c^4 \left( \frac{\partial^2 v}{\partial P^2} \right) = \frac{v^3}{2c^2} \left( \frac{\partial^2 P}{\partial v^2} \right)$$
(8)

where the sound speed is defined by:

$$c^{2} = \left(\frac{\partial P}{\partial \rho}\right)_{s} = -v^{2} \left(\frac{\partial P}{\partial v}\right)_{s} > 0$$
(9)

The dynamic behaviour of the compressible fluids has a direct relation with the fundamental derivative. For an ideal gas  $\Gamma = (\gamma+1)/2$  is always greater than one. However, Zeldovich and Raizer [17] found that  $\Gamma$  will be negative for a van der Waals substance in the vapour phase near the saturation line, at the pressure somewhat below the critical pressure. It then leads to an inverted gas dynamic behavior [18]. Therefore, in this region (the inversion zone), there is a possibility of generation of rarefaction shock waves. Also, when  $\Gamma$  is close or equal to zero, entropy is small (albeit high enough to avoid condensation) that leads to improving efficiency in the turbomachinery [19]. Although, the desire is to design the turbomachinery for this condition without having negative  $\Gamma$ , accurate estimation of  $\Gamma$  is challenging due to the uncertainty in the speed of sound in the vicinity of the critical point. This issue is highlighted in supercritical turbomachinery where the fundamental derivative depends on the area variation in the supercritical region. In this study, the value of inlet conditions is chosen carefully to avoid condensation in order to quantify the maximum efficiency without reaching the inverse zone for the fundamental derivative.

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# 4. Modelling setup

Simulations were carried out at fixed initial conditions for two different vane numbers. The performance of both has been compared to understand the effect of the throat area. CFX 17.1 was employed to perform single passage steady state calculations. The diffuser mesh was generated in ANSYS-TurboGrid. An ATM-optimised topology was employed inside the impeller (see Fig. 1), considering diffuser flow path meshes with approximately 10<sup>6</sup> nodes. Also, in order to accurately capture the friction losses, careful grid refinement was performed close to the blade boundaries. Two different vane numbers (13 and 17) were investigated. The compressor stage operating conditions for each case were kept the same.

To simulate the real gas effect, the Span-Wagner EOS model was used to accurately generate the flow properties [10]. For this purpose, an RGP (real gas property) format table was created to implement the variable properties in the CFX code. The user-defined table includes CO<sub>2</sub> features such as specific heat ratio and density near the critical point which fluctuates due to the phase change effect. These characteristics are created by the NIST REFPROP 8.0 fluid property database. The generated property files were combined with a MATLAB code to create a lookup table as an input of TASCflow RGP in ANSYS CFX 17.1.



Fig. 1. Supercritical CO<sub>2</sub> compressor stage, the diffuser mesh by TurboGrid 17.1 and the throat area (At).

Turbulence k-e and total energy including the viscous work term were used for the  $CO_2$  fluid, with pressure 75 bar and temperature 305 K defined as inlet boundary conditions with flow direction normal to the boundary. Outlet average static pressure of 145 bar was chosen as the outlet boundary condition. The compressor wheel speed was chosen to be 80,000 rpm and the Reynolds number at the inlet of the diffuser  $10^{+7}$ . A parametric check on convergence was employed by monitoring the momentum, energy, pressure ratio, efficiency and mass flow imbalance to ensure that these reached limits; the reduction of all RMS features residual below  $10^{-4}$ .

## 5. Results

Flow simulations close to the critical point were performed to demonstrate the effect of supercritical conditions on the compressor diffuser operation. As it can be seen in Fig. 2, the Mach number for VN17 is greater than unity at the throat area. In the model VN17, the compressibility of the flow is significant, and since the diffuser span is small compared to the impeller dimensions, it will develop instability in the compressor performance. Also, from this figure, it can be concluded that the velocity into the VN17 diffuser is close to supersonic conditions that will lead to a quite narrow operating range.



Fig. 2. Mach number filed at 50% span for diffusers with inlet impeller stagnation pressure of 75 bar and inlet diffusers pressure around 125 bar.

The results also demonstrate the effect of the cross area on the inlet pressure. The models for the two vane numbers have a 15% difference in throat cross sectional area and both could achieve the target pressure ratio, close to 2. The throat Mach number in VN17 reaches 1.2. This increase will lower the back pressure because of the shock after the flow becomes supersonic. The blockage in the diffuser throat impacts on the diffuser inlet flow. Therefore, VN17 has lower inlet pressure compared to the VN13. In Fig. 3, for model VN13 much of the pressure recovery occurs between 0.4 and 0.8 streamline location (S/C), which is the mid-vane space. The maximum pressure drop over average area for this model happens in the semi-vaneless space; and there is again a slight pressure drop around 0.2 S/C. This drop in model VN17 reaches to its minimum between 0.2 S/C and 0.3 S/C.

The difference in pressure for VN13 and VN17 can be explained by the density fluctuations over the area shown in Fig. 4. In 5% S/C, semi-vaneless space, both models predict similar density values. However, in 25% S/C approximately the throat area, VN17 has sudden drop while VN13 does not show any changes. This density reduction in VN17 leads to higher radial velocity which leads to instability.



Fig. 3. Diffuser inlet to outlet distribution of pressure in streamline location.

The blade surface distributions of the speed of sound, in Fig. 4, show more clearly the real gas effects occurring at supercritical pressure. The speed of sound for vapour  $CO_2$  has a minimum around 148 m/s at the critical point. In

VN17, this parameter decreases to its minimum (230 m/s) around 20% S/C followed by a strong increase. However, for VN13, the speed of sound continues to increase. The minimum for this model is 255 m/s and occurs at 5% S/C. This difference in the minimum speed of sound of the two vane numbers causes the differences in the respective flow characteristics at the trailing edge.

Moreover, the results show that the changes in density and speed of sound in the semi-vaneless space (5% S/C) have opposite trends. This characteristic will lead to higher pressure drop in the narrower throat. Therefore, the location of the sudden reduction in density and speed of sound demonstrates the effect of throat area on these parameters. It can be concluded that VN17 with the higher number of blades, at high speeds will have a higher probability to stall. The higher number of blades therefore leads to a smaller operating range.



Fig. 4. Hub (0) to Shroud (1) surface distribution of density and sound speed in 5%, 25% and 50% streamline location (VN13:---, VN17:--).

#### 6. Conclusions

In this investigation, firstly an explicit representation and characterisation of the real gas effects of the fluid on the one-dimensional internal flow behaviour and related mechanisms have been studied. Secondly, computational fluid dynamics modelling has been used to study the internal flow of a supercritical CO<sub>2</sub> compressor diffuser (with two-dimensional radial shape) when operating close to the critical point. By considering the change in cross-sectional area (by changing the number of vanes), we have investigated the relationship between the sCO<sub>2</sub> real gas behaviour and existing conventional design tools which suggest that lower number of blades lead to more stable performance.

The flow modelling was performed with ANSYS CFX 17.1, including a generated lookup table from REFPROP for  $CO_2$  real gas properties. Comparisons of the results of the CFD analysis of the designed blades demonstrate that consideration of the behaviour of the sCO<sub>2</sub> can lead to optimal designs. The results show that the model with 17 vanes

can lead to flow instability and higher pressure drop at the throat of the diffuser compared to the 13 vane diffuser. However, further investigations are needed to confirm this outcome for higher and lower incidence angles on the leading edge of the diffuser for non-ideal gas flows.

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