SUPERCRITICAL CO$_2$ NUMERICAL MODELLING AND TURBOMACHINERY DESIGN

Alireza Ameli
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Dissertation for the degree of Doctor of Science (Technology) to be presented with due permission for public examination and criticism in the Auditorium 1316 at Lappeenranta-Lahti University of Technology, Lappeenranta, Finland on the 16th of April, 2019, at noon.

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Lappeenrantaensis 849
Supercritical CO\textsubscript{2} Brayton cycles have attracted significant attention in recent years on the basis that they can achieve higher thermal efficiency at relatively lower turbine inlet temperature in comparison to conventional power cycles. Because a higher density is achieved near the critical point, the turbomachinery required is relatively compact. Fluid thermophysical properties near the critical point change non-linearly and sharply, thereby impacting the simulation and design processes. These rapid changes cause instabilities in the numerical modelling and experimental measurements. Coupling the real gas equation of states directly with the solver increases the simulation time significantly. Also, in some locations extremely near the critical point, an equation of states cannot predict the fluid properties. This thesis aims to address these issues. First, a method was developed which is possible to overcome the instabilities in the numerical simulations in near-critical point applications by using in-house code to generate a look-up table of the properties. After that, the look-up table was generated using different equation of states at different resolutions. The comparison between the look-up tables generated using different equation of states at different resolutions was conducted in different operating conditions near and far from the critical point. The possibility of condensation forming near the critical point was investigated and the study was extended by modelling the non-equilibrium condensation inside a converging-diverging nozzle in the vicinity of the critical point. During the last stage of the thesis, the compressor design procedure was studied using individual enthalpy loss models. Due to the small size of the compressor near the critical point, and the high density, skin friction loss attracted more attention. A further study on the skin friction loss and friction coefficient was conducted and, finally, the most accurate compressor design procedure for the near-critical point applications was developed using different loss correlations and validating the findings against the numerical simulations and experimental measurement.

Keywords: centrifugal compressor, radial turbine, brayton cycle, real gas, skin friction
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Last but not least, my dear wife, Faegheh. Thank you for being my best friend and wife over the past 12 years. Without your patience and love, I would not be able to complete my doctoral dissertation.

Alireza Ameli
March 2019
Lappeenranta, Finland
To my lovely wife, who always supports me.
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Abstract

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This dissertation was written based on the following publications. The publishers have granted their permission for the papers to be included in this dissertation.


Author's contribution

I am the principal author, planner and investigator of all papers. All co-authors reviewed the articles and gave suggestions for improvements.
Nomenclature

In the present work, variables and constants are denoted using italic style, vectors are denoted using bold regular style, and abbreviations are denoted using regular style.

Latin alphabet

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>b</td>
<td>impeller width</td>
<td>m</td>
</tr>
<tr>
<td>C</td>
<td>absolute velocity</td>
<td>m/s</td>
</tr>
<tr>
<td>c_f</td>
<td>skin friction coefficient</td>
<td>–</td>
</tr>
<tr>
<td>c_p</td>
<td>specific heat capacity at constant pressure</td>
<td>J/(kgK)</td>
</tr>
<tr>
<td>d</td>
<td>diameter</td>
<td>m</td>
</tr>
<tr>
<td>D</td>
<td>diffusion factor</td>
<td>–</td>
</tr>
<tr>
<td>e</td>
<td>wall roughness</td>
<td>–</td>
</tr>
<tr>
<td>g</td>
<td>acceleration due to gravity</td>
<td>m/s^2</td>
</tr>
<tr>
<td>G</td>
<td>Gibbs free energy</td>
<td>J</td>
</tr>
<tr>
<td>h</td>
<td>enthalpy</td>
<td>J/kg</td>
</tr>
<tr>
<td>H</td>
<td>head coefficient/height</td>
<td>–/m</td>
</tr>
<tr>
<td>J</td>
<td>nucleation rate</td>
<td>1/kg s</td>
</tr>
<tr>
<td>K_n</td>
<td>Knudsen number</td>
<td>–</td>
</tr>
<tr>
<td>L</td>
<td>length/latent heat</td>
<td>m/ J/kg</td>
</tr>
<tr>
<td>m</td>
<td>molecular mass</td>
<td>kg</td>
</tr>
<tr>
<td>ṁ</td>
<td>mass flow rate</td>
<td>kg/s</td>
</tr>
<tr>
<td>n</td>
<td>unit normal to the surface</td>
<td>–</td>
</tr>
<tr>
<td>N</td>
<td>droplet number per unit of volume</td>
<td>–</td>
</tr>
<tr>
<td>p</td>
<td>pressure</td>
<td>Pa</td>
</tr>
<tr>
<td>r</td>
<td>radius/droplet radius</td>
<td>m</td>
</tr>
<tr>
<td>s</td>
<td>entropy</td>
<td>kJ/kg K</td>
</tr>
<tr>
<td>S</td>
<td>splitter blade/source term</td>
<td>–</td>
</tr>
<tr>
<td>t</td>
<td>tip clearance distance</td>
<td>m</td>
</tr>
<tr>
<td>T</td>
<td>temperature</td>
<td>K</td>
</tr>
<tr>
<td>U</td>
<td>tangential impeller speed</td>
<td>m/s</td>
</tr>
<tr>
<td>W</td>
<td>relative velocity</td>
<td>m/s</td>
</tr>
<tr>
<td>X</td>
<td>Cartesian coordinate</td>
<td>–</td>
</tr>
<tr>
<td>Z</td>
<td>compressibility factor/number of blades</td>
<td>–</td>
</tr>
</tbody>
</table>

Greek alphabet

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>α</td>
<td>volume fraction</td>
</tr>
<tr>
<td>β</td>
<td>critical point exponent</td>
</tr>
<tr>
<td>ζ</td>
<td>Markov loss coefficient</td>
</tr>
</tbody>
</table>
### Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\eta$</td>
<td>efficiency</td>
<td>–</td>
</tr>
<tr>
<td>$\pi$</td>
<td>pressure ratio</td>
<td>–</td>
</tr>
<tr>
<td>$\rho$</td>
<td>density</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>surface tension</td>
<td>J/m$^2$</td>
</tr>
<tr>
<td>$\tau_w$</td>
<td>wall shear</td>
<td>MPa</td>
</tr>
<tr>
<td>$\phi$</td>
<td>flow coefficient</td>
<td>–</td>
</tr>
<tr>
<td>$\omega$</td>
<td>specific turbulent dissipation/rotational speed of the rotor</td>
<td>s$^{-1}$</td>
</tr>
</tbody>
</table>

### Dimensionless numbers

- **Re**: Reynolds number

### Superscripts

- *: related to the critical droplet

### Subscripts

- $\alpha$: axial
- BL: blade loading
- c: critical
- cl: clearance
- DF: disk friction
- h: hub
- hb: hydraulic diameter of the blade passage
- I: incidence
- l: liquid
- L: leakage
- M: mixing
- r: rough/reduced property
- R: recirculation
- s: isentropic/static condition/smooth/saturation
- SF: skin friction
- t: at the tip/total condition
- TC: tip clearance
- u: circumferential component
- v: vapor
- w: relative
- 1: inlet of the impeller
- 2: outlet of the impeller
- 3: inlet of the diffuser
- 4: outlet of the diffuser/inlet of the volute
- 5: outlet of the volute
- $\infty$: free stream condition
### Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D</td>
<td>two dimensional</td>
</tr>
<tr>
<td>3D</td>
<td>three dimensional</td>
</tr>
<tr>
<td>CFD</td>
<td>computational fluid dynamics</td>
</tr>
<tr>
<td>EOS</td>
<td>equation of state</td>
</tr>
<tr>
<td>RANS</td>
<td>Reynolds-averaged Navier-Stokes</td>
</tr>
<tr>
<td>RGP</td>
<td>real gas properties</td>
</tr>
<tr>
<td>RMS</td>
<td>root mean square</td>
</tr>
<tr>
<td>SST</td>
<td>shear stress transport</td>
</tr>
<tr>
<td>SW</td>
<td>Span and Wagner</td>
</tr>
<tr>
<td>URANS</td>
<td>unsteady state Reynolds-averaged Navier-Stokes</td>
</tr>
</tbody>
</table>
1 Introduction

1.1 Motivation and background

The need to produce electricity sustainably and at a lower cost has dominated much of the recent energy-related research and development. Our everyday lives are dependent on a continuous supply of energy, particularly for electricity and heating purposes. There is no doubt that even a small increase in the efficiency of power cycles can considerably save energy resources. A significant element of the electricity that is consumed in the world is produced using energy conversion cycles. The most common energy conversion cycles are Rankine or Brayton cycles i.e. steam and gas turbine power plants. Even a small increase in cycle efficiency can generate an enormous gain in electricity production and decrease the use of primary energy sources. In general, closed gas turbine cycles are more compact and simpler and can be constructed in a shorter period of time. Different fluids such as helium, SO$_2$, and CO$_2$ can be employed as a working fluid with different heat sources such as biomass, solar, waste heat, gas, and coal.

The selection of the working fluid is considerably constrained by environmentally impacts, accessibility, cost, and thermophysical properties. Taking advantage of the real gas properties near the critical point, such as the high dependency of density to pressure and temperature, is a pre-eminent way to enhance cycle performance and efficiency. In addition to exploiting the effects of the real gas properties, the moderate critical temperature of the working fluid plays a crucial role in the improvement of the cycle performance. Based on the thermodynamics point of view, a higher cycle efficiency can be achieved when the cycle rejects the heat at the lower temperature. Contrarily, if the working fluid critical temperature is excessively low, problems arise in the cooling process due to the lower limit set by the terrestrial ambient temperature. Also, condensing cycles can increase the possibility of cavitation inside the pump. Therefore, there is an inherent need for fluid that has a critical temperature near the ambient temperature (Dostal, Hejzlar, & Driscoll, 2006). Sorokin (Sorokin, 1979) investigated the use of Nitrogen Tetroxide (N$_2$O$_4$) as a working fluid instead of ideal gas inside a Brayton cycle. Regardless of the attractive thermophysical properties of the N$_2$O$_4$, the toxicity of the working fluid can have major environmental impacts. Zhao and Peterson (Zhao & Peterson, 2008) investigated the performance of hydrogen as the working fluid for the Brayton cycle. In their study, to achieve the 40% cycle efficiency using hydrogen, the turbine inlet temperature was increased to 850 °C due to the critical properties of the gas. The use of alternative working fluids in the supercritical cycle other than CO$_2$ was also studied by Zhao and Peterson (Zhao & Peterson, 2008). Alternative pure working fluids, which have a critical temperature in the suitable region, are straight-chain hydrocarbons. However, they are flammable and have low thermal stability. Fluorohydrocarbons, on the other hand, has a high global warming potential and is very expensive. The combination of CO$_2$ and benzene in the supercritical regenerative cycles has also been studied (Zhao & Peterson, 2008) and a low turbine inlet temperature (400 °C) was used. The research concluded that it was possible to modify the critical temperature through the use of
mixtures. However, one problem associated with the use of mixtures is the low thermal stability of organic compounds, which limit the maximum cycle temperature and, thus, the cycle efficiency.

In recent times, the supercritical carbon dioxide (sCO\(_2\)) Brayton cycle has attracted more attention from scholars on the basis that it offers a relatively higher thermal efficiency at a relatively lower turbine temperature. The sCO\(_2\) Brayton cycle takes advantage of the moderate critical temperature (304.13 K) and gas properties of the working fluid. CO\(_2\) is non-toxic, incombustible, easily accessible, and relatively economical. Compared to refrigerants and chlorofluorocarbons, it does not have negative impacts on the depletion of the ozone layer and effective global warming potential (Zhang, Xu, Liu, Zhang, & Dang, 1998; Riffat, Afonso, Oliveira, & Reay, 1997). A previous study by Angelino and Invernizzi (Angelino & Invernizzi, 2001) found that the efficiency of a sCO\(_2\) Brayton cycle is enhanced if the inlet boundary conditions of the compressor are set near the critical point. A lower compressibility factor results in less compression work and, subsequently, decreases the power input of the cycle. Since the compressor is operating in the vicinity of the critical point, considerable deviation between the predicted performance and flow behaviour using ideal gas assumption compared to the real gas models is expected. Moreover, the liquid-like density and gas-like viscosity of the fluid near the critical point results in more compact turbomachines compared to those in the standard power cycles. The inconsistence behaviour of the thermophysical properties of a fluid close to the critical point gives rise to instabilities in the simulation and design procedures. These instabilities are more profound inside the compressor since the operating conditions of the compressor inside a sCO\(_2\) Brayton cycle are closer to the critical point than the turbine. These instabilities and the associated measurement difficulties have been recently addressed in the literature (Conboy et al., 2012; Iverson, Conboy, Pasch, & Kruizenga, 2013; S. G. Kim, 2014; Y. M. Kim, Kim, & Favrat, 2012; Lettieri, Yang, & Spakovszky, 2015). Moreover, it was noticed that in a compressor operating near the critical point, there is possibility of condensation as a result of local flow acceleration (Pecnik, Rinaldi and Colonna, 2012). The non-linear behaviour of the thermophysical properties can also mitigate high uncertainties in the experimental measurements. Furthermore, as the operating conditions get closer to the critical point, the uncertainty is notably increased (Lee, Baik, Cho, Cha, & Lee, 2016). Figure 1 contains an example to illustrate the CO\(_2\) isobaric specific heat variations in the vicinity of the critical point.
1.2 Objectives

The main objectives of this research were as follow:

- Investigate the numerical constraints of modelling and simulate the turbomachinery (radial compressor and turbine) in the supercritical region.
- Study the effect of the boundary condition and accuracy of the real gas properties on the performance of the turbomachinery (radial compressor and turbine).
- Search the evidence concerning the condensation inside the compressor near the critical point.
- Analyze the skin friction loss inside the centrifugal compressor near the critical point.
- Develop a compressor design method for near-critical point applications.

To meet the objectives of the research, at the outset of the study, a shrouded impeller of a centrifugal compressor excluding the diffuser and volute was modelled. During this
stage, the main focus of the study was on numerical modelling and the accurate identification of the real gas properties (Publication I). The investigation was continued by modelling the whole stage, including the tip clearance and vaned diffuser, in different boundary and operating conditions near the critical point (Publication II). During the compressor simulation and modelling procedures, small regions were found in which the thermophysical properties of fluid fell below the critical point and there was a possibility of condensation forming. Further investigations were carried out to study the condensation possibilities near the critical point (Publication IV). In addition, the sCO\textsubscript{2} radial turbine simulation and modelling in different boundary and operating conditions was studied. Different real gas models were examined in a variety of boundary conditions in the supercritical region (Publication V). Finally, by studying the turbomachinery design methods, a compressor design method was developed based on the modified individual enthalpy loss correlations. The results indicated that this was more accurate than the conventional enthalpy loss correlations in the near-critical point applications (Publications III and VI). All numerical studies were compared and validated against the experimental measurements.

The dissertation consists of two main parts:

First, a summary of the investigated topics is given followed by the conclusions and achievements. In the second part, the published papers are presented. These are referred to as Publication I, Publication II, Publication III, Publication IV, Publication V, and Publication VI.
2 Numerical investigations of turbomachinery in the supercritical region

In a sCO$_2$ Brayton cycle, compressors operate closer to the critical point than the turbines. As a result of sharp changes in the fluid properties, it is challenging to numerically simulate and design a compressor in the sCO$_2$ cycle. Due to the relatively higher pressure and lower mass flow rate in the sCO$_2$ Brayton cycles compared with the steam power cycles, especially re-compression layout, centrifugal compressors are preferred to the axial ones (Hoffmann & Feher, 197; Iverson et al., 2013; Lee, Lee, Yoon, & Cha, 2014). Consequently, this dissertation places a strong emphasis on the centrifugal compressor. However, a radial turbine has also been studied to compare and investigate the effect of real gas models on the turbomachine performance and flow field in the supercritical dome and relatively far from the critical point.

2.1 Experimental test loop

To validate the study of the numerical constraints near the critical point, experimental measurements are required. There is lack of open-access experimental data from sCO$_2$ test loops in the literature. The only semi-open access geometry and measurement data are available from the sCO$_2$ re-compression test loop in the Sandia National Laboratory (Conboy et al., 2012; S. A. Wright, Conboy, & Rochau, 2011). The Sandia sCO$_2$ test loop is a split-flow re-compression Brayton cycle using two single-stage centrifugal compressors as the main and recompression compressors (see Figure 2). The main compressor shaft has the maximum designed rotational speed of 75000 RPM and the maximum designed pressure ratio of the cycle is 1.8. However, in the measurement, the maximum shaft speed of 75000 RPM was not achieved because of sealing, bearing, and windage loss problems (S. Wright, 2017). In the experimental procedure, the rotational speed varied from 45000 to 65000 RPM, while most measurements were conducted at 50000 RPM. A wide range of operating conditions for the main compressor have been measured: near the critical point, in the liquid side, in the vapour side and even in the saturation area. In this research, only the operating range extremely near the critical point is of interest.
2.2 Studied geometries and computational grid

The dimensions of the Sandia sCO₂ main compressor were derived from the literature (Conboy et al., 2012; S. A. Wright et al., 2011), and missing parameters, like the axial length of the impeller, was estimated based on the well-derived correlation by Aungier (Aungier, 2000). The main dimensions of the impeller and vaned diffuser are summarized in Table 1. The volute was not modelled due to the lack of information about the geometry. Even though the geometry could be easily estimated using correlations, modelling the volute does not provide much additional information and would incur significant additional numerical efforts.

Table 1. Dimensions of the main Sandia centrifugal compressor.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Impeller diameter ratio (\frac{d_2}{d_1})</td>
<td>1.99</td>
</tr>
<tr>
<td>Impeller diameter</td>
<td>37.36 (mm)</td>
</tr>
<tr>
<td>Exit blade height</td>
<td>1.71 (mm)</td>
</tr>
<tr>
<td>Blade tip angle (minus is backswept)</td>
<td>-50 (deg)</td>
</tr>
<tr>
<td>Blade thickness</td>
<td>0.76 (mm)</td>
</tr>
<tr>
<td>Inlet blade angle at tip</td>
<td>50 (deg)</td>
</tr>
<tr>
<td>Tip clearance (constant)</td>
<td>0.25 (mm)</td>
</tr>
<tr>
<td>Exit vaned diffuser angle</td>
<td>71.50 (deg)</td>
</tr>
<tr>
<td>Diffuser blade divergence angle</td>
<td>13.17 (deg)</td>
</tr>
</tbody>
</table>
2.3 Numerical methods

The geometry of the impeller was created using BladeGen (ANSYS® Academic Research, 2017a) and a fully structured grid was generated using Turbogrid (ANSYS® Academic Research, 2017b). In the first stage of the research (Publication I), the impeller was assumed to be shrouded and no tip clearance was modelled. Also, in the first step of the research, the diffuser was not modelled. This simplified the simulation and made it possible to concentrate only on the numerical methods and the accuracy of the real gas properties. In the second phase of the research (Publication II), the whole compressor, including the tip clearance and vaned diffuser, were modelled to include the effect of the tip clearance flow and rotor-stator interaction on the accuracy of the prediction of the compressor performance. In addition, a wide range of the backpressures and operating conditions were studied in the second stage. Figures 3 illustrates the compressor and mesh that were studied in Publication II.

Figure 3. Geometry and mesh of the studied centrifugal compressor.

Mesh dependency tests were performed for both studied models. For the shrouded compressor, increasing the number of cells to more than around 440,000 did not generate any significant changes in the stage efficiency and pressure ratio while, for the unshrouded case, including the diffuser, this amount was increased up to 1.5 million cells. The quality of the grids was also examined using Jacobian and skewness factors. The maximum skewness among the cells was below 0.7, which is an acceptable value for the complex geometries involved. Sufficient small cells were generated near walls to ensure the value of $y^+$ remained below unity.

2.3 Numerical methods

Reynolds Averaged Navier-Stokes (RANS) equations were coupled with one of the most common linear eddy viscosity turbulence models: Shear-Stress Transport $k - \omega$ SST (Menter, 1994). Two-equation turbulence models can predict the characteristic and physics of the majority of flows especially in industry applications. The SST model was
introduced to accurately predict the flow separation under an adverse pressure gradient by employing the transport effects in the eddy viscosity equation. This model has been highly recommended for boundary layer simulations and a range of validation studies have proven that the SST model offers a superior performance to other two-equation turbulence models (Jaatinen-Värrä et al., 2016; Mani, Ladd, & Bower, 2004; Park & Kwon, 2004; Rumsey, 2010). This model integrates the advantages of the standard $k - \varepsilon$ (far from the wall) and the standard $k - \omega$ turbulence models (near the wall). Also, to access the full advantages of the SST model, at least 10 nodes inside the whole boundary layer are required (ANSYS® Academic Research CFX, 2017).

Moreover, the total energy model was used, to capture the effect of both kinetic energy and enthalpy transport. The viscous work term was added to the total energy model which represents the work due to the viscous stress. This term enables internal heating as a result of viscosity. Even though some recent studies have not included the viscous work term within the energy equation, this term is included in this study because the molecular viscosity in the viscous sublayer near the walls has a significant effect on the boundary layer profile. It is worth mentioning that the turbulence viscosity dominates this term away from the walls and, as a result, the viscous work term can be neglected far from the walls.

The high-resolution scheme (second order) was used to discretize the advection and turbulence equations. Due to the convergence difficulties associated with the high-resolution scheme, the results were first generated with the first order scheme (upwind) before the simulation was continued by increasing the order of the schemes. The convergence criteria for the CFD simulations were based on decrease of the Root Mean Square (RMS) of continuity, mass, momentum and energy residuals below $10^{-4}$; stability of the stage efficiency; and decrease the mass and energy imbalances (difference between inlet and outlet) below $10^{-3}$ percent in each zone. In the steady state simulations, including those involving a vaned diffuser (Publication II), the frozen rotor interface was set between the stationary and rotating zone. The frozen rotor model is robust and uses less computational resource than the other frame change models. In the transient simulations (Publications III and V), the transient blade row interface employing the Fourier Transformation was set to capture the losses as a result of rotor-stator interaction. The Fourier Transformation interface model can be applied in all flow regimes as well as the full range of pitch ratios (ANSYS® Academic Research CFX, 2017).

### 2.4 Real gas EOS models comparison

The critical point represents the point at which the phase boundary between the liquid and gas vanishes. Above the critical point, fluid is a gas that has the liquid like density (high density and low viscosity), which has the highest isobaric specific heat along the pseudo-critical line. Although, in some recent research, it has been noticed that the fluid is not homogeneously distributed in the supercritical region (Banuti, 2015; Simeoni et al., 2010), The Widom line separates it into two separate regions with liquid-like and gas-
like properties. This behaviour of the fluid has influence on the turbomachinery design and numerical simulations for the near-critical point applications. The thermophysical properties of a fluid near its critical point have strong dependency on the temperature and pressure, which causes sharp changes. These strong changes make the computational fluid dynamic (CFD) simulations unstable and challenging to perform. The low compressibility factor (around 0.2) of the fluid at the critical point causes the fluid to behave like a real gas and employing the ideal gas assumption results in a significant deviation from the experimental data. Even some well-developed real gas equation of states (EOS) are not able to accurately predict the fluid behaviour in the vicinity of the critical point.

To find the most accurate EOS model in the supercritical region, the main radial turbine of the Sandia sCO\textsubscript{2} test loop was analysed numerically in various operating conditions using different EOS (Publication V). The operating conditions of the studied radial turbine are shown in a T-S diagram in Figure 4. Three off-design points and one design point were selected for this investigation. Points A, B, and C were the off-design points and the operating condition D was the design point.

![Figure 4. Radial turbine boundary and operating conditions.](image)

Among the most well-known cubic EOS models that are employed for the real gas simulations, those presented by Peng Robinson (PR) (Peng & Robinson, 1976), Soave-Redlich-Kwong (SRK) (Soave, 1972), and Span and Wagner EOS model (SW) (Span & Wagner, 1996) were selected to be compared against the ideal gas EOS model and, subsequently, validated with experimental measurements (Vilim, 2011). Among the various EOS models that are available, the Span and Wagner (SW) model has been widely employed in the sCO\textsubscript{2} simulations near and far from the critical point (Baltadjev, 2015;...
Numerical investigations of turbomachinery in the supercritical region

Chu & Laurien, 2016; S. G. Kim et al., 2014; Kulhánek & Dostál, 2011; Lee et al., 2014; Wang, Guenette, Hejzlar, & Driscoll, 2004). This model was developed particularly for CO\textsubscript{2} and can calculate the CO\textsubscript{2} thermophysical properties from the triple point up to 1100 K and 800 MPa.

If the real gas EOS models are coupled directly to the flow solver, the computational time increases dramatically. Also, in points at which the properties are extremely close to the critical point, due to the singularity, no properties are calculated and, consequently, the simulation is diverged. To reduce the computational effort and time, an external look-up table of real gas properties (RGP) using different EOS models was generated that can be coupled with the CFD flow solver. The developed Fortran code was combined with the NIST REFPROP data-base (Lemmon, Huber, & McLinden, 2013) to export nine main fluid properties: specific enthalpy, speed of sound, specific volume, specific heat at constant volume, specific heat at constant pressure, partial derivative of pressure with respect to specific volume at constant temperature, specific entropy, dynamic viscosity, and thermal conductivity. The exported properties were stored in two RGP tables: one for the liquid and one for the gas. It is important to note that the fluid properties in the supercritical region are the same in both RGP tables. Spinodal and saturation curves were generated with extreme care, especially near the critical point, as they play a crucial role in the multiphase and near-critical point simulations. To generate the RGP table, pressure and temperature were used to drive the properties from the REFPROP libraries. It was done in this order, because in many cases operating conditions like temperature and pressure can be estimated easily. For an example, in the compressor simulations, the pressure ratio and outlet temperature can be estimated. But using the enthalpy or density as an input for the table generation is not fully straight forward in some cases. However, solver reads the RGP table of properties in a different way. For each real gas EOS model, the RGP table was generated with different resolutions. In addition, setting the constant critical values were crucial for this comparison. The RGP table was generated for a wider range than the operating condition because, at the outset of the iterations, some cells have properties beyond the operating range and the solver applies clipping or linear-extrapolating methods. Due to the non-linear behaviour of the fluid properties, especially near the critical point, clipping and linear-extrapolating methods significantly decrease the numerical accuracy.

2.4.1 EOS comparison results

As expected, all EOS models, even the ideal assumption, achieved almost the same accuracy in the design point (D) because of its relatively far distance from the critical point and high value (near unity) of the compressibility factor (Z). The comparison revealed that the SW EOS model was more accurate in all off-design points (A, B and C) inside the supercritical dome. For the turbine off-design conditions, there was no significant deviation between the different RGP resolutions. Full details regarding the EOS and RGP resolution accuracy test are given in Publication V.
2.5 Compressor boundary conditions and RGP look-up table

The RGP table should be generated according to the boundary and operating conditions of the simulating case. In the Sandia test loop measurement, many boundary and operating conditions were tested. The highest efficiency and performance were achieved as the inlet of the compressor became closer to the critical point (Conboy et al., 2012; S. A. Wright et al., 2011; S. A. Wright, Radel, Vernon, Rochau, & Pickard, 2010). The nearest inlet boundary conditions of the Sandia main compressor to the critical point (306 K and 7.69 MPa) were set as the inlet boundary condition of the compressor (reduced pressure and temperature values normalized value by the critical value are 1.042 and 1.006, respectively). The selected rotational speed of the compressor was 50,000 RPM and the machine Mach number was 0.293, which is defined as the ratio of the tip speed divided by the speed of sound at the inlet.

For the shrouded impeller study (Publication I), only one operating condition was modelled as the main aim of this study was perform RGP dependency and real gas accuracy tests. The mass flow rate of 3.6 kg/s (flow coefficient 0.049) was set as the outlet boundary condition in the shrouded impeller. For the whole stage compressor simulation, different back pressures from 8.7 MPa to 9.5 MPa with 0.1 MPa intervals were set as the outlet boundary condition. The operating condition of the compressor can be seen in Figure 5. As can be observed, the inlet boundary condition is on the Widom line. Isobaric specific heat reaches the highest value on this line at different temperatures and pressures, which makes the simulation unstable. The RGP table range that was generated for the whole stage is shown in Figure 6.

![Figure 5](image)

Figure 5. Operating conditions of the centrifugal compressor. Blue dot indicates the inlet and blue squares locate the outlet boundary conditions.
To investigate the effect of the RGP table resolution in the same range on the compressor performance and flow field, different table resolutions were generated ranging from low resolution (0.4 K and 0.08 MPa step sizes for temperature and pressure, respectively) to high resolution (0.1 K and 0.02 MPa step sizes for temperature and pressure, respectively). It was noticed that using the highest table resolution at the beginning of the simulation made the calculation unstable due to sharp changes in the properties near the critical point (see Figure 7). There are some limitations associated with creating the RGP look-up table using REFPROP. When the resolution of the table is increased, there is a possibility to place a point extremely near the critical point, causing divergence in the generation of the table. The reason for this behaviour is that the real gas EOS models cannot calculate the fluid properties adjacent to the critical point due to the extremely non-linear variation of the fluid properties. Therefore, there was a need to find the optimum resolution for the look-up table. To do so, simulations were performed using the lowest table resolution and were continued by replacing the RGP table with higher resolution RGP table on a step-by-step basis. This procedure was continued step by step to achieve the result with the highest resolution RGP table and the result was insensitive to the look-up table resolution. Also, in the lowest RPG resolution table, the highest peaks of the fluid properties were skipped to achieve a smooth convergence as an initial solution.
2.6 RGP resolution effects on the flow field

A comparison of the flow field inside the impeller proved that the RGP resolution has a significant impact on the compressor performance and flow field. It worth mentioning that deviation difference (calculated according to the local values and the properties given by REFPROP) between low and high table resolutions are not notable. By contrast, the effects on the flow field and performance are worthy of attention. As an example, Figure 8 illustrates the isobaric deviation between three RGP tables (200, 300, and 400 points) and the REFPROP at two different constant pressures: At the inlet (7.69 MPa) and near the outlet of the compressor (10 MPa).
Figure 8. Isobaric specific heat deviation at constant pressure inlet and outlet.

Figure 9 shows the Mach number around the main blade leading edge. Even though the boundary conditions were set the same in simulations using low-to-high RGP resolutions, the different looked-up values for the fluid properties like density and speed of sound, cause dissimilarity in the flow fields. Moreover, by keeping the geometry and boundary conditions the same, changes in the RGP table resolution affected the velocity triangles along the impeller (different looked-up properties). A higher flow acceleration at the suction side of the main blade can be observed when a higher resolution RGP table was employed (see Figure 9).
2.6 RGP resolution effects on the flow field

The deviation between the low and high RGP table resolution results gets bigger as the critical point is approached. When the operating conditions move further away from the critical point, this deviation decreases significantly. Moreover, there is no significant difference in the deviation between the tables of 300 and 400 points. The non-dimensional temperature at 70% of span also showed the deviation between the low- and high-resolution RGP table, see Figure 10.

Figure 9. Mach number around the leading edge. The lower figure is for the highest RGP resolution.

Figure 10. Non-dimensional temperature at 70% span.
Comparing the density contour inside the impeller proved that the RGP resolution has a significant effect on the magnitude of the calculated properties. Even though the pattern of the profiles looks the same, the differences in the magnitude affect the flow downstream and, eventually, the performance of the compressor. In addition, the density difference between the side of the blades, affects the blade wake and back flow downstream. Figure 11 shows the density contour inside the impeller at $r/r_2 = 0.8$ and $r/r_2 =1$. S and M indicate the splitter and main blades respectively.

Figure 11. Density profiles inside the impeller at different RGP resolutions.

### 2.7 The effect of RGP resolution on the performance

Performance sensitivity according to the RGP resolution was examined using four table resolutions in the operation range presented in Figure 6. Figure 12 shows the influence of the RGP table resolution on the centrifugal compressor performance in terms of the isentropic total-to-total efficiency.
2.7 The effect of RGP resolution on the performance

As the resolution of the RGP table is increased, the predicted performance map is getting closer to the experimental measurements. By increasing the RGP table resolution more than 400 point in the mentioned range, no significant change in the compressor efficiency was observed. It should be mentioned that the external losses and the volute did not model in the CFD simulations. At that stage, more operating conditions than those presented in Figure 12 (higher and lower back pressures) were simulated; however, due to some instabilities in the simulations, the results were ignored. By further increasing the backpressure (decreasing the flow coefficient to below 0.031), few separations were observed inside the impeller at the suction side of the main blade, leading to the rotating stall. Moreover, by increasing the flow coefficient over 0.55 (back pressure below 8.8 MPa), the diffuser pressure recovery dropped sharply because of the negative incidence on the vane’s leading edge. Moreover, the compressor performance near the critical point is extremely sensitive to the operating pressure and temperature. As it was discussed in Publication I, even a minor change in temperature ~0.5 °C can lead to 1-2% difference in the efficiency.

The main step in the design of a Brayton cycle involves finding the suitable pressure ratio. For the Sandia sCO₂ Brayton cycle, this pressure ratio was 1.18. By setting the optimum pressure ratio constant, different boundary conditions near the critical point were investigated.

Fifteen different boundary conditions with a constant pressure ratio were studied (see Figure 13). Reduced values at the inlet were from 1.006 to 1.03 and 1.04 to 1.23 for the temperature and pressure respectively. Small intervals of 0.6 K and 0.1 MPa were selected and the effects of the boundary conditions variations on the compressor performance when the pressure ratio was constant were studied.
Figure 13. Boundary conditions of the studied 15 cases.

By keeping the pressure ratio constant and progressively moving the inlet boundary condition to the critical point, the isentropic efficiency was increased almost linearly. This finding is in agreement with previous studies (G Angelino, 1968; G Angelino & Invernizzi, 2001; Gianfranco Angelino, 1969). Figure 14 illustrates the compressor efficiency trend at all simulated points. Case 1 is the closest to the critical point while Case 15 is the farthest away.

Figure 14. sCO₂ compressor isentropic efficiency trend.

As the critical point was approached, the compressibility factor dropped, which led to a larger deviation between the specific volume of real gas and that given by the ideal gas assumption. Furthermore, as the critical point neared, the difference between the average values of the compressibility factor at the inlet and outlet decreased and the difference between the average density values at the inlet and outlet increased (see Figure 15). By setting the inlet boundary condition of the compressor relatively far from the critical
point, the speed of sound increased (22% from Case 1 to 15), which reduced the machine Mach number from 0.29 to 0.24 at a constant rotational speed. The higher Mach number caused a greater density variation inside the compressor with the same pressure ratio and rotational speed. Also, the greater machine Mach number decreased the stage volume ratio, indicating the higher compressibility of the fluid (Ludtke, 2004). Therefore, the efficiency of the compressor was enhanced as the inlet boundary conditions neared the critical point if the rotational speed and stage pressure ratio were held constant.

Figure 15. sCO$_2$ density change along the impeller
2 Numerical investigations of turbomachinery in the supercritical region
3 Possibility of condensation near the critical point

During the numerical investigations of the sCO$_2$ centrifugal compressor, a small region was observed near the suction side of the main blade leading edge at which the fluid properties fell below the critical point. Consequently, there is the possibility of condensation in that region. More investigations were conducted to model and estimate the non-equilibrium condensation near the critical point (Publication I and IV). Due to the flow acceleration at the suction side of the blades, the temperature and pressure of the fluid dropped in accordance with variations in the flow coefficients. If the inlet boundary condition of a compressor is extremely close to the critical point or saturation curves, fluid properties may cross the saturation curves. The effect of the supercritical condensation inside a centrifugal compressor has been previously studied (Lettieri, et al., 2015) using a non-dimensional criterion associate with the nucleation time and expansion rate. It was concluded that condensation might not develop when the operating condition of the compressor is far from the critical point. However, near the critical point, the two-phase effects are expected to become more significant. Some researchers have addressed the difficulty of non-equilibrium condensation modelling in the high-speed flows in converging-diverging nozzles with CO$_2$ as a working fluid (Masafumi, et al., 2009; Nakagawa, et al., 2008; Yazdani, et al., 2014). In this study, the fluid properties in the metastable region (between the spinodal and saturation curves) was generated in the RGP generator code by using bilinear cubic extrapolation of the saturation properties to the spinodal curve.

The supercooling degree is defined as follows:

$$\Delta T = T_s(p_v) - T_v$$

(1)

where $T_s$ is the saturation temperature at vapour pressure ($p_v$) and $T_v$ is the temperature of the vapor. Crossing the saturation curves is a prerequisite for droplet generation; however, it is not enough. The residence time of the properties inside the metastable region is another key issue. In the first stage of investigating the possibility of condensation near the critical point, a converging-diverging nozzle was selected to exclude geometry and physics complications. The aim of this was to validate the well-known non-equilibrium theories that predict the location of condensation and the effect it has on the flow field (Publication IV).

Among the different experimental measurement conducted by Nakagava et al. (Nakagawa, Berana, & Harada, 2008), the closest boundary conditions to the critical point were selected in a way that was designed to replicate the conditions of the sCO$_2$ centrifugal compressor. Inlet reduced pressure and temperature were 1.2 and 1.02 respectively. While the reduced outlet pressure was below the critical point at 0.53. The geometry and dimensions of the studied case can be seen in Figure 16.
3.1 Non-equilibrium model

Based on the two fundamental theories for non-equilibrium phase change models, nucleation and droplet growth, it was assumed that nucleation produces the initial droplets of the liquid phase, while the phase transition was covered by the supercritical droplet growth (Kantrowits, 1951). More details about the non-equilibrium condensation model can be found in Gerber (Gerber, 2008) and Publication IV. Hence, this chapter is limited to a general description of the model and its challenges near the critical point.

The supercritical droplet means the droplet is larger than the critical radius, which is defined as below:

\[ r^* = \frac{2\sigma T_c}{\rho_l L \Delta T} = \frac{2\sigma}{\rho_l \Delta G_v} \quad (2) \]

where \( \rho_l \) is the liquid density, \( \sigma \) is the surface tension, \( L \) is the latent heat and \( \Delta G_v \) is the Gibbs free energy change of the vapour. Different surface tension models can be found in the literature (Hakim, Steinberg, & Stiel, 1971). According to the previous comparison study (Jianxin & Yigang, 2009), a semi-empirical correlation for the surface tension was selected (Jianxin & Yigang, 2009) on the basis that it offers highest accuracy in the near-critical point applications. The equation is function of reduced temperature (\( T_r \)), reduced pressure (\( P_r \)) and critical compressibility factor (\( Z_c \)) as follows:
3.2 Results and discussion of the validation case

\[
\sigma = \left(-0.951 + \frac{0.432}{Z_c}\right)(1 - T_r)^{11/3}(p_c^2 T_c)^{1/3}.
\]  

(3)

\[
Z_c = \frac{1}{R} \left(\frac{P_c V_c}{T_c}\right).
\]  

(4)

This model was coupled with the flow solver by means of a user-defined expression language. The Gibbs free energy in Ansys CFX was calculated as follows:

\[
\Delta G_v = \frac{L \Delta T}{T_s}.
\]  

(5)

The Gibbs free energy of the vapour changes in the vicinity of the critical point and is extremely small, which entails that the critical radius equation has an unrealistic large value, in a scale of millimetres. To overcome this issue, the critical radius was calculated in the post process based on Eq. 2 (left side) and the average value was set as a constant to achieve a realistic droplet size. Using the data presented in Figure 17, the averaged value of \(10^{-8} m\) was estimated.

Figure 17. Critical radius distribution along the centreline of the nozzle.

3.2 Results and discussion of the validation case

The non-equilibrium condensation model was used to simulate the flow in a nozzle near the critical point. The saturation pressure was compared with the experimental saturation pressure along the nozzle (see Figure 18). The saturation pressures in the experimental
measurements were calculated from the measured temperature along the nozzle. The calculated pressure using CFD simulation were in good agreement with the experimental measurements. However, because of droplet condensation, a slight deviation between the CFD and measurements data was observed near the outlet. This deviation can be attributed to the lack of accuracy of the classical nucleation theory near the critical point, numerical error and experimental measurement uncertainties. Figure 19 shows the liquid mass fraction, supercooling degree, surface tension variation and Mach number profiles inside the nozzle. The flow became supersonic in the upstream side (throat) but the onset of the phase change occurred close to the outlet.

Figure 18. Saturation pressure variation along the nozzle

Figure 19. Liquid mass fraction, supercooling, surface tension and Mach number.
3.3 Possibility of condensation inside the compressor

After validation of the supercritical condensation inside the nozzle, the study was progressed to investigate the possibility of condensation forming inside the compressor near the critical point. This part of the research is yet to be published and is currently under review for journal publication. Therefore, only a short description of the methods and results is presented herein. The positive supercooling degree was measured to identify the region in which there was a possibility of condensation forming (see Figure 20). Even though it seems that the located volume with possibility of condensation (red colour) is relatively small, but this volume increases significantly as the flow coefficient increases with a same inlet boundary conditions (see Figure 21).

Figure 20. Volume of the positive supercooling degree (50000 RPM-peak efficiency).
Figure 21. Volume with the positive supercooling degree at different flow coefficients.

The inlet boundary conditions of the studied cases were exactly above the critical point; therefore, in the expansion process, the fluid state path intersected with the saturation curve at the critical point. Eventually, without entering the metastable region, the fluid properties directly fell into the unstable region (see Figure 22).

Figure 22. Temperature-density phase diagram of CO$_2$ based on SW EOS and fluid state path along the streamline in Case D of Figure 20
3.3 Possibility of condensation inside the compressor

Extrapolating the properties into the unstable region generated an unrealistic result, even from a qualitative standpoint of view. Consequently, the flow solver was forced to clip the properties on the spinodal curves which decreased the numerical accuracy. To overcome this inaccuracy, the fluid expansion path inside the unstable zone was estimated using a constant cooling rate. Using this assumption, the state of the fluid inside the unstable zone and, consequently the condensation completion time could be estimated using Eq. 6 (Binder & Stauffer, 1976) (see Figure 22).

\[
\tau = \left( \frac{8\pi}{15} \left[ \frac{D \beta \Delta T}{T_c - T} \right]^{1.5} J \right)^{-0.4}
\]  

Where \( D \) is the diffusion coefficient which is estimated as \( D = \bar{D}(1 - T_r)^{5\nu} \), and \( \bar{D} \approx 10^{-3} \) cm\(^2\)/s and \( \nu \approx 0.64 \). \( \beta \approx 0.35 \) is the critical-point exponent and \( J \) is the nucleation rate, which is estimated as follows (Binder & Stauffer, 1976)

\[
J \approx 10^{30} \left[ \frac{\Delta T}{T_c - T} \right]^{6.06} \exp(-0.7 \left[ \frac{\Delta T}{T_c - T} \right]^{-2}).
\]  

In the studied centrifugal compressor, the fluid state path did not even cross the metastable region and entered the unstable region directly through the critical point. Studies by Binder (Binder, 1987) and Langer and Schwartz (Langer & Schwartz, 1980) proved that theory in deriving \( \tau \) is also valid when the phase transition starts by spinodal decomposition.

To calculate the completion time, the temperature and density of the fluid at the location in which the deepest penetration was observed in the unstable zone are required. To do so, it was assumed that the cooling rate, as given by the Lagrangian derivative of temperature \( \dot{T} = -\frac{\Delta T}{\Delta t} \), remains constant after entering the unstable zone. First of all, the average cooling rate for some stream lines before crossing the saturation curve was calculated. Then, the residence time of the fluid, \( \delta t \), inside the unstable zone was estimated (see Figure 23). Finally, by keeping the cooling rate constant, the estimated final temperature, \( T_2 \), was calculated by \( T_2 = 16 \ T_1 - T \times \delta t \). The same method was used to estimate the final density. Even though estimating the final density and temperature using this method is not without error, there is a need to estimate the magnitude of the completion time for the purpose of comparing this with the residence time. Also, by investigating the extreme case and conditions (case E in Figure 21), we tend to overestimate the residence time and cooling rate. Thus, the possible error introduced within this method will not loosen the criterion for condensation. The comparison between the volumes at which there is a possibility of condensation forming according to different flow coefficients is shown in Figure 23.
3 Possibility of condensation near the critical point

3.4 Completion time VS. residence time

In this section, by comparing the condensation completion time with the residence time of the particles, the possibility of condensation forming is examined. The estimated density, temperature, completion and residence times for the most extreme case (Case E in Figure 21) are provided in Table 2. A comparison of the completion and residence times reveals that the condensation has sufficient time for completion. Due to uncertainties pertaining to the final state of the fluid that are inherent in this method, as an alternative approach, different ranges of the temperature and supercooling degree were compared with the residence time. According to Figure 24, if the lowest temperature of the fluid during the flow acceleration reached 290 K and 300 K, to avoid condensation, the supercooling degree should not cross the limits of 4 K and 1.5 K respectively. In other words, these limits reveal that the impact of the critical slowing down is not significant enough to avoid condensation forming because of the extremely large nucleation rates near the critical point. Any system reacts to small perturbations increasingly slowly as the operating conditions approach the critical point. In other words, for a near-critical system, the time scales which characterizing the relaxation process upon small disturbances, significantly increase. This behaviour is called ‘critical slowing down’ and is observed in numerous systems as diverse as ecosystems, financial markets (Scheffer et al., 2009; Scheffer et al., 2009) and also physical processes such as magnetization and phase transition (Scheffer et al., 2009; Scheffer et al., 2009). Figure 25 illustrates the comparison between nucleation rates for 290 K and 300 K. The nucleation rates are significantly higher at 300 K because of the eradication of the surface tension near the critical point.
Table 2. Estimated values for the extreme case (E).

<table>
<thead>
<tr>
<th>Residence time</th>
<th>0.06 m sec</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lowest density</td>
<td>464 kg/m³</td>
</tr>
<tr>
<td>Lowest temperature</td>
<td>292 K</td>
</tr>
<tr>
<td>Completion time</td>
<td>0.005 m sec</td>
</tr>
<tr>
<td>Residence time/completion time</td>
<td>12 -</td>
</tr>
</tbody>
</table>

Figure 24. Comparison between residence time and completion times for $T=290$ K and $T=300$ K over different supercooling degrees.

Figure 25. Comparison between nucleation rates for $T=290$ K and $T=300$ K over different supercooling degrees.
In conclusion, a comparison of the residence time of the fluid particle and completion time inside the positive supercooling region revealed that, condensation formed. It should be noticed that different centrifugal compressor designs and operating conditions can significantly affect the residence and completion times and should be investigated on a case-by-case basis. However, the theory for phase transition starting from the unstable region is still incomplete unless an accurate description of the thermophysical properties of the fluid inside the unstable region is provided.
4.1 Compressor design methodology

4 Centrifugal compressor design for the near-critical point applications

The last stage of the research described in this dissertation involved discussing the centrifugal compressor design based on the individual enthalpy loss models using the sCO\textsubscript{2} working fluid. One commonly used approach to compressor sizing involves the use of the $n_e - d_s$ diagram by Balje and Japikse (Balje & Japikse, 1981). This method can be used to size turbomachinery for conventional working fluids; however, it does not achieve high accuracy in the supercritical region applications (Lee et al., 2014). Therefore, in the current study, the precise performance prediction of the centrifugal compressor was obtained by means of CFD simulations and 1-D mean line analysis. The majority of individual enthalpy loss correlations are derived based on the ideal gas assumption or from experimental measurements using air. Therefore, there is a need for further investigation and validation of these models for near-critical point applications.

Because of the high density (low specific volume) of the fluid near the critical point, the size of the turbomachine is reduced. The relatively smaller flow coefficient in this situation makes the compressor passage narrower. Consequently, the extremely high skin-friction losses caused by the imposed shear force on the mean fluid inside the boundary layer significantly limit the efficiency of the compressor (Aungier, 2000). Thus, this chapter focuses on the skin-friction loss estimation methods and the effect they have on the compressor performance near the critical point.

4.1 Compressor design methodology

The compressor mean-line design code is based on the most common equations for turbomachinery design, Euler and continuity as follows:

$$h_{t_2} - h_{t_1} = U_2C_{u_2} - U_1C_{u_1}$$

(7)

$$\dot{m} = \rho A C_{a_1}$$

(8)

where $C_{a_1}$ stands for the circumferential velocity and subscripts 1 and 2 indicate the inlet and outlet of the impeller, respectively. The velocity triangles were calculated at the hub, shroud, and mean line radiiuses. The schematic of the velocity triangles used in this research is presented in Figure 26.
The fluid properties at each step were derived directly from the REFPROP based on the SW EOS model. After computing the velocities and angles at the inlet and outlet, the values were updated by incorporating the enthalpy losses.

The existing literature presents a wide variety of proposed enthalpy correlations for the compressor design. Oh et al. (Oh, Yoon, & Chung, 1997) examined different correlation sets for performance prediction of the centrifugal compressor and proposed the set loss models (see table 3). This set of loss correlations has been validated in the supercritical region with acceptable accuracy (Liu, Luo, Zhao, Zhao, & Xu, 2018; Wang et al., 2004; Lee et al., 2014). Enthalpy loss correlations can be divided into two types: internal and external (parasitic) losses. Internal losses include incidence, blade loading, tip clearance, mixing and skin friction losses. External losses include disk friction, leakage, and recirculation losses.

Table 3. Studied individual enthalpy loss correlations (Oh, Yoon, & Chung, 1997).

<table>
<thead>
<tr>
<th>Losses</th>
<th>Correlations</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Incidence</td>
<td>$\Delta h_i = f_i \left( \frac{W_{u_1}^2}{2} \right)$</td>
<td>(Conrad, Raif, &amp; Wessels, 1979)</td>
</tr>
<tr>
<td>Blade loading</td>
<td>$\Delta h_{BL} = 0.05D_T^2U_Z^2$</td>
<td>(Coppage &amp; Dallenbach, 1956)</td>
</tr>
<tr>
<td>Tip clearance</td>
<td>$\Delta h_{TC} = 0.6 \left( \frac{t_{c1}}{b_2} \right) C_{u_2}$</td>
<td>(Jansen, 1967)</td>
</tr>
</tbody>
</table>
4.2 Skin-friction coefficient

In this part, the skin friction coefficient is calculated based on the most well-known correlations which were integrated into the mean-line code. The validation case is the Sandia main centrifugal compressor, for which the dimensions were given in chapter 2. To select the most accurate model, results are compared with the unsteady CFD simulations and the experimental data of the Sandia sCO₂ main compressor over a range of operating conditions.

4.2.1 Mean-line

The skin friction correlation proposed by Jansen (\(\Delta h_{SF}\)) (Jansen, 1967), \(L_p\) incorporates the passage length and \(\bar{W}\) is the mean relative velocity through the impeller, which are calculated as below:

\[
\begin{align*}
\Delta h_{ML} &= 0.5 \left( \frac{C_2}{\cos \alpha_2} \right)^2 \left( \frac{(1 - \epsilon) - \frac{b_3}{b_2}}{1 - \epsilon} \right)^2 \\
\Delta h_{SF} &= 2c_f \frac{L_p}{d_{rb}} \bar{W}^2 \\
\Delta h_{DF} &= c_f \frac{\bar{p}r_2^2 U_2^3}{4 m} \\
\Delta h_{L} &= \frac{\dot{m}_i U_1 U_2}{2m} \\
\Delta h_{R} &= 8 \times 10^{-5} \sinh(3.5\alpha_2^2) D_f^2 U_2^2
\end{align*}
\]

To consider the effects of the diffuser and volute losses on the compressor performance prediction, the empirical correlations proposed by Zhu and Sjolander (Zhu & Sjolander, 1987) were used as follows:

\[
\begin{align*}
\Delta h_{F} &= \frac{p_{t4} - \kappa_d (p_{t3} - p_{t3})}{p_{t4} - \kappa_d (p_{t4} - p_{t4})} \\
\Delta h_{R} &= \frac{p_{t5} - \kappa_s (p_{t5} - p_{t5})}{p_{t4} - \kappa_s (p_{t4} - p_{t4})}
\end{align*}
\]
4 Centrifugal compressor design for the near-critical point applications

\[ L_b = \frac{\pi}{8} \left[ d_2 - \frac{d_t_1 + d_{h_1}}{2} - b_2 + 2L_x \right] \left( \frac{4}{\cos \beta_{t_1} + \cos \beta_{h_1} + 2 \cos \beta_2} \right) \] (11)

\[ \bar{W} = \frac{(2W_2 + W_{t_1} + W_{h_1})}{4} \] (12)

The axial length of the impeller, \( L_x \), is calculated using Aungier’s correlation which is the function of the flow coefficient, \( \Phi \), (Aungier, 2000) as follows:

\[ L_x = d_2 \left( 0.014 + \frac{0.023d_2}{d_{h_1}} + 1.58\Phi \right). \] (13)

The hydraulic diameter, \( d_{hb} \), for an annular simple passage can be assumed as the passage width, but to generate a more realistic estimation of \( d_{hb} \), Jansen’s recommendation was used as follows (Jansen, 1967):

\[ d_{hb} = d_2 \left( \frac{\cos \beta_2}{\pi + \frac{Z}{d_2 \cos \beta_2}} \right) + \frac{0.5 \left( \frac{d_{t_1} + d_{h_1}}{d_2} \right) \left( \frac{\cos \beta_{t_1} + \cos \beta_{h_1}}{2} \right)}{\left( \frac{d_{t_1} + d_{h_1}}{d_{t_1} - d_{h_1}} \right) \left( \frac{\cos \beta_{t_1} + \cos \beta_{h_1}}{2} \right)}. \] (14)

The most important parameter in the enthalpy loss correlation is the skin friction coefficient, \( c_f \), because it is the only parameter that can be affected by the sharp real gas properties changes. Jansen (Jansen, 1967) proposed the skin friction factor equation which was derived based on the pipe flow and as a function of Reynolds number as follows:

\[ c_f = 0.0412 (Re)^{-0.1925} \] (15)

\[ Re = \frac{\bar{\rho} \bar{W} d_{hb}}{\mu}. \] (16)

Eq. 15 was derived based on the pipe flow, but the curvature shape of the impeller passage requires the higher value of the skin friction coefficient. However, Jansen (Jansen, 1967) also recommended the constant value of 0.006 for the skin friction coefficient over a wide range of applications.

Another approach that is commonly used to calculate the skin friction coefficient for the turbulent flows is the model proposed by Schlichting (Schlichting, 1949), which is written as follows:

\[ c_f = 0.0412 (Re)^{-0.1925} \] (15)

\[ Re = \frac{\bar{\rho} \bar{W} d_{hb}}{\mu}. \] (16)
4.2 Skin-friction coefficient

\[
\frac{1}{\sqrt{4c_{f_s}}} = -2\log\left(\frac{e}{3.71d_{hb}}\right) \tag{17}
\]

\[
\frac{1}{\sqrt{4c_{f_r}}} = -2\log\left[\frac{2.51}{Re_{hb}\sqrt{4c_{f_s}}}\right] \tag{18}
\]

Where \(c_{fs}\) and \(c_{fr}\) denote the skin friction coefficient for the smooth and rough surfaces respectively. The ratio of the peak-to-valley surface roughness \(e\) is estimated based on surface material and finish (The Sandia main compressor was made by aluminium 6061 T6 and consequently, the wall roughness is around 0.000005).

Owing to the fact that the centrifugal compressors operate over a wide range of operating conditions, a correlation for the skin friction loss and the skin friction factor, in particular, should be employed that can comprehensively cover the laminar and turbulent flows along with the effects of the surface characteristics. Therefore, the weighted averaged model proposed by Aungier (Aungier, 2000) was also examined. This is written as follows:

\[
c_f = c_{fs} + (c_{fr} - c_{fs})(1 - 60/(Re_{hb} - 2000)e/d_{hb}). \tag{19}
\]

Aungier suggested the use of the outlet passage width as a hydraulic diameter in the weighted averaged model; however, using the hydraulic diameter proposed by Jansen (Eq. 12) generated a more accurate result in the current research. For better understanding, skin friction coefficient based on the Jansen model, Eq. 15, is indicated by \(C_{f(JA)}\) and the recommended value (0.006) is shown by \(c_{f(RE)}\). The weighted averaged model proposed by Aungier is named as \(c_{f(WA)}\).

4.2.2 CFD simulations

The Sandia sCO₂ main compressor was simulated using the unsteady approach. Numerical models, mesh and RGP dependency tests and convergence criteria were explained in chapter 2. The only difference is that, for this part of the research to achieve more accurate results, unsteady simulations were performed to capture the effects of the rotor-stator interaction on the performance of the centrifugal compressor.

The fundamental equation of the skin friction coefficient is as follows:

\[
c_f = \frac{\tau_w}{2\rho_\infty U_\infty^2} \tag{20}
\]

where \(\tau_w\) is the wall shear stress, and \(\rho_\infty\) and \(U_\infty\) are the free stream density and velocity, respectively. In a relatively simple geometries and physics like pipe/duct flows, estimating the boundary layer thickness and, consequently, free stream values are
4 Centrifugal compressor design for the near-critical point applications

straightforward. In the recent research conducted by Tiainen et al. (Tiainen et al., 2017), different methods were examined and the most accurate procedure for estimating the free stream locations was proposed. In the previously mentioned research, the boundary layer thickness was calculated as the distance from the wall and the location at which the velocity is 99.5% of the adjacent point velocity. This assumption is formulated as follows:

\[ \frac{dU}{dN} = 0.005 \]
\[ U_{n-1} = 0.995U_n \]
\[ U_\infty = U_n \]

where \( N \) is the normal vector to the wall. In the previous study by Tiainen et al. (Tiainen et al., 2017) the location of the free stream velocity and, consequently, the boundary layer thickness were estimated in the blade-to-blade direction along the impeller. In this study, the same method was used to estimate the free stream values in both blade-to-blade and span wise (hub-to-shroud) directions. Some surfaces in the stream-wise direction along the impeller were generated at which the generated surfaces intersect all walls (hub, shroud and blades). Free stream values were estimated on the lines aligned with span-wise and blade-to-blade directions (see Figure 27). By using this method, the wall shear stress can be calculated from the CFD results at the intersections of the surfaces with all walls. Figure 28 illustrates the wall shear stress distribution at 90% of the meridional distant in the peak efficiency off-design point simulation.

Figure 27. Locations along the stream-wise direction from the main blade leading edge (MB-L) to the blade trailing edge (B-T).
4.2 Skin-friction coefficient

Figure 28. Wall shear stress distribution at 90% of the meridional distance.

In the same meridional distance (90%), Figure 29 depicts the normalized relative velocity distribution and the estimated location of the free stream velocity (circles).

Figure 29. Normalized relative velocity in the blade-to-blade direction at 90% of meridional distance. Circles locate $U_{n-1} = 0.995U_n$.

After estimating the free stream values and the wall shear stress distribution, all these values were averaged at each generated surface along the impeller passage. The skin friction coefficient was calculated based on the averaged values along the impeller for all off-design simulations. Figure 30 compares the calculated skin friction coefficient based on the CFD results and mean-line models along the impeller for the peak efficiency off-design point.
As exhibited in Figure 30, the skin friction coefficient is not constant along the flow passage. The trend shows that the skin friction coefficient increases from the inlet to the outlet of the impeller. However, near the leading edges of the blades, the skin friction factor reaches a peak because of local flow acceleration. The averaged value of the CFD results in all off-design points are in good agreement with the weighted averaged model by Aungier, which incorporated the hydraulic diameter proposed by Jansen, \( c_f(\text{RE}) \) model.

The constant value recommended by Jansen, \( c_f(\text{RE}) \), still has better accuracy than the friction coefficient value on the basis of pipe flow, Eq. 15. Figure 31 shows the Sandia main compressor efficiency calculated by the different friction coefficients in the mean-line code, URANS simulation, and the experimental measurement at 50000 RPM. Employing the pipe flow-based skin friction coefficient, \( c_f(\text{RE}) \), the compressor efficiency is over-predicted, while the trend of the efficiency remains similar to the measurements. Both the recommended value and the weighted averaged model, \( c_f(\text{RE}) \) and \( c_f(\text{WA}) \), predict the efficiency in close proximity to the experimental data, while the weighted averaged models are more closely aligned with the measurements. The URANS simulations over-predict the compressor efficiency because of absence of external losses, volute, and uncertainties pertaining to the numerical and fluid properties.
After selecting the most accurate skin friction coefficient, $c_f(\text{WA})$, individual enthalpy loss shares on the Sandia design point were calculated (see Figure 32). As expected, skin friction loss contributed to more than 50% of the total losses and around 73% of the internal losses of the studied compressor. Due to the extreme importance of the skin friction calculation for the near critical point applications, more experimental data is needed to confirm the proposed statement pertaining to the most accurate skin friction coefficient model. The external and other internal losses (except skin friction loss) computed based on the well-known developed models in the literature (Table 3). Most of those models were developed based on the ideal gas assumptions, which influence should be studied in detail in the future. This might also be one of the reasons why the predicted disk friction loss is relatively low. Moreover, the comparison between the internal losses and the CFD simulation was performed (see Figure 33), which shows a good agreement between the result in the absence of the external losses.
4 Centrifugal compressor design for the near-critical point applications

4.3 Stage efficiency correlations

In this part of the study, different stage efficiency correlations were used to design the investigated compressor and compare it with the developed individual enthalpy loss model. The commercial compressor design code, Vista CCD (PCA Engineers Ltd, 2016), was used in combination with two different well-developed stage efficiency correlations:
4.3 Stage efficiency correlations

Casey-Robinson (M V Casey and C J Robinson, 2006) and Casey-Marty (Casey & Marty, 1986). Both studied correlations are actually stage efficiency correlations rather than individual enthalpy loss correlations. These correlations estimate the polytropic efficiency as a function of the flow coefficient. The pros and cons of the stage efficiency approach are explained as follows. The methods listed above essentially avoid estimation of the individual components of loss in a compressor stage and, instead, rely on correlations of efficiency as a function of non-dimensional overall performance parameters such as flow coefficient and specific speed. On the one hand, attempting to calculate the individual losses arising from several independent sources of loss can result in an incoherent overall loss formulation, which may have little chance of yielding an efficiency that compares well with the test experience (no doubt there are exceptions to this general statement). On the other hand, the simpler methods used in stage efficiency models do not offer the designer direct information about the sources of inefficiency at a particular stage. Rather, this is left to the designer's knowledge of the implications of, say, flow coefficient or specific speed. In addition, the higher density of CO$_2$ in the near-critical point applications, in comparison with air, may affect the Reynolds number and Power Input Factor (PIF) corrections, which considerably improve the accuracy of efficiency prediction. More details on the mentioned design approach based on the efficiency correlations can be found in the research proposed by Robinson et al. (Robinson, Casey, & Woods, 2011). Figure 34 illustrates the comparison between these models at the Sandia compressor design point. The results of these two correlations show slight deviations from the URANS simulation and the enthalpy-based model predictions of outlet temperature, power, and efficiency. Arguably, if the fluid properties are calculated with extreme care, the studied stage efficiency correlations can predict the compressor performance with an acceptable level of accuracy. However, the validity of this argument needs to be verified with further near-critical experiments in the future.

![Figure 34](image-url)
5 Conclusions

5.1 sCO₂ properties in the vicinity of the critical point

Due to growing interest in the sCO₂ Brayton cycle as an alternative for near-future energy production, the numerical investigations of the sCO₂ turbomachinery design and simulation in the near-critical point applications are essential. The first stage of this thesis demonstrated that, large changes in the fluid thermophysical properties near the critical point have an effect on the numerical accuracy and stability. Coupling the real gas equation of states directly to the solver would raise the computational time and cost significantly. Therefore, an external look-up table of properties (RGP table) was generated using the developed code, the properties of which were derived from the NIST REFPROP database. Different EOS models using the diverse range of resolutions were examined on the Sandia radial turbine operating in the supercritical dome. The SW EOS model proved to be more accurate than the other studied cubic EOS models, especially near the critical point. The selected EOS model was used to simulate the map of the Sandia centrifugal sCO₂ compressor and compare the data with experimental measurements. The investigation of the CFD results showed that there was a strong dependency between the compressor performance and flow field and the RGP table resolution. It was observed when the RGP table resolution was increased in a same range, the predicted compressor efficiency trend was more closely aligned with the experimental data. Also, the use of a lower RGP range resulted in different interpolated properties at the compressor inlet, which affected the velocity triangles and, eventually, the flow field inside the studied turbomachines.

The challenges pertaining to the sharp changes in the fluid properties, which caused instabilities in the numerical simulations, were overcome by setting the table range wider than the operating range and increasing the table resolution step by step. In the extended study, the full studied centrifugal compressor was simulated in different boundary conditions while the pressure ratio was kept constant (the most optimum pressure ratio for the studied cycle). The findings revealed that by approaching the critical point, the compressor efficiency was increased almost linearly while the pressure ratio and rotational speed were held constant. However, in some operating points where the inlet boundary conditions were extremely close to the critical point or saturation curves, due to local flow acceleration on the suction side of the blades, the possibility of condensation/cavitation was observed. Even though the volume of the positive supercooling degree was relatively small, when the flow coefficient and, correspondingly, the supercooling degree volume were increased, the droplets were expected to have a noticeable effect on the compressor performance and flow field.
5.2 sCO₂ condensation

Due to flow acceleration at the suction side of the compressor blades, fluid properties crossed the critical point/saturation curves and the supercooling degree became positive. Therefore, there was a possibility that condensation would form. A study using the classical nucleation and droplet growth theories in the supercritical region was performed and the possibility of condensation forming inside the sCO₂ centrifugal compressor was evaluated. Fluid properties were cubic extrapolated up to the spinodal curves to generate the metastable properties. The generated tables were used to model the non-equilibrium condensation inside a converging-diverging nozzle in the supercritical dome and the results were compared with the experimental data. It was concluded that the classical nucleation and droplet growth theories can predict the location of shock accurately in accordance with the experimental data. However, the calculated pressure trend along the nozzle showed that these models lacked accuracy near the critical point. In the non-equilibrium condensation model, the fluid properties occasionally crossed the spinodal curves and ended up in the unstable region. Due to the lack of information about the fluid properties in the unstable region, the properties were clipped to the spinodal curves.

Finally, an investigation was performed to study the possibility of condensation forming inside the compressor by calculating the final states of the fluid inside the unstable zone, residence time, and completion time. A comparison of the residence time and completion time for the most extreme case showed that condensation occurred inside the Sandia sCO₂ centrifugal compressor. However, the design and operating conditions of the compressor affected the possibility of condensation forming and should be studied on a case-by-case basis.

5.3 sCO₂ compressor design methodology

In the last stage of the thesis, a centrifugal compressor design code that was based on the individual enthalpy loss models for the near-critical point was developed. It was noticed that, due to the relatively small size of the turbomachines as a result of high density of the working fluid near the critical point, skin friction loss played a significant role in all internal and external losses. Therefore, more attention was paid to the skin friction losses and, especially, the skin friction coefficient. Due to the wide operating range of the compressor, a model including turbulence and laminar as well as wall finish was utilized. The weighted averaged model proposed by Aungier, which incorporated the hydraulic diameter by Jansen, proved to achieve the best accuracy among the studied models. It was also observed that the skin friction coefficient and, consequently, the friction loss was not constant along the impeller. Using the skin friction coefficient correlations that were proposed for the pipe flows affected the accuracy of the compressor performance prediction with a large deviation from the experimental measurements. The mean-line code results were compared with the URANS simulations and the experimental results
from the Sandia test loop. The weighted averaged skin friction coefficient model exhibited the best agreement with the experimental measurements.

Furthermore, the compressor design methodology based on the stage efficiency correlation was compared with the developed enthalpy-based model and the CFD simulations. The comparison revealed that the studied stage efficiency correlations (Casey-Robinson and Casey-Marti) showed only marginal deviation from the design point data and the CFD result if the fluid properties were selected appropriately and accurately. In conclusion, for near-critical point applications, the modified individual enthalpy based-model and the studied stage efficiency correlations could predict the compressor performance with an acceptable level of accuracy. However, the validity of this statement should be validated in future by further sCO$_2$ experimental measurements.

5.4 Recommendations

Some of the following recommendations (I and IV) have already been investigated by the author; however, due to the publication time and review process, the results are not included in the thesis.

I- The effect of condensation and corresponding losses on the centrifugal compressor performance and flow field should be investigated. In addition, even though the SW model was developed especially for CO$_2$, it is still unable to predict the fluid properties extremely close to the critical point. More developments and improvements are recommended to achieve the numerical result with the lowest possible uncertainties caused by the EOS model.

II- The application of classical nucleation and droplet growth theories resulted in good accuracy for the shock location prediction. However, the pressure distribution confirmed the lack of accuracy of these models when applied to near-critical point applications. Therefore, more investigations are recommended to increase the level of accuracy of these models for the near-critical point applications.

III- More sCO$_2$ turbomachinery experimental data is needed to develop general design methodologies for near-critical point applications. Moreover, other enthalpy loss models that are based on the ideal gas assumption or measurement using air should be investigated in detail.

IV- The effect of the non-homogenous supercritical region and crossing the Widom line on the turbomachinery and heat exchanger performance and flow field should be studied.
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Publication I

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Numerical Investigation of the Flow Behaviour inside a Supercritical CO₂
Centrifugal Compressor

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Numerical Investigation of the Flow Behavior Inside a Supercritical CO₂ Centrifugal Compressor

Centrifugal compressors are among the best choices among compressors in supercritical Brayton cycles. A supercritical CO₂ centrifugal compressor increases the pressure of the fluid which is very close to the critical point. When the supercritical fluid is compressed near the critical point, wide variations of fluid properties occur. The density of carbon dioxide at its critical point is close to the liquid density which leads to reduction in the compression work. This paper explains a method to overcome the simulation instabilities and challenges near the critical point in which the thermophysical properties change sharply. The investigated compressor is a centrifugal compressor tested in the Sandia supercritical CO₂ test loop. In order to get results with the high accuracy and take into account the nonlinear variation of the properties near the critical point, the computational fluid dynamics (CFD) flow solver is coupled with a look-up table of properties of fluid. Behavior of real gas close to its critical point and the effect of the accuracy of the real gas model on the compressor performance are studied in this paper, and the results are compared with the experimental data from the Sandia compression facility. [DOI: 10.1115/1.4040577]

Introduction

One of the most important ways of managing the growth in energy consumption is energy efficiency. Energy conversion cycles are the major part of the electricity production in the world, where Brayton and Rankine cycles are the most common energy conversion processes. A small increase in these cycle efficiencies would achieve a significant gain in electricity production and would save primarily energy sources.

The supercritical organic Brayton cycle has a higher cycle efficiency with the relatively low maximum temperature compared to simple Brayton and Rankine cycles, and the efficiency is closer to the Carnot efficiency [1]. Also, the cycle can utilize several energy sources such as biomass, solar, and waste heat. Due to significant impact of the compressor performance on the cycle efficiency, flow analysis for the supercritical compressors is crucial.

The concept of using supercritical CO₂ as a medium in a closed compression loop Brayton cycle was investigated by Angelino [2]. In Angelino studies, carbon dioxide as working fluid for several condensation cycles was investigated and it was seen that for the high turbine inlet temperature (650°C) single heating carbon dioxide cycle shows better performance than reheat steam cycle. One of the most important advantages of using supercritical CO₂ in Brayton cycle is the higher conversion efficiency achievement according to its moderate values of pressure and temperature.

There have been prior researches about other supercritical fluids as working fluid in a Brayton cycle. For instance, N₂O₄ was evaluated by Sorokin [3], but according to the high corrosiveness and toxicity of the fluid, it was stated as an unsuitable medium. Moreover, organic fluids like hydrocarbons have critical temperature between 30 and 40°C and they have been used in geothermal power generation, but are not good options as a working fluid due to negative effects on the ozone layer and radiation instabilities.

Carbon dioxide close to its critical point has very high density (close to liquid) which leads to lower compression work. Supercritical CO₂ as working fluid in Brayton cycle has been studied in the literature [4,5]. There are a few investigations [6–8] about design of the turbomachines working with fluids close to their critical points. Mostly studies are based on one-dimensional model including real gas effects [9,10].

A numerical investigation about the effect of the real gas on the centrifugal compressor has been carried out by Baltadjiev et al. [11]. It was observed that by reaching to the critical point, compressor choke margin is decreased by 9%. This was because of the increment in the isentropic exponent. Furthermore, a performance map of a centrifugal compressor working with supercritical CO₂ was studied by Rinaldi et al. [12]. A numerical three-dimensional simulation was done with the in-house code and the results were compared to the experimental data over a range of back pressures, and a potential of using computational fluid dynamics (CFD) simulation to improve the design of turbomachinery working with supercritical working fluid was demonstrated.

In this paper, an investigation of the flow behavior close to the critical point and the effects of look-up table resolution on the flow field and the performance of the supercritical CO₂ centrifugal compressor are studied. This is important because even small changes in the simulation accuracy and the resolution of the look-up table of thermodynamic properties can have a significant effect on the compressor performance and flow field in vicinity of the critical point. In addition, this study presents the limitations of the simulation accuracy close to the critical point because of high nonlinear behavior of the flow properties.

Geometry and Mesh of Studied Case

Studied centrifugal compressor is a single stage centrifugal compressor operating in the test loop facility at Sandia supercritical compression loop [9]. Major dimensions of the compressor are mentioned in Table 1. Utilizing the design dimensions of impeller and the blade design software [13], geometry of the impeller was modeled. Fully structured grids were generated and the quality of mesh was
examined by Skewness and Jacobian factors. Most of the grids have skewness below 0.7, although some grids close to the sharp and complex locations have skewness about 0.8. According to the complexity of the geometry, these values are acceptable. Beside the structured grid quality check, quite small grids close to walls ensure that $y^+$ at all walls is close to unity.

The total number of cells approximately 440,000 was found to be sufficient according to the mesh dependency tests, which is presented in Fig. 1.

Mesh dependency test was done by using nondimensional static pressure ratio and isentropic efficiency. Lowest resolution real gas properties (RGP) table (which is discussed in detail in next chapter) was used for mesh dependency check. Figure 2 shows grids of supercritical CO$_2$ impeller with moderate resolution. Tip clearance and vaned diffuser are not modeled in this study. However, the aim of this study is to investigate the effect of the accuracy of the thermodynamic model and it is estimated that these details are not affecting results in this respect.

### Numerical Procedure

The finite volume flow solver ANSYS CFX 16.0 [14] was used for all simulations in this study. Second-order discretization was implemented to solve Reynolds-averaged Navier–Stokes equations coupled to two additional equations of $k-\omega$ shear stress transport turbulence model of Menter [15]. Steady-state

### Table 1 Impeller design dimensions [9]

| Impeller diameter ratio, $d_2/d_1$ | 1.993 |
| Exit blade height, $H_2$ | 0.00171 m |
| Blade trailing edge angle (back swept) | 50 deg |
| Number of blades (splitter and main blades) | 12 |
| Inlet blade angle at tip | 50 deg |
| Thickness of blade | 0.000762 m |

![Fig. 1 Mesh dependency tests](image1)

![Fig. 2 Geometry and grids of the supercritical CO$_2$ impeller](image2)
simulation was done for one passage of impeller consisting of the main and splitter blades. Viscous work term was added to the total energy equation in order to solve the energy equation. Intensity of 5% was prescribed at the inlet boundary condition with zero velocity angle.

Moreover, convergence criteria of steady-state simulations in this study were based on constant values of root-mean-square of momentum, energy and mass below $10^{-5}$, stability in the isentropic efficiency, and stability and reduction of difference of the mass flow between inlet and outlet less than $10^{-5}$ percent.

Static pressure and temperature were defined as inlet boundary conditions with 76.9 bar and 306 K, respectively. Reduced pressure and temperature values are 1.042 and 1.006, respectively. These values are slightly higher than CO$_2$ critical values (304.13 K and 73.77 bar). Shaft speed is 50,000 rpm (machine Mach number is 0.293 which is defined as the ratio of tip speed of the blade at the inlet) and the mass flow rate of 3.6 kg/s (flow coefficient is 0.049 which is defined as $\frac{Q}{\rho_1 U_1 d_2}$) was set as the outlet boundary condition. In the experimental approach, several shaft speeds were conducted from 25,000 to 60,000 rpm but most of the experiments were done with shaft speed of 50,000 rpm. In the experimental measurements, the inlet temperature and pressure were kept between 304.3–307 K and 77–81 bar, respectively. These values and experimental procedures were presented by Wright et al. [16].

**Fluid Property Table**

Thermophysical properties of fluid close to the critical point change nonlinearly. Figure 3 demonstrates the nonlinear behavior of isobaric specific heat of CO$_2$. Nonlinear thermophysical behavior of CO$_2$ near the critical point can be simulated by using an external look-up table of properties. A thermodynamic look-up table of properties of CO$_2$ such as enthalpy, entropy, pressure, temperature, density, and specific heat in constant pressure and volume has been generated by in-house FORTRAN code and coupled with the flow solver ANSYS CFX v16.

The abovementioned properties were taken from the widely used multipurpose NIST REFPROP 9.0 database [17]. Due to lack of accuracy of the two-parameter equation of states (EOS) like Van der Waals EOS [18], especially close to critical point, Span and Wagner (SW) [19] model has been used. SW EOS model is written in terms of Helmholtz energy and applies a completely different method concentrating specially on CO$_2$. The SW EOS covers fluid region from triple point up to 1100 K and 800 MPa for temperature and pressure, respectively, and it has been recommended in vicinity of the critical point with higher accuracy compared to other EOS models [20].

All of the required properties and their derivatives have been stored in two separate tables, one for vapor region and the other for liquid zone. This approach has been used in order to reduce the error of interpolation close to the saturation line. Same approach was used by Pecnik et al. [21]. An extra high resolution saturation table has been generated and coupled with the lookup table separately. These tables were coupled with the in the format of RGP file. In RGP file, saturation lines were computed accurately to ensure that in each iteration proper properties and table have been used by CFX.

Moreover, the large changes in thermodynamic properties close to the critical point are demanding high resolution of look-up tables. The number of tables from very low resolution to high resolution was generated. The ranges of all tables are the same and presented in Fig. 4. Pressure range for tabulated region starts from 50 bar to 300 bar and the temperature range is from 20°C to 150°C. These values are selected to prevent extrapolating of the solver at the beginning of the simulation which reduce the numerical accuracy.

The tabulated region presented in Fig. 4 was created with different resolutions. Resolution of the first table was 100 points for pressure and 100 points for temperature. Intervals of the pressure and temperature in the first table were 2.5 bar and 1.3 K, respectively. The second table was generated with 300 points for pressure and temperature. The last table was defined with resolution of 500 points for pressure and 500 points for temperature in the same range as previous tables. Also, in all tables, more points were generated at the saturation lines (1000). Interval of the pressure and temperature in the highest resolution table which was used in simulation was 0.5 bar and 0.26 K, respectively.

In order to overcome the instabilities of the simulation in vicinity of the critical point, a few steps are suggested as follows:

At first, a solution with lowest resolution was achieved while in the production of the table, critical values should be skipped. In other works, intervals should be selected accurately to jump over the critical values and high peaks. Then, the result was used as an initial solution for higher resolution table and continued to get the result with highest resolution table gradually. This work has been done due to high instability of simulation with high-resolution RGP table. After each computation, the results were compared to the REPROP database in order to check the error of the table.

Two of the nine main properties of the fluid, which were used in RGP tables, were selected to check the accuracy of the table near critical point. Density and entropy were selected as test candidates due to wide fluctuations of these properties and high sensitivity to small pressure and temperature changes.
Accuracy of Real Gas Properties Table

Accuracy of the tables were tested by comparing the converged result of the simulation with REFPROP data. Three spanwise surfaces from inlet to outlet of the impeller at 0.3, 0.5, and 0.7 of span were selected and temperature, pressure, density, and entropy of all nodes were exported. The selected data were compared to the REFPROP data as a function of the pressure and temperature of the result files. According to the results, flow acceleration close to the leading edge at the suction side of the main blade induces the thermodynamic state to pass the critical point and to fall into the saturation region. It causes some inaccurate calculation in this area.

Figure 5 shows an example of the accuracy of entropy at 0.7 spanwise surface from inlet to outlet of the impeller. Compared to other surfaces, differences are more obvious in this spanwise surface. Average error in the lowest resolution is about 3%, and in the highest resolution, the result is around 0.29%. Some points very near the critical point or even exactly at the critical point have an error around 14%. This is because of linear interpolation of thermodynamic properties and the lack of information about fluid behavior near the critical point. It causes around 12% different isentropic efficiency between these two cases.

One common accuracy check of the RGP table is only checking the accuracy of the table before the simulation using inlet and outlet states of the simulations. It should be pointed out that in this study, accuracy check was done after the convergence of simulations. During the simulation, the flow solver uses some interpolation, clipping, and extrapolation methods to predict the properties among the table properties. Therefore, it is important to check the accuracy of lookup table over the whole simulated domain.

Two extra surfaces at inlet and outlet of the impeller were modeled to investigate the accuracy at those areas separately. Mass flow averaged of properties was used at inlet and outlet surfaces. Table 2 shows the results of the accuracy comparison in the case of entropy and density. Moreover, increasing the RGP table resolution does not have a significant effect on the computational cost.

With the higher resolution table 1000 × 1000, very sharp fluctuations in properties close to the critical point occurred and it leads to divergence of the simulation even with very small time steps. In addition, REFPROP using SW mode is not able to predict the thermodynamic properties very close to the critical point. To compare the fluctuations range of the tables, specific heat in constant pressure (C_p) was selected as a candidate property and accurate plot of its fluctuations versus temperature and pressure is presented in Fig. 6. It shows the highest peaks of C_p in different pressures and temperatures.

With lower resolution, smooth curves are shaped near the critical point, but by increasing the resolution, sharp peaks and nonlinear behavior are more pronounced. Moreover, the highest amount of specific heat too close to the critical point changes rapidly by increasing the resolution of table, and thus, stability of the simulation encounters problem.

In the simulation of a compressor in vicinity of the critical point, sometimes fluid properties drop into the subcritical area and liquid properties of the working fluid are returned by the real gas model. By using the single-phase table, which includes only the supercritical region, the solver diverges due to the discontinuous fluctuation. Also, using the extrapolation method in that area decreases the accuracy of the simulation. It should be mentioned that this phenomenon is not seen far from the critical point. So, due to mentioned table accuracy tests and investigations, multiple tables (both liquid and supercritical regions plus extra saturation line tables) with resolution of 500 × 500 and mentioned range are found to be sufficient according to the complexity and instabilities of the simulations.

Compressor Performance

In the experimental test loop, several shaft speeds were tested. The operation and boundary conditions are described in detail by Conboy et al. [5]. Inlet conditions were 306 K and 76.9 bar for static temperature and static pressure, respectively, and constant mass flow rate 3.6 kg/s was adjusted at outlet in order to get a

![Fig. 5 Entropy error (%) at 70% span: (a) lowest resolution (100 × 100) and (b) highest resolution (500 × 500)](image)

![Fig. 6 Fluctuations of C_p versus temperature and pressure (resolution gets higher from left to right: 100, 500, and 1000)](image)
Experimental compressor map was measured by Conboy et al. [16]. Experimental impeller efficiency was calculated based on experimental data presented by Wright et al. [16]. Better agreement between the simulated efficiency of the impeller with higher resolution tables and the experimental efficiency of the impeller implies that the accuracy of the RGP table is with the sufficient resolution. Although difference between the mass averaged enthalpy and entropy at inlet and outlet of both results with lowest and highest accuracy is less than 2%, isentropic efficiency difference is around 12%. Interval of the pressure and temperature in the first table was 2.5 bar and 1.3 K, respectively. Interval of the pressure and temperature in the highest resolution table was 0.5 bar and 0.26 K. Efficiency about 67% was achieved for higher resolution table, while larger efficiency around 79% was observed for lowest resolution table. According to Table 3, the resolution of RGP table does not have a significant effect on the pressure ratio of the compressor. The efficiency was calculated above the experimental efficiency for each case. This is due to the absence of tip clearance and corresponding losses. The compression in T-s diagram with different RGP resolution tables can be seen in Fig. 7. The resolution, i.e., accuracy of the look-up table, is clearly affecting the entropy at the inlet of the compressor because the temperature and the pressure are the same in each simulation. Vicinity of the highest resolution table operation condition to pseudo-critical line causes significant instability and sharp variation of specific heat in that area.

Real Gas Flow Behavior

Changes in the look-up table accuracy and resolution can have significant influence on the real gas flow behavior close to critical point. Furthermore, one of the main difficulties in real gas simulations occurs due to high negative incidence angle at the leading edge of the blades. The flow accelerates at the suction side of the leading edge and thermodynamic properties fall into subcritical region. Flow velocity is higher near the shroud side of the impeller at the leading edge and subcritical region is more observable in this area. Local Mach number increases at the suction side of the leading edge and there is possibility of flow separation. Wide variation of fluid properties in small area causes lots of instabilities in simulation.

By comparing the velocity and local speed of sound fields in lowest and highest resolution results, it was found out that higher Mach number and possibility of separation of the bubbles at the suction side is due to influence of the RGP table on the flow behavior in that area. By increasing the resolution of the RGP table, wider thermodynamic properties variations and fluctuations can be captured, while more instabilities of simulations are occurred. As it was mentioned before, SW EOS model is developed especially for CO₂ and it has been implemented successfully in several studies [11,12,20,21], but even this EOS model cannot predict fluid properties too close to the critical point. Another limitation of simulations is size of RGP table and effects of that on the flow behavior inside the supercritical compressor. Due to the same mesh, boundary conditions (pressure and temperature), and convergence criteria in all cases, this error is estimated as the influence of the RGP table resolution on the flow behavior. In order to investigate the effects of RGP table resolution on the flow field, pressure, temperature, and Mach number flow fields are studied.

Speed of sound in real gas according to the SW model is not only the function of temperature. Also, small areas of flow acceleration can be seen close to the trailing edge of the blades. Mach number field at 70% span around the leading edge of the main blades is presented in Fig. 8. Greater nonlinear behavior of the thermodynamic properties near the critical point can be captured by higher resolution RGP table. Non-dimensional temperature and pressure with inlet values at 70% of the span are illustrated in Figs. 9 and 10, respectively. Subcritical region at the suction side of leading edge of the main blade is observable and it is more significant for higher resolution of table.

Conclusion and Discussion

This paper presented a numerical investigation of a centrifugal compressor operating with CO₂ in the operation conditions close to the critical point. Sandia centrifugal compressor has been selected to be simulated and three-dimensional CFD simulations were performed. Comparison between different resolution RGP tables was conducted and the influence of the table resolution on the fluid properties changes was investigated.

Compressor performance in the case of isentropic efficiency was compared with experimental results and better agreement was

![Fig. 7 Operation conditions of the simulations](image)

![Fig. 8 Mach number at leading edge of the main blade. The left figure is for highest and the right one is for lowest resolution tables.](image)
achieved with higher resolution tables. The accuracy of the gas properties on compressor performance was discussed and it can be concluded that small changes in fluid properties close to the critical point lead to a significant impact on the compressor performance.

Behavior of real fluid shows the high sensitivity of the flow behavior to very small changes in properties and table resolution in vicinity of the critical point. High gradients in gas properties at the vicinity of the critical point are causing instabilities and difficulties to obtain converged results. Although by increasing the table accuracy, computational costs and simulation instabilities are increased rapidly, and as it was mentioned, even the most accurate EOS models for CO₂ like SW EOS are not able to predict the properties too close to the critical point. On the other hand, by using low-resolution table, sufficient accuracy cannot be achieved. So, by increasing the resolution of RGP table gradually, sufficient resolution and accuracy are accomplished in this paper.

Due to acceleration of the flow near the leading edge of the main blade, thermodynamic properties of the flow fall into subcritical region and possibility of condensation in that area is raised. Lower speed of sound at the suction side of the leading edge in higher resolution result leads to higher Mach number, and consequently, greater subcritical area was noticed. Due to lack of experimental information about this phenomenon in compressor and very small area of expected subcritical region, appropriate model for condensation problems is not used in this paper, but for higher rotational speeds and mass flow rates, the effects of this phenomenon are expected to be more significant.

Acknowledgment

The authors gratefully acknowledge the financial support of the Graduate School of Lappeenranta University of Technology.

Nomenclature

\[ \begin{align*}
    h &= \text{enthalpy (kJ/kg)} \\
    H &= \text{height (m)} \\
    k &= \text{turbulent kinetic energy (m}^2/\text{s}^2) \\
    p &= \text{pressure (MPa)} \\
    Q &= \text{mass flow rate (kg/s)} \\
    s &= \text{entropy (kJ/kg K)} \\
    T &= \text{temperature (K)} \\
    U &= \text{speed (m/s)} \\
\end{align*} \]

Greek Symbols

\[ \begin{align*}
    \eta &= \text{efficiency} \\
    \pi &= \text{pressure ratio} \\
    \rho &= \text{density (kg/m}^3) \\
    \alpha &= \text{specific turbulent dissipation (s}^{-1}) \\
    \varphi &= \text{flow coefficient} \\
\end{align*} \]

Subscripts

\[ \begin{align*}
    \text{ex} &= \text{experimental} \\
    \text{h} &= \text{hub} \\
    \text{i} &= \text{inlet of the impeller} \\
    \text{q} &= \text{quasistatic} \\
    \text{g} &= \text{outlet of the impeller} \\
\end{align*} \]

Abbreviations

EOS = equation of state
RGP = real gas properties
SW = Span and Wagner

References


Ameli, A., Afzalifar, A., Turunen-Saaresti, T., and Backman, J.

Effects of Real Gas Model Accuracy and Operating Conditions on Supercritical CO₂ Compressor Performance and Flow Field

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Effects of Real Gas Model Accuracy and Operating Conditions on Supercritical CO2 Compressor Performance and Flow Field

Rankine and Brayton cycles are common energy conversion cycles and constitute the basis of a significant proportion of global electricity production. Even a seemingly marginal improvement in the efficiency of these cycles can considerably decrease the annual use of primary energy sources and bring a significant gain in power plant output. Recently, supercritical Brayton cycles using CO2 as the working fluid have attracted much attention, chiefly due to their high efficiency. As with conventional cycles, improving the compressor performance in supercritical cycles is major route to increasing the efficiency of the whole process. This paper numerically investigates the flow field and performance of a supercritical CO2 centrifugal compressor. A thermodynamic look-up table is coupled with the flow solver, and the look-up table is systematically refined to take into account the large variation of thermodynamic properties in the vicinity of the critical point. Effects of different boundary and operating conditions are also discussed. It is shown that the compressor performance is highly sensitive to the look-up table resolution as well as the operating and boundary conditions near the critical point. Additionally, a method to overcome the difficulties of simulation close to the critical point is explained.

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1 Introduction

Supercritical Brayton cycles are superior to conventional cycles in several aspects. Depending on the working fluid, the cycle efficiency can be enhanced with a relatively low temperature at the turbine inlet. The characteristics of supercritical CO2 cycles were studied in detail by Dostal [1]. Invoking the ideal gas assumption, they concluded that the turbine operating range of pressure (while the pressure ratio is constant) does not have a significant influence on the turbine performance, and the work output is mainly determined by the pressure ratio. Dostal et al. also stated that the fluid in the turbine behaves like an ideal gas except at very high pressure ratios. It was claimed that this pattern is the same also for a compressor operating with an ideal gas and performance mainly depends on the pressure ratio, as opposed to the operating pressure range. However, since a supercritical compressor operates close to the critical point, significant deviations in the compressor performance and flow conditions can be expected between results calculated using a real gas model and those using an ideal gas model. Supercritical compressor work changes significantly as a function of the pressure ratio as well as the operating pressure. The current work shows that compressor work is affected not only by the pressure ratio but also by changes to the operating pressure range.

Thermodynamic properties of CO2 near the critical point exhibit nonlinear behavior. Sharp changes in fluid properties affect the accuracy of numerical simulations and introduce considerable uncertainties into experimental measurements. This inaccuracy and uncertainty becomes more pronounced when approaching the critical point [2]. Issues related with compressor design and numerical simulation in the vicinity of critical point have been addressed in the literature [3–5]. Moreover, it has been shown that in centrifugal compressors operating near the critical point with low flow coefficient, flow acceleration around the suction side of the main blade leading edge causes the fluid thermodynamic state to cross the saturation line and, therefore, condensation can occur [6].

An investigation by Angelino and Invernizzi [7] indicated that the efficiency of supercritical compressor and the supercritical Brayton cycle increases when the compressor inlet conditions become close to the critical point. This improvement in the efficiency stems from the reduction in the compressibility factor of CO2 near the critical point. Thus, investigation of the flow field and compressor performance near the critical point is essential. Rinaldi et al. [8] computed the centrifugal compressor performance map in the supercritical region at different rotational speeds and demonstrated the potential of using the computational fluid dynamics (CFD) simulations to improve the compressor aerodynamics in the supercritical region. Current paper in addition to performing the compressor map investigates the impact of the real gas model on compressor performance and flow field. Also, the possibility of condensation is investigated by creating the metastable region and calculating the supercooling degree. Moreover, effects of the operating conditions when getting far from the critical point at constant pressure ratio on the compressor have been studied and compressor performance at the critical point has been estimated.

This paper is structured as follows: First, brief descriptions of the studied centrifugal compressor, experimental test loop, and computational domain are provided. Then, the numerical methodology and convergence criteria along with the accuracy of the look-up table for the thermodynamic properties are discussed. The effect of look-up table resolution on the flow field and compressor performance in different operating conditions is investigated in the next step. Thereafter, to investigate the influence of pressure ratio and operation conditions on compressor performance, a wide
operating range is studied and the simulated results compared with experimental data. Finally, the location in the studied supercritical centrifugal compressor where condensation possibly occurs is defined by applying a simple criterion.

2 Studied Centrifugal Compressor

The studied compressor is a single-stage centrifugal compressor tested in the Sandia supercritical CO₂ compression test loop facility [9]. Main compressor dimensions are summarized in Table 1. The unshrouded impeller includes six main blades and six splitter blades, while the diffuser has 17 wedge-shaped vanes. Commercial blade modeler software [10] was used to model the compressor from the initial blade geometry. The structured mesh was subsequently generated using ANSYS turbo grid [11] in structured format with sufficiently fine cells near the walls to ensure the values of y⁺ close to unity.

Different grids were tested to check the grid dependency by comparing the nondimensional isentropic efficiency of the modeled compressor at 50 kpm shaft speed. Nondimensional efficiency was calculated by dividing the isentropic efficiency of the simulation by the isentropic efficiency of the coarsest grid. The isentropic efficiency of the centrifugal compressor was calculated according to the following equation:

\[ \eta_s = \frac{h_2 - h_1}{h_2^* - h_1} \quad (1) \]

Isentropic enthalpy (\(h_{2s}\)) has been calculated by assuming the constant entropy and calling the enthalpy from the reference fluid thermodynamic and transport properties database (REFPROP) by using the inlet entropy (from the CFD result) and the outlet pressure. Due to lack of data from the Sandia reports regarding the location of the probes at the compressor inlet and information about the exact boundary conditions (static or total), static boundary conditions were defined and all efficiencies were computed as total to static.

Figure 1 shows the mesh dependency test for the studied centrifugal compressor. Four different grid resolutions with around 500 k, 1000 k, 1500 k, and 2000 k cells were generated with the same mesh topology. Since the efficiency remains almost unchanged after 1.5 \( \times 10^6 \) cells and to reduce the computational costs, the grid with 1.5 \( \times 10^6 \) cells is employed in all simulations in this study. The quality of the structured grid was examined by the Jacobian and skewness factors. Most of the cells had skewness close to unity.

3 Boundary Conditions and Numerical Methods

The critical pressure and temperature of CO₂ are 7.377 MPa and 304.13 K, respectively. In the experimental measurements, inlet temperature range was between 304 K and 306 K and the inlet pressure range was between 7.7 MPa and 8.14 MPa. The impeller rotational speed in the experimental measurements was varied from 25 kpm to 60 kpm while most of the measurements were conducted at 50 kpm. A commercial Navier–Stokes flow solver ANSYS cfx 17.1 [12] was used for the steady-state simulations in this study. In addition, RANS equations were closed through the two equation k–\(\omega\) shear stress transport turbulence model of Menter [13]. Convergence criteria of the simulations were based on reduction of root-mean-square momentum, mass and energy residuals below 10⁻³, reduction and stability of the imbalance (difference between inlet and outlet) mass flow rate, energy, and momentum at each zone below 10⁻³, and the stability in the stage isentropic efficiency along the simulations. Turbulence intensity of 5% with zero velocity angle was prescribed at the inlet, and the reference pressure was set to zero.

Second-order discretization (high resolution) methods were used. Total energy model, including the viscous work term, was defined and all walls were assumed as nonslip. Frozen rotor interface was defined between the stationary and rotating zones [12].

In the first part, Sec. 4.1, the effects of the different resolutions of the fluid properties look-up table on the flow field performed on the studied compressor are studied. Afterward, by setting the inlet conditions to constant values (305.95 K and 7.69 MPa) and varying the back pressure from 8.7 to 9.5 MPa with 0.1 MPa intervals, a compressor map is calculated and compared to experimental data [14].

In section five, the most optimum pressure ratio (1.18) of the compressor according to the experimental measurements is kept constant and different operating conditions are applied to investigate the effect of boundary condition on performance in the supercritical region. The closest inlet pressure ranges from 7.7 MPa to 9.1 MPa, i.e., normalized inlet pressures with respect to the critical point are from 1.04 to 1.233. In addition, inlet temperature varies from 306.11 K to 313.82 K, corresponding to normalized temperatures of 1.004–1.032, respectively. The compressor performance is calculated at 50 kpm with different back pressures (the machine Mach number, which is defined as the ratio of impeller tip speed to the speed of sound at the inlet, ranges from 0.23 to 0.29).

4 Real Gas Properties Table

4.1 Effect on the Compressor Performance. Strong variation of the fluid properties causes high instabilities in the numerical

Table 1 Main compressor design dimensions [11]

<table>
<thead>
<tr>
<th>Table 1 Main compressor design dimensions [11]</th>
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<tr>
<td>Impeller diameter ratio (d_i/d_{14}):</td>
</tr>
<tr>
<td>Impeller diameter:</td>
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<tr>
<td>Exit blade height:</td>
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<tr>
<td>Blade tip angle (minus is backswept):</td>
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<tr>
<td>Blade thickness:</td>
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<td>Inlet blade angle at tip:</td>
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<td>Tip clearance (constant):</td>
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<td>Exit vane diffuser angle:</td>
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<td>Diffuser blade divergence angle:</td>
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simulations and experimental measurements. As an example, Fig. 3 shows the specific heat at constant pressure near the critical point. To overcome the instabilities in the simulation near the critical point, an in-house FORTRAN code was developed to generate an external look-up table of properties, which was coupled with the flow solver. The real gas properties (RGP) table includes nine main properties: specific entropy, specific enthalpy, speed of sound, specific volume, specific heat at constant pressure and volume, dynamic viscosity, thermal conductivity, and partial derivative of pressure with respect to specific volume at constant temperature.

The fluid properties for the external RGP tables were imported from the multipurpose NIST REFPROP [15] database, which employs Span and Wagner (SW) equation of state (EOS) [16]. SW EOS is a real gas model that has been developed especially for CO2. This EOS has previously been evaluated and investigated for near critical point simulations [3,17]. SW EOS is formed in terms of Helmholtz energy and covers thermodynamic properties of CO2 from the triple point up to 1100 K and 800 MPa for temperature and pressure, respectively. Liquid and vapor properties are stored in separate tables. In the supercritical region, both liquid and vapor tables have the same value for each property. In this study, according to the operating conditions, RGP table ranges are 290–330 K and 3.6–11.6 MPa for temperature and pressure, respectively (normalized table ranges with respect to the critical values are 0.95–1.09 for temperature and 0.49–1.57 for pressure). The tabulated region of the look-up table is wider than the operating conditions to prevent extrapolating or clipping routines by the solver in the initial stage of simulation. Figure 4 shows the RGP table and operation ranges in the p-T diagram in this study.

There are limitations to generating the RGP table using REFPROP. Increasing the resolution of the table places some points too close to the critical point, causing divergence in generating the table. The reason for this behavior is that even the SW EOS model is not able to calculate the fluid properties adjacent to the critical point. Another constraint is the stability of the simulation procedure and eventually these instabilities cause divergence in the calculation. To overcome these instabilities and acquire sufficient accuracy for the RGP table, an optimum resolution for the look-up table has to be found.

The results of three RGP tables with different resolution from 100 to 300 points for temperature and pressure are presented and compared in details in this study. Higher resolution table (400) did not affect the result and performance of the compressor. But, by increasing the resolution more than 400 point in the mentioned range of the look-up table, simulation becomes unstable and error becomes significant, because, some points are placed extremely close to the critical point, which causes divergence in table generation due to lack up accuracy of the EOS. To avoid diverging in the extremely dense look-up tables, some points are clipped or extrapolated, which decrease the accuracy of the simulation significantly. The range of all the tables is identical and only the number of points in each table is different. This lowest resolution table was used to obtain an initial solution, and this result was then used as an initial solution for calculation with a higher resolution table. This procedure was continued to achieve the result with the highest resolution RGP table for which the result is insensitive to the look-up table resolution. More details regarding the difficulties in simulation and a method to overcome this issue were provided previously by authors [6]. Figure 5 shows the RGP table accuracy of the span-wise surface from the inlet to outlet of the centrifugal compressor at 0.7 span. The error is calculated according to the local values and the properties given by REFPROP.

Figure 6 illustrates the table accuracy at constant pressures 7.69 MPa (inlet) and 10 MPa. The accuracy of the table 100 is not included in Fig. 6 in order to better distinguish the differences between tables. Highest differences in the error is in vicinity of the critical point, while by getting farther, error decreases significantly. Moreover, there is no significant difference in the errors between table 300 and 400.

The inlet condition of the simulations in this part of the study is in the vicinity of the pseudo-critical line, which indicates the highest isobaric heat capacity at different pressures and temperatures. Simulating close to the pseudo-critical line causes lots of difficulties and instabilities in simulations due to the highly nonlinear behavior of the fluid properties. Figure 7 shows the operation conditions of the simulations (for the 300 points RGP table) and the location of the pseudo-critical line.

Results of different RGP tables are compared with modeled and experimental measurements conducted at Sandia [18]. Figure 8 shows the influence of the RGP table resolution on the performance map of the centrifugal compressor in terms of the isentropic efficiency. The flow coefficient is calculated according to Eq. (2). By increasing the RGP table resolution from 100 to 400, trends of the efficiency variation become closer to the experimental
measurements. Although, there is no significant change between results of tables 300 and 400. The numerical results show higher efficiency compared with the experimental measurements due to some uncertainties related to external losses such as windage losses, flow leakage, and disk friction, which are not included in the CFD simulations. Furthermore, the volute was not modeled as its geometry is not available in the literature. The trend of the isentropic efficiency with the highest resolution table displays a better agreement with experimental and modeled data compared to the lower resolution table results. Averaged error at the inlet and outlet surfaces is presented in Table 2.

In this study, it is argued that even around 0.5% error in the look-up table can have a significant impact on the performance of the compressor when it is operating near the critical region. Difference in the efficiencies mostly comes from accuracy of the properties calculation at the inlet, because the inlet boundary condition is closer to the critical point. By increasing the number of points from 300 to 400, averaged error and compressor performance almost remained constant, while the time and cost of the simulation were increased.

4.2 Effect on the Flow Field. In this part, all boundary conditions in all cases were identical (305.9 K and 7.69 MPa at the inlet and 8.7 MPa at the outlet), while the resolution of the RGP table was altered. Consequently, different flow field behavior is expected at the downstream flow. The boundary conditions were chosen based on the highest flow coefficient and acceleration near the suction side of the blades, which cause strong variations in the properties.

Closest points to the critical point need extensive attention to be calculated accurately. Accordingly, the sensitivity of the flow field to the resolution of the RGP tables is greater in those regions, such as at the suction side of the main blade leading edge. A comparison between local Mach number and the relative velocity vectors around the leading edge of the main blade for different RGP table results is shown in Fig. 10.

By using different resolution tables, different velocities at the impeller inlet are calculated due to the difference between the interpolated densities by each table and consequently mass flow.
rate, even with the constant boundary conditions. By calculating different velocities at the inlet, the velocity flow angle at the blade is changed, which results in different expansion rates at the suction side of the main blade, as shown in Fig. 10. The averaged velocity flow angle with respect to the axial axis at the main blade leading edge changes from around 35 deg to 46 deg when the table resolution is increased from 100 to 300 points. Using the higher resolution table, a higher Mach number can be seen at the suction side of the main blade due to the flow angle being closer to the design point (50 deg).

By investigating the density field inside the impeller, it is noticed that even though the pattern of the density contour is almost similar in different RGP table results, the magnitudes of the property (density) are different. These differences can affect the flow behavior in downstream as well as the compressor performance. Figure 11 illustrates the density profile inside the impeller at \( r/r_2 = 0.8 \) and \( r/r_2 = 1 \). Signs S and M in the following figures indicate the splitter and main blades, respectively.

Differences in density on the pressure and suction sides of the main and splitter blades affect the blade wake and back flow at the impeller outlet. Backflow at the impeller outlet and blade wake can be investigated by studying the radial velocity field. Radial velocity contours at \( r/r_2 = 1.01 \) are shown in Fig. 12. Due to higher acceleration of the flow at the leading edge of the main blade with the higher resolution table, radial velocity at the flow passage between the main blade suction side and splitter pressure side is higher, while at the suction side of the splitter, it is decreased. By increasing the table resolution more than 300, difference in the flow field was not observed. According to the RGP
table accuracy tests, multiple RGP tables (two regions with the saturation line table) with resolution of 300 x 300 for mentioned operating range and intervals of 0.0267 MPa and 0.133 K for pressure and temperature were found to be sufficient.

5 Effects of the Operation Conditions

Optimization of the cycle pressure ratio is the main step in design of a Brayton cycle. In this section, by setting a constant pressure ratio (1.18) at the most optimum pressure ratio according to the experimental measurements, the influence of the operating conditions on the compressor performance in supercritical region is studied. Operating conditions of the studied cases are presented in Fig. 13 (points are numbered from 1 to 15, from left to right). All inlet boundary conditions are placed on the constant entropy line to meet the sharp variation of the thermodynamic properties near the critical point. Inlets reduced temperature and pressure range with respect to the critical point from 1.006 to 1.03 for temperature and 1.04 to 1.23 for pressure. Intervals for the inlet temperature and pressure are 0.6 K and 0.1 MPa. Quite small intervals were chosen to investigate the influence of small changes in the boundary conditions on the compressor performance with constant pressure ratio.

According to Fig. 14, with the constant pressure ratio, the isentropic efficiency increases almost linearly as the inlet conditions approach the critical point. By extrapolating the linear trend, it can be estimated that the efficiency at the critical point could be around 72.1%, while the highest efficiency in simulated cases is 71%. Figure 15 illustrates the nondimensional torque of the rotor. The torque of the centrifugal compressor was calculated according to the following equation:

\[
\tau = \left[ \frac{\tau \times (E) \, dA}{\tau \times (E)} \right] \, d
\]

The variation in efficiency as a result of small changes in the boundary conditions in the vicinity of the critical point while the pressure ratio is constant can be explained as follows: Approaching the critical point, the compressibility factor reduces and the compressor efficiency increases. Reduction of the compressibility factor indicates larger deviation of the specific volume of a real gas from that given by the ideal gas assumption. When the compressibility factor is not constant, enthalpy and internal energy of the real fluid depend not only on the temperature but also on pressure. The compressibility factor at the inlet and outlet of all simulated cases is presented in Fig. 16. Difference between inlet and outlet the compressibility factors reduces as the critical point is approaching. The minimum difference in the compressibility factors is at point 1 (closest point to the critical point), where it is about 6.7%, and this difference increases up to 8.1% for the last point. Moreover, the density changes from the inlet to the outlet of the compressor increases approaching the critical point while the pressure ratio is constant. Higher density change (smaller specific volume change) from inlet to outlet of the compressor at constant pressure ratio results in a reduction of the impeller work and subsequently enhances the compressor performance [19].

Figure 17 illustrates the nondimensional mass averaged density change with respect to the inlet density versus the pressure ratio.
of the compressor in 100 surfaces with equal intervals from the inlet to the outlet of the compressor.

The studied centrifugal compressor was designed for a certain design point. As discussed in the previous section, small changes in the boundary conditions at the inlet (even smaller than 1 K and 0.1 MPa) can have a significant impact on the fluid properties. Far from the critical point, cases number 1 to 15, properties at the inlet like speed of sound increases (22%), which leads to decrease in the machine Mach number from 0.29 to 0.24. Rise in the machine Mach number results in decrease in the stage volume ratio. The machine Mach number, stage volume ratio, determines the sizing of the through-flow area of the stage and results in volumetric overloading [19]. Although the ratio of the mass flow and the density is constant in these 15 cases, by decreasing the effective area of the flow (due to back-flow at the inlet), velocity at the inlet is increased from case 1 to 15. The change of inlet velocity alters the velocity triangle at the blades and causes misalignment of the relative velocity vector with the blade angle, which increases the incidence loss.

6 Possibility of Condensation

Near the suction side of the main blade leading edge (due to flow acceleration), flow properties cross the saturation curve(s), and there is the possibility of condensation. Positivity of the supercooling degree is used as a measure to identify the region with a possibility of condensation. For the metastable region and at the vapor part, the saturation curve has to be substituted by the upper spinodal curve as demonstrated in Fig. 18. Bilinear cubic extrapolation of the saturation properties to the spinodal curve (extending the trends of the properties to the spinodal curve) was done by an in-house FORTRAN code to calculate the properties in the metastable region. More details regarding the metastable region and spinodal decomposition are under the research and will be published in near future by the current authors. The supercooling degree ($\Delta T$) is calculated according to the below equation:

$$\Delta T = T_s(p_v) - T_v$$

where $T_s$ is the saturation temperature at vapor pressure ($p_v$) and $T_v$ is the temperature of the vapor. The positivity of supercooling degree is used as a measure to identify the region with a possibility of condensation. Figure 19 shows the volume of the positive supercooling degree near the blade leading edge.

Due to the proximity of the compressor inlet condition to the critical point, in the course of expansion, the fluid state path intersects with the saturation line at a location very close to the critical point. Therefore, without entering the metastable region, the thermodynamic state of fluid immediately becomes unstable for which thermodynamic properties cannot be defined by SW EOS. It is noted that SW EOS is only correct for the stable region its extrapolation into the unstable region leads to unreasonable results even from a qualitative standpoint. Therefore, cfx has to calculate the fluid properties based on the values on the spinodal curves. In other words, the properties are clipped to the spinodal curves.

It is typically assumed that the condensation is not significant because the region with a positive supercooling degree is confined to a very small volume. However, high flow coefficients or rotational speeds can increase this volume and consequently the chance of condensation.

7 Discussion and Conclusion

The influence of the accuracy of real gas properties on compressor performance and flow fields was investigated in this study. To study the effects of operating conditions on compressor performance in the vicinity of the critical point, flow fields for a wide range of operating conditions were simulated and the results were compared with experimental measurements.

The proximity of the inlet operating condition to the pseudocritical line and critical point causes instabilities in the simulations and nonlinear behavior of the thermophysical properties of the flow. External look-up tables of properties using the SW EOS model were exported from REFPROP and coupled to the flow solver to overcome the instabilities problem.

By decreasing the RGP table interval sizes, the trend of the efficiency with different back pressures became closer to the experimental measurements. It was observed that a small change in the inlet boundary condition affects the density and mass flow rate, and consequently the velocity at the impeller inlet. This can affect the velocity triangle at the blades.

To study the effects of the operating conditions on compressor performance, by keeping the pressure ratio constant, 15 cases with Fig. 18 Spinodal limits built into the table

Fig. 19 Volume of the positive supercooling degree

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different operating conditions were investigated and the trends of the efficiency change and compressor torque were calculated. It was seen that when approaching the critical point, compressor efficiency gradually increases while compressor torque decreases. By studying the density change from the inlet to the outlet of the compressor, it was seen that when approaching the critical point, density change and as machine Mach number increase, which causes the enhancement in compressor performance. At the last part, by locating where supercooling degree becomes positive in the compressor, the region with possibility of the condensation was shown. It is also discussed that the fluid thermodynamic state becomes unstable, which leads to clipping the properties to the spinodal curve as the SW EOS is not valid in the unstable region.

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Nomenclature

\( a \) = unit vector parallel to the rotational axis
\( A \) = surface of all rotational parts (N/m²)
\( c_v \) = specific heat capacity at constant pressure (kJ/kg K)
\( d \) = diameter (m)
\( h \) =enthalpy (kJ/kg K)
\( k \) = turbulent kinetic energy (m²/s²)
\( M \) = main blade
\( n \) = unit vector normal to the surface
\( p \) = pressure (MPa)
\( r \) = radius (m)
\( s \) = entropy (kJ/kg K)
\( S \) = splitter blade
\( T \) = temperature (K)
\( U \) = speed (m/s)
\( Z \) = compressibility factor

Greek Symbols

\( Q \) = mass flow rate (kg/s)
\( \eta \) = efficiency
\( \rho \) = density (kg/m³)
\( \tau \) = torque (kg m²/s²)
\( \sigma \) = total stress tensor (N/m²)
\( \omega \) = flow coefficient

\( \sigma \) = specific turbulent dissipation (s⁻¹)

Subscripts

\( ex \) = experimental
\( h \) = hub

I = liquid
\( s \) = isentropic/saturation
\( v \) = vapor
1 = inlet of the impeller
2 = outlet of the impeller
3 = inlet of the vane diffuser
4 = outlet of the vane diffuser

References


Publication III

Ameli, A., Afzalifar, A., Turunen-Saaresti, T., and Backman, J.

Centrifugal Compressor Design for Near-Critical Point Applications

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1 Introduction

Supercritical organic Brayton cycles offer several advantages over the traditional energy conversion cycles. In supercritical organic Brayton cycles, depending on the working fluid, the cycle efficiency can be increased with comparatively low maximum cycle temperature; thus, different energy sources (such as biomass, coal, solar, and waste heat) can be utilized. Later, there has been a growing interest toward supercritical organic Brayton cycles and especially toward cycles where the working fluid is carbon dioxide. Higher density of the working fluid near the critical point results in more compact turbomachines and heat exchangers compared to the typical Brayton cycles [1]. Even a seemingly marginal improvement in the compressor design can considerably decrease the annual consumption of primary energy sources and brings a noteworthy gain in power plant output. The study by Angelino and Invernizzi [2] indicated that the efficiency prediction and off-design performance have to be obtained by the computational fluid dynamic (CFD) calculations and one-dimensional mean-line analysis. Several researchers, such as Conrad et al. [5], Coppage et al. [6], Jansen [7], Aungier [8], and Rodgers [9], proposed loss models for turbomachinery design. Later, Oh et al. [10] examined the loss models and suggested an optimum set of loss correlations among all available loss models. Most loss models were derived based on the ideal gas assumption suitable for low-density steam or air. However, a careful examination needs to be done to validate these models in near-critical point applications. Due to high density (low specific volume) of the CO₂ near the critical point, the compressor size is considerably reduced. As a result of this reduced size, the friction loss caused by the shear force imposed on the working fluid in the boundary layer plays the significant role among all of the internal losses. Moreover, as

Centrifugal Compressor Design for Near-Critical Point Applications

The supercritical CO₂ (sCO₂) Brayton cycle has been attracting much attention to produce the electricity power, chiefly due to its higher thermal efficiency with the relatively lower temperature at the turbine inlet compared to other common energy conversion cycles. Centrifugal compressor operating conditions in the supercritical Brayton cycle are commonly set in vicinity of the critical point, owing to smaller compressibility factor and eventually lower compressor work. This paper investigates and compares different centrifugal compressor design methodologies in close proximity to the critical point and suggests the most accurate design procedure based on the findings. An in-house mean-line design code, which is based on the individual enthalpy loss models, is introduced to the skin friction loss calculation to establish an accurate one-dimensional design methodology. Moreover, compressor performance is compared to the experimental measurements. [DOI: 10.1115/1.4040691]

Fig. 1 Specific heat in constant pressure variation near the critical point. The dot shows the critical point location.
noted by Aungier [8], centrifugal compressors operate in a wide range of regimes; therefore, a general correlation for the skin friction loss and specifically skin friction factor is needed to cover the laminar and turbulent flows as well as the effect of the surface finish on the wall friction. Thus, the current work focuses on the skin friction coefficient to examine the available loss models in the near-critical applications.

In this paper, an in-house mean-line code to design a centrifugal compressor in the supercritical region is developed. It is noticed that skin friction loss has the biggest share among other loss correlations, which comes from high density and compact size of the turbomachine. Therefore, the code employs different skin friction factor correlations to evaluate their accuracy. To find the most accurate skin friction factor estimation method, different skin friction coefficient models are compared against the three-dimensional unsteady CFD simulations, and the compressor performance prediction based on different skin friction models is compared with the experimental measurements conducted at Sandia national laboratories [11].

In the first part of the paper, compressor design methodologies are discussed and the details of individual enthalphy loss models are presented. Due to the high importance of the skin friction loss in the supercritical CO2 compressor design, more attention has been paid on this loss model. Then, the centrifugal compressor is modeled based on the different stage efficiency correlations at the design point and results are compared with the experimental data, mean-line in-house code, and CFD results.

2 Turbomachine Design Methodologies

In this section, the in-house mean-line design code (AlFa CCD [12]) for supercritical centrifugal compressor, based on the individual enthalphy loss models, is presented in details. To design a centrifugal compressor based on the stage efficiency correlations, the commercial centrifugal compressor design code, Vista CCD [13], employing three different stage efficiency correlations has been used. Results are validated using CFD simulations and experimental data by the Sandia national laboratory [11].

The AlFa CCD code computes the fluid properties employing the multipurpose NIST REFPROP 9 [14], which is based on Span and Wagner (SW) equation of state (EOS) [15]. SW EOS covers the CO2 properties from the triple point up to 1100 K and 800 MPa for temperature and pressure, respectively. SW EOS has been used and validated by several researchers in the near critical point applications and it has been suggested as the most accurate EOS for CO2 in the supercritical region [4,16–19]. In the Vista CCD tool, fluid properties are imported via an external look-up table, which derived from the SW EOS model. The resolution dependency of the look-up table was tested and discussed in detail in the previous study by present authors [19].

AlFa CCD code input parameters are inlet total conditions, impeller enthalphy loss models, and is presented in details. To design a centrifugal compressor based on the stage efficiency correlations, the commercial centrifugal compressor design code, Vista CCD [13], employing three different stage efficiency correlations has been used. Results are validated using CFD simulations and experimental data by the Sandia national laboratory [11].

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In the AlFa CCD code, velocity triangles have been calculated at the hub, mean line radius and the shroud. After calculations of the velocities at the inlet and outlet of the impeller and importing the thermodynamic properties for each location from the REFPROP, the loss correlations can be calculated to update the

\[ \Delta h_1 = f_1 \frac{W_{1}^2}{2} \]

(3)

where \( W_1 \) is the difference between the tangential components of the relative velocity and the blade metal angle. At the design point, flow angle is assumed to be parallel with the blade leading edge metal angle and consequently the incidence loss is zero.

The boundary layers on the blades cause momentum losses, which can be estimated by blade loading loss model of Coppage et al. [6] as follow:

\[ \Delta h_{BL} = 0.05D_f^2 U_{t1}^2 \]

(4)

where \( D_f \) in which the diffusion factor, is given by

\[ D_f = 1 - \frac{W_e}{W_t} + \frac{0.75((U_{e1}C_{e2} - U_{e1}C_{e3})/U_{t1}^2)}{Z \left( 1 - \frac{d_1}{d_2} \right) + 2(d_1/d_2)} \]

(5)

where \( Z \) is the total number of the blades. The diffusion factor defines the diffusion in the impeller passage as well as the blade loading distribution along the impeller.

Skin friction loss is caused by the flow friction at the walls of the impeller and commonly it is calculated based on the model proposed by Jansen [7]

\[ \Delta h_{f} = 2\pi r \frac{f_{r}}{4} \frac{W^2}{

\]

where \( W \) is the mean relative velocity through the passage, \( f_r \) is the average hydraulic diameter of the blade passage, and \( c_f \) is the skin friction factor. For calculating the Reynolds number, the

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\]

where \( W \) is the mean relative velocity through the passage, \( f_r \) is the average hydraulic diameter of the blade passage, and \( c_f \) is the skin friction factor. For calculating the Reynolds number, the
averages of density and viscosity are computed using the values at the impeller inlet and outlet. The flow length, \( L_D \), is estimated as:

\[
L_D = \frac{\pi}{8} \left[ d_2 - \delta h_{t1} + \delta h_{t2} \right] \left( \frac{4}{\cos \beta_{r1} + \cos \beta_{r2} + 2 \cos \beta_{t}} \right)
\]

(7)

and the axial length of the impeller, \( L_A \), is calculated by Aungier’s correlation [8] as:

\[
L_A = d_2 [0.014 + 0.02 \delta h_{a1} / d_{h1} + 1.58 \delta (2)]
\]

(8)

Jansen [7] proposed the common model to calculate the skin friction which is derived on the basis of pipe flow and it reads as:

\[
c_f = 0.0412 \left( \frac{Re}{10^{12}} \right) \]

(9)

\[Re = \frac{5 \pi D h_{a}}{h} \]

(10)

Due to curvature shape of the blade passage of the impeller, the skin friction coefficient is higher than the value estimated by Eq. (9). According to the literature and the suggestion by Jansen [7], an average value of 0.006 results in a good agreement with the experimental data. The density and viscosity are computed as the average values of the inlet and outlet of the impeller have been used to calculate the Reynolds number in Eq. (9).

Another common approach to calculate the skin friction factor in the turbulent flows (\( Re > 2000 \)) was proposed by Schlichting [20] as follows:

\[
\frac{1}{\sqrt{4 \xi_1}} = -2 \log \left( \frac{e}{3.71 b_1} \right)
\]

(11)

\[
\frac{1}{\sqrt{4 \xi_2}} = -2 \log \left( \frac{2.51}{R_{2m} \sqrt{4 \xi_2}} \right)
\]

(12)

where \( e \) is the ratio of the peak to valley surface roughness, which is based on the material and surface finish (Sandia compressor material is aluminum 6061 T6 [11]). Skin friction factors for fully smooth and fully rough surfaces are shown by \( \xi_1 \) and \( \xi_2 \), respectively.

Owing to the fact that the operating conditions of centrifugal compressors expand over a broad range, a correlation for the skin friction loss, and in particular skin friction factor, should be used which can encompass the laminar and turbulent flows as along with the influence of the surface characteristics on the wall friction [8]. Thus, the weighted-average model proposed by Aungier [8,20] is examined, which reads as:

\[
c_f = c_{f1} + (c_{f2} - c_{f1})(1 - 60/(Re - 2000)^{0.6})
\]

(13)

For a simple annular passage, hydraulic diameter can be assumed as the passage width. However, to provide a more realistic representation for \( d_h \), the expression proposed by Jansen [7] is used in this work, which is written as:

\[
d_h = d_2 \left( \frac{\cos \beta_2}{\pi} + \frac{0.5 \delta d_{h1} \delta d_{h2}}{b_2} \right) + d_2 \left( \frac{\cos \beta_{r2}}{\pi} + \frac{0.5 \delta d_{h1} \delta d_{h2}}{b_2} \right)
\]

(14)

In this paper, the skin friction coefficient proposed by Jansen [7] (Eq. (9)) is noted as \( c_{fJA} \), and the weighted averaged model proposed by Aungier [8] (Eq. (13)) is named as \( c_{fA} \). Also, the recommended value by Jansen [7] for the skin friction coefficient (0.006) is named \( c_{fJ} \), see Table 1. In the studied models, hydraulic diameter of the compressor passage proposed by Jansen [7] (Eq. (14)) is used.

One of the significant factors which contribute to the total loss in the centrifugal compressor is the tip clearance. In the unshrouded impellers, a considerable pressure difference between the suction and pressure sides of the blades forces the flow to cross the tip clearance and increase the loss. The model proposed by Jansen [7] shows good agreement with the experimental measurements even in the low specific speed centrifugal compressors. Pressure difference along the clearance gap is calculated based on the blade loading, and the total pressure losses are estimated using the loss factors in the contraction and expansion processes:

\[
\Delta p_{REC} = 0.6 \left( \frac{\delta_{1}}{b_{2}} \right) C_{a2} \times \frac{4 \pi}{b_{2} Z} \left( \frac{r_{2}^{2} - r_{1}^{2}}{r_{2} - r_{1}} \left( 1 - \frac{\rho_{2}}{\rho_{1}} \right) \right) C_{f1} C_{a2}
\]

(15)

where \( \delta_{1} \) is the normal distance of the tip clearance. Due to the strong sensitivity of density to temperature and pressure, especially at the inlet being in close proximity of the critical point, an accurate calculation of the properties using the properties of REPPPROP is applied to calculate the tip clearance loss.

The trailing edge thickness leads to nonuniform flow velocity distribution at the impeller outlet generating the mixing loss. To quantify the mixing loss at the impeller outlet, the following expression, by Johnston and Dean [21], is employed:

\[
\Delta p_{h} = 0.5 \left( \frac{C_{f2}}{\cos \beta_{2}} \right)^{2} \left( \frac{1 - \epsilon}{\epsilon} \right) \frac{b_{2}^{2}}{2 \delta_{h}} \frac{1}{1 - \epsilon}
\]

(16)

where \( \epsilon \) is the dimensionless fraction of blade to blade space covered by the wake. In the aforementioned model, it was assumed that there is no variation of the relative velocities of the jet and relative flow in the wake.

After updating the centrifugal compressor performance by employing the internal loss models, parasitic losses are calculated to take account of the extra work for rotating the compressor. Consideration of the seal leakage is crucial for predicting the input work of the impeller. The empirical leakage loss model by Aungier [8] is derived matching the predicted work curves for open impellers. It is assumed that almost half of the leakage mass flow reentered into the blade passage. This model is expressed as:

\[
\Delta L_{L} = \frac{m_{L} C_{f} U_{L}}{2 \mu} \]

(17)

where \( U_{L} \) is the velocity of the leakage flow, which is a function of pressure difference between the two sides of the clearance and it is expressed as

### Table 1: Studied skin friction models

<table>
<thead>
<tr>
<th>Jansen based on pipe model [7]</th>
<th>Weighted average model [7,8]</th>
<th>( C_{fJA} )</th>
<th>( C_{fA} )</th>
</tr>
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<tr>
<td>Jansen recommendation [7]</td>
<td>( C_{fJ} )</td>
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The average pressure difference across the clearance is derived from the angular momentum variations through the impeller

\[ \Delta p_s = \frac{m(r_2C_{u2} - r_1C_{u1})}{2} \]

and the leakage flow is calculated as

\[ m_l = \rho_lU_lA_l \]

(19)

The recirculation loss has been calculated according to the empirical model by Oh et al. [10], which is expressed as

\[ \Delta p_{rec} = 8 \times 10^{-5}\sinh(3.5a_r^2)D_2^{1.2} \]

(21)

where diffusion factor can be estimated according to Eq. (5). The disk friction loss, caused by frictional force on the rotating disk, is calculated by the model of Daily and Nece [22], which reads as

\[ \Delta p_d = \frac{6\pi 1}{4m} \]

(22)

To include the effect of the diffuser and the volute losses on the compressor performance, models proposed by Zhu and Sjolander [23] are used as follows:

\[ p_{n1} = p_{n1} - \kappa \alpha (r_1 - r_2) \]

(23)

\[ p_{n2} = p_{n2} - \kappa \alpha (r_1 - r_2) \]

(24)

where \( \alpha \) and \( \kappa \) are design target constants for diffuser and volute (values range from 0.01 to 0.2), respectively.

2.2 Studied Case and Numerical Methods. To the knowledge of authors, the only available experimental data of a sCO₂ compressor has been provided by the Sandia reports [11, 24]. The studied case is the main centrifugal compressor in the Sandia split-flow re-compression sCO₂ Brayton cycle. The unshrouded impeller of this compressor includes six main and six splitter blades, while the diffuser employs 17 wedge-shaped vanes. Main compressor dimensions are summarized in Table 2.

The compressor was modeled by using BladeGen [25] and fully structured grids were generated using ANSYS Turbo Grid [26]. Mesh dependency test was done by computing the total to static pressure and stability of the imbalance (difference between inlet and outlet in each zone) of mass flow rate, energy and momentum smaller than 10⁻³%, reduction and stability of the stage isentropic efficiency. Turbulence intensity of 5% with zero velocity angle was defined at the inlet. Two rotations of the impeller found to be sufficient to achieve the converge result (720 deg). The second-order accuracy was used for spatial discretization. Total energy model, including the viscous work term, was defined and all walls were assumed as nonslip. Transient blade row interface employing the Fourier Transformation was defined between the impeller and the vaned diffuser to capture the losses occurred in the transient situation as the flow is mixed between the rotating and stationary zones. The Fourier Transformation interface can be applied for compressible as well as incompressible flows for all range of pitch ratios. Although for smaller pitch ratios (near the unity), time transformation interface is recommended due to more efficient calculations; in this case, because of the relatively high pitch ratio between the zones, Fourier transformation has been used [29].

An external real gas properties (RGP) look-up table has been coupled with the flow solver. RGP table resolution is gradually increased by getting closer to the critical point and critical density curve. The table covers sufficiency wide ranges of temperature and pressure to prevent clipping or extrapolating of the properties. For near the critical point, the resolution dependency of RGP table was done and presented by authors [19, 27]. Boundary conditions at the inlet were set as total pressure and total temperature with reduced values (normalized by critical value) of 1.042 and 1.006 for pressure and temperature, respectively. The static pressure, with the reduced range of 1.16 to 1.33, was set as the outlet boundary condition.

3 Skin-Friction Loss Comparison

The share of the individual loss models at the design point is presented in Fig. 4. It can be seen that due to relatively small size of the compressor and high density, skin friction accounts for the major proportion of the enthalpy losses and it amounts to more than 50% of total losses and around 73% of internal losses (based on the \( c_{f_{in}} \) model).

For the postprocessing of the CFD results, the fundamental equation for the skin friction coefficient is used, which reads as

\[ c_f = \frac{\tau_w}{\frac{1}{2} \rho_u U_s^2} \]

(25)

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Fig. 3 Geometry and mesh of the studied centrifugal compressor and the structured grid. The volute has not been modeled due to lack of geometrical information. Unsteady Reynolds-Averaged Navier-Stokes (URANS) equations were closed through the two equation \( k-\omega \) shear stress transport turbulence model of Menter [28]. Convergence criteria of the CFD simulations were based on reduction of root-mean-square of momentum, mass and energy residuals below 10⁻⁶%, reduction and stability of the imbalance (difference between inlet and outlet in each zone) of mass flow rate, energy and momentum smaller than 10⁻³% and the stability of the stage isentropic efficiency. Turbulence intensity of 5% with zero velocity angle was defined at the inlet. Two rotations of the impeller found to be sufficient to achieve the converge result (720 deg). The second-order accuracy was used for spatial discretization. Total energy model, including the viscous work term, was defined and all walls were assumed as nonslip. Transient blade row interface employing the Fourier Transformation was defined between the impeller and the vaned diffuser to capture the losses occurred in the transient situation as the flow is mixed between the rotating and stationary zones. The Fourier Transformation interface can be applied for compressible as well as incompressible flows for all range of pitch ratios. Although for smaller pitch ratios (near the unity), time transformation interface is recommended due to more efficient calculations; in this case, because of the relatively high pitch ratio between the zones, Fourier transformation has been used [29].

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where \( \tau_w \) is the shear stress at walls and \( U_\infty \) is the free-stream velocity. In complex flows, such as flows in centrifugal compressors, a major problem arises in defining the free-stream velocity. Different methods to estimate the free-stream velocity in the centrifugal compressor were presented and compared in the work by Tiainen et al. [30]. In the aforesaid work, for comparison of different methods, the boundary layer thickness was assumed as a distance between the wall surface and the location, where the velocity is 99.5% of the adjacent point velocity. This assumption can be formulated as

\[
\frac{dU}{dn} = 0.005 \quad (26)
\]

\[
U_{\infty - 1} = 0.995U_{\infty} \quad (27)
\]

\[
U_{\infty} = U_{n} \quad (28)
\]

where \( n \) is the normal direction with respect to the wall. It is noted that in the work by Tiainen et al. [30], the free-stream velocity was estimated only along the blade-to-blade direction, while in the present study, the free-stream velocities are calculated along both blade-to-blade and hub-to-shroud directions. To calculate the free-stream velocity, 11 surfaces at the stream-wise locations intersecting with all walls (hub, shroud, and blades) were generated. Free-stream velocities are calculated at each surface, on two lines aligned with hub-to-shroud and blade-to-blade directions at middle of the passages and middle of the blades, respectively (see Fig. 5).

Figure 6 illustrates the wall shear stress at 90% of the blade passage in the peak efficiency point. For the same location, normalized relative velocity distribution and the estimated free-stream velocity are shown in Fig. 7.

After calculating the shear stress at the walls, free-stream velocity and density, the parameters are averaged in each surface. Figure 8 shows the skin friction coefficient from the CFD simulation, the weighted averaged model \( c_{f,WA} \), \( c_{f,JA} \), and the constant value \( c_{f,RE} \) (at the peak efficiency among the studied off-design cases). CFD simulations show a significant change in the skin friction coefficient along the meridional distance.

Results show that calculating the skin friction coefficient based on the pipe flow approximation, \( c_{f,JA} \), despite of employing the blade passage hydraulic diameter, is not able to predict values close to the CFD simulation. Figure 9 shows the one-dimensional...
AlFa CCD code result versus the CFD simulations and experimental measurements at 50,000 rpm. For the all off-design points, the weighted averaged model, $\text{CF}_{\text{WA}}$, provides the best agreement with the CFD simulations as well as the experimental measurements. Simulations are performed for a wide range of backpressures. By further increase/decrease the back pressure beyond the presented cases in Fig. 9, instability of the simulation increased and leading to divergence of the CFD simulations, consequently those results are not presented. Due to absence of the external loss effects on the compressor performance in the CFD simulations, results show higher efficiency compared with the measurement. It can be seen that by calculating the skin friction coefficient based on the weighted averaged model, $\text{CF}_{\text{WA}}$, to take account the turbulence and laminar flows as well as the effect on the surface finish, better agreement with the experimental data can be achieved. In the extreme case, there is almost 2% difference between the curves denoted by $\text{CF}_{\text{WA}}$ and $\text{CF}_{\text{JA}}$ in Fig. 9, which indicates the importance of the skin friction coefficient calculation accuracy.

To exclude the influence of external losses on the comparison accuracy, the normalized (with respect to the inlet enthalpy) internal losses inside the impeller are compared at the studied off-design points, see Fig. 10. It is noticed that the model using $\text{CF}_{\text{JA}}$ still has the closest values to the URANS simulation, and the pipe model ($\text{CF}_{\text{PA}}$) underestimates the internal losses amount. Although the recommended value by Jansen ($\text{CF}_{\text{RE}}$) can predict the internal loss efficiently, the weighted averaged model $\text{CF}_{\text{WA}}$ still has the most acceptable trend.

4 Stage Efficiency Correlations

In this chapter, different centrifugal compressor design methods are compared at the design point of the Sandia supercritical CO$_2$ compressor. Although the highest rotational speed which was achieved in the experiment was about 65,000 rpm, the most of the stable measurements were conducted at 50,000 rpm. Figure 11 shows the deviation of the predicted outlet temperature, power, and total polytropic efficiency achieved by different methodologies from the model proposed by Sandia [31]. With the Rodgers correlation, the iteration did not converge near the critical point, and it is not presented in the comparisons.

In order to design the compressor based on the stage efficiency correlation, Vista CCD code [13] was used. There are three options for the main correlations: Casey–Robinson [32], Casey–Marty [33], and Rodgers [34]. All three are actually stage efficiency correlations rather than loss correlations. The first two of these three correlations give polytropic efficiency as a function of flow coefficient. In fact, Rodgers’ method is the stage isentropic efficiency in form of a function of specific speed. Specific speed, $N_S$, and flow coefficient, $\phi$, can be computed as follows:

$$N_S = \frac{\sqrt{\dot{m} \rho}}{\sqrt{\text{MPA} \ D \ H_0}} \quad (29)$$

$$\phi = \frac{\dot{m}}{U_d \ D^2} \quad (30)$$

Furthermore, it is possible to modify the efficiencies given by these three formulations in Vista CCD using a Reynolds’ number correction factor which itself employs a “basis” compressor stage efficiency at a standard Reynolds number. Another correction, namely the power input factor (PIF) influences power input and impeller outlet temperature, as opposed to the pressure losses. PIF is employed to account for the temperature rise through disk friction. The value of PIF is estimated empirically from the flow coefficient.

In essence, the methods discussed above do not estimate the individual components of loss in a compressor stage as they use efficiency correlations which receive dimensionless overall performance parameters such as flow coefficient and specific speed. The pros and cons of this approach are explained as follow. On the one hand, calculating the individual losses caused with independent sources and natures of loss can lead to an incoherent overall loss formulation which may occasionally result in efficiency prediction, which is not in good agreement with test experiment. On the other hand, the methods relying on efficiency correlations provide no direct information on the origin of a particular stage loss, instead the designer has to approximate the
contribution of loss sources based on parameters such as flow coefficient or specific speed. However, the Reynold’s number and PIF corrections, which considerably improve the accuracy of efficiency correlations, may be influenced by the higher density of CO₂ in supercritical cycles, in comparison with air. More details on the preliminary design approach based on the efficiency correlations can be found in the work by Robinson et al. [35].

5 Conclusion

A mean-line code including individual enthalpy loss models was developed to predict the compressor performance operating in vicinity of the critical point. It was shown that, because of the relatively small size of the compressor near the critical point, skin friction loss becomes significant and consequently precise prediction of the skin friction coefficient is crucial to realistically estimate the compressor performance. As the centrifugal compressor works over a wide range of the operating conditions, a general formulation has to be used to cover turbulence and laminar flow regimes as well as the surface finish impact. Therefore, the model proposed by Aungier, \( c_{\text{f,mean}} \), was used to take account of transition between the laminar and turbulent regimes along with surface roughness. Using the wall shear stress and the free stream velocity obtained from the CFD calculations, skin friction coefficients along the meridional distance of the impeller were estimated. It was observed that by incorporating the equation for the hydraulic diameter of the impeller, proposed by Jansen, into the Angier’s model, the results are improved with respect to the CFD and the experimental data. In addition, the importance of the skin friction coefficient calculation accuracy and its effect on the compressor performance prediction were investigated. It was seen that the weighted averaged model, \( c_{\text{f,mean}} \), gives the best agreement with the experimental measurements and URANS results.

Moreover, to examine the accuracy of the stage efficiency correlations, for designing the compressor near the critical point, two correlations (Casey–Robinson and Casey–Marly) were compared with the mean-line code, CFD simulations and compressor design point data from the Sandia laboratory. The results of these two correlations showed only marginal deviations from the CFD and enthalpy based mean-line code predictions of outlet temperature, power and efficiency. As a result, it can be argued that even in vicinity of the critical point, if the fluid properties are calculated accurately, these correlations are able to provide acceptable accuracy when compared to more complicated and computationally demanding methods such as CFD. It is noted that, the validity of this argument needs to be verified with further near-critical experiments in future.

Acknowledgment

The authors gratefully acknowledge PCA Engineers for making VistaCCD available and Mr. Peter Came for his assistance in explaining the correlations. Also, authors gratefully acknowledge the financial support of the Graduate School of Lappeenranta University of Technology.

Nomenclature

\( h \) = impeller width
\( C \) = absolute velocity
\( c_f \) = skin friction coefficient
\( c_p = \text{specific heat capacity in constant pressure (kJ/kg K)} \)
\( d \) = diameter (m)
\( e \) = wall roughness (m)
\( b \) = enthalpy (kJ/kg)
\( H \) = head coefficient
\( k \) = turbulent kinetic energy (m²/s²)
\( m \) = mass flow rate (kg/s)
\( n \) = normal to the surface
\( p \) = pressure (MPa)

Greek Symbols

\( \varnothing \) = flow coefficient
\( \eta \) = efficiency
\( \rho \) = density (kg/m³)
\( \tau \) = wall shear (MPa)
\( \omega \) = specific turbulent dissipation (s⁻¹)

Subscript

a = axial
BL = blade loading
c1 = clearance
DF = disk friction
\( \text{h} \) = hub
\( \text{hb} \) = hydraulic diameter of the blade passage
\( L \) = leakage
\( M \) = mixing
\( r \) = rough
\( R \) = recirculation
\( s \) = isentropic/static/smooth
SF = skin friction
\( t \) = total
\( \text{TC} \) = tip clearance
\( u \) = circumferential component
\( w \) = relative
I = inlet of the impeller
O = outlet of the impeller
3 = inlet of the vane diffuser
4 = outlet of the vane diffuser/inlet of the volute
S = outlet of the volute

References


Publication IV

Ameli, A., Afzalifar, A., and Turunen-Saaresti, T.

Non-Equilibrium Condensation of Supercritical Carbon Dioxide in a Converging-Diverging Nozzle

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Non-equilibrium condensation of supercritical carbon dioxide in a converging-diverging nozzle

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Abstract. Carbon dioxide (CO₂) is a promising alternative as a working fluid for future energy conversion and refrigeration cycles. CO₂ has low global warming potential compared to refrigerants and supercritical CO₂ Brayton cycle ought to have better efficiency than today’s counter parts. However, there are several issues concerning behaviour of supercritical CO₂ in aforementioned applications. One of these issues arises due to non-equilibrium condensation of CO₂ for some operating conditions in supercritical compressors. This paper investigates the non-equilibrium condensation of carbon dioxide in the course of an expansion from supercritical stagnation conditions in a converging-diverging nozzle. An external look-up table was implemented, using an in-house FORTRAN code, to calculate the fluid properties in supercritical, metastable and saturated regions. This look-up table is coupled with the flow solver and the non-equilibrium condensation model is introduced to the solver using user defined expressions. Numerical results are compared with the experimental measurements. In agreement with the experiment, the distribution of Mach number in the nozzle shows that the flow becomes supersonic in upstream region near the throat where speed of sound is minimum also the equilibrium reestablishment occurs at the outlet boundary condition.

NOMENCLATURE

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GREEK SYMBOLS

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1. Introduction

Supercritical Brayton cycles have several advantages over conventional ones. For Supercritical Brayton cycles, depending on the working fluid, a higher cycle efficiency can be achieved with the relatively low temperature at the turbine inlet.

A previous study by Angelino and Invernizzi [1] indicated that the efficiency of the supercritical compressor and therefore, supercritical Brayton cycle becomes higher when the compressor inlet operation condition approaches the critical point. Previous studies showed that for low flow coefficient compressors operating in the vicinity of the critical point, due to the flow acceleration near the suction side of the main blade leading edge, the fluid state crosses the saturation curve and therefore, there is the possibility of spontaneous condensation [2-3]. Accordingly, an investigation of the non-equilibrium condensation of the supercritical carbon dioxide (SCO$_2$) is essential. Near the critical point, fluid has non-linear behavior and the behavior of the fluid is very sensitive to temperature and pressure. Previous studies discussed the difficulties of the compressor design and numerical calculations near the critical point [2, 4-5].

Numerical and thermophysical investigations of the formation of the dispersed phase in the rapid expansion of SCO$_2$ were studied in literature [6,7] and it was concluded that the most important factor which has a significant effect on the pressure and flow fields inside a supercritical nozzle is the inlet pressure. Moreover, the pressure at the inlet can alter the location at which the pressure goes below the critical pressure and consequently it changes location changes of onset of dispersed phase formation.

Furthermore, the impact of the supercritical condensation inside a centrifugal compressor was studied [8] by a non-dimensional criterion, which is related to the nucleation time and expansion rate. It was reported that condensation might not occur when the inlet boundary condition is far from the critical point. However, near the critical point, the effects related to phase transition are expected to become more significant.

The non-equilibrium condensation for high-speed flows in converging-diverging nozzles has been investigated for different fluids in many works such as [9-13]. The latent heat release due to condensation leads to a pressure drop or rise in the converging or diverging part of a nozzle, respectively. To isolate the unnecessary difficulties of modelling the condensation in supercritical fluids and focus on the essential elements of the model, the non-equilibrium condensation in a converging-diverging nozzle is selected for investigation to keep the flow complexity to a minimum. It is hoped that the current work provides a validation basis for modeling condensation in centrifugal compressors in future.

This work applies the numerical model developed by Gerber [14] to predict the flow field in the course of spontaneous condensation. The focus is on the prediction of the location of condensation and its effects on the flow field.

2. Experimental, theoretical and numerical procedures

2.1. Experimental setup

In the experimental measurements (which numerical results in this paper are compared with) performed by Nakagawa et al. [11] different converging-diverging nozzles with the same divergence angles and different boundary conditions were used. The shape and dimensional parameters of the nozzle are shown in Figure 1. The nozzle was rectangular due to ease construction and the heat transfer through the walls was reported to be too small to affect the experiment. The nozzle with the closest inlet conditions to the critical point is selected for the numerical investigation in this study, which has a divergence angle $\theta$ of 0.48°.
2.2. Non-equilibrium model

The foundations for almost all non-equilibrium phase change models are laid upon the prediction of the new phase evolution in forms of two consecutive stages described by the nucleation and droplet growth theories. It is believed that initially the condensation is favored by nucleation providing the first droplets of the liquid phase. Then, the phase transition is governed by the growth of supercritical droplets, which ideally quenches the nucleation and reestablishes the equilibrium [15]. The supercritical term is referred to the droplets larger than a critical radius, \( r^* \), which is calculated according to the theory developed by Gibbs and Thomson for the equilibrium between a vapor with supersaturation ratio \( S \) and a liquid droplet. Here by use of Clausius-Clapeyron equation [16], critical radius \( r^* \) is related to the supercooling degree, \( \Delta T \), and the specific enthalpy of evaporation, \( L \), as below,

\[
r^* = \frac{2\sigma}{\rho_l \ln(S)} \approx \frac{2\sigma T_s}{\rho_l L \Delta T}, \quad \Delta T = T_s(\rho_v) - T_v
\]

where \( T_s \) is the saturation temperature at vapor pressure, \( p_v \), \( \rho_l \) is the liquid density and \( \sigma \) is surface tension. The calculation of the surface tension of the liquid carbon dioxide is based on a semi-empirical formulae proposed by Brock and Bird [17] using critical pressure, temperature and volume to express the liquid’s surface tension as follows

\[
\sigma = \left(-0.951 + \frac{0.432}{Z_c}\right)(1 - T_r)^{1/9} \left(P_v T_c\right)^{1/3}
\]

where \( T_r \) and \( Z_c \) are reduced temperature and critical compressibility factor, respectively. These parameters are given as follow

\[
T_r = \frac{T}{T_c}
\]

\[
Z_c = \frac{1}{R} \left(\frac{P_v}{T_c}\right)
\]

where subscript \( c \) refers to the critical state of the variables. Several expressions of surface tension equation are available in the literature [18-20]. A comparison between these surface tension models and experimental data was conducted by Jianxin and Yigang [21] and it was concluded that close to the critical point and in the range of interest in this article, Brock and Bird model has the highest accuracy. Therefore, this model was implemented to the flow solver by means of a user defined CFX Expression Language (CEL).
Despite decades of research after formulating the classical nucleation theory by Becker and Döring [22] and Zeldovich [23], the classical nucleation theory is still the most popular approach to model the nucleation process. Also, here the formation rate of critical droplets per unit volume \( J \) is computed by the Becker and Döring expression for the classical theory of the homogenous steady nucleation as follows

\[
J = \frac{\rho^2}{\rho_l} \left( \frac{2\sigma}{\pi m} \right)^{1/2} \exp \left( -\frac{4\pi r^{2} \sigma}{3kT} \right).
\]  

A growing droplet absorbs monomers of the vapor phase through molecular collisions. Simultaneously, the droplet needs to give away the latent heat released by the condensation of monomers into the droplet. Due to large amount of the latent heat, of the droplet growth is dictated by the rate of heat transfer between the droplet and the vapor [24]. As the droplet temperature is unknown, one needs to iteratively solve the heat and mass transfer equations to obtain the growth rate. Although, the iterative method can be discarded applying the following estimation for a droplet temperature

\[
T_l = T_s - \Delta T \frac{r}{r^*}
\]  

The details of the non-equilibrium model were provided by Gerber, in [26]. Here only a general description about the model in accordance with choices and assumptions made in this work are given. For the continuous and dispersed phases, the discretized transport equations are solved in an Eulerian reference frame. The model can also benefit from the so-called Source Specific capability to divide the liquid phase into separated groups based on their locations of nucleation/introduction. The mass and energy transfer between the dispersed phases and the continuous one are handled through source terms. Similar to the continuous phase, the dispersed phases are also evolving in the form of volume fractions. Thus, the conservation equations for the continuous and the dispersed phases are expressed using their volume fractions respectively denoted by \( \alpha_v \) and \( \alpha_l \), along with the constraint \( \alpha_v + \sum_{i=1}^{n_l} \alpha_l = 1 \)

\[
\frac{\partial (\alpha v \rho)}{\partial t} + \frac{\partial (\alpha v \rho u_j)}{\partial x_j} = -\sum_{i=1}^{n_l} S_{1,i} - \sum_{i=1}^{n_l} S_{2,i}
\]  

\[
\frac{\partial (\alpha l \rho)}{\partial t} + \frac{\partial (\alpha l \rho u_j)}{\partial x_j} = S_{1,l} + S_{2,l}
\]  

Above equations define the mass conservation for each phase and they are connected by means of source terms \( S_{1,i} \) and \( S_{2,i} \). The mass transfer from the continuous phase to the dispersed one, induced by nucleation is computed by \( S_{1,i} \), and \( S_{2,i} \) accounts for the growth/decay of a dispersed phase as follows

\[
S_{1,i} = m^* \alpha_v J
\]  

\[
S_{2,i} = \left( \frac{3\rho \alpha}{r} \frac{dr}{dt} \right)_l, \quad r_l = \left( \frac{3\alpha_l}{4\pi N_l} \right)^{1/3}
\]  

where \( m^* \) is the mass of a critical droplet, \( \alpha \) is the volume fraction. Moreover, the droplet number \( N_l \) of each dispersed phase must be conserved.
\[ \frac{\partial (\alpha N)}{\partial t} + \frac{\partial (\alpha N u_j)}{\partial x_j} = S_{1,l} \]  

(11)

In the same manner as with the mass conservation equations, by neglecting the relative acceleration between phases and discarding energy equations for dispersed phase, the conservation of momentum and energy for the continuous phase yield as below

\[ \frac{\partial (\alpha p u_i)}{\partial t} + \frac{\partial (\alpha p u_i u_j)}{\partial x_j} = -\alpha \frac{\partial p}{\partial x_j} + \frac{\partial (\alpha \tau_{ij})}{\partial x_j} - \sum_{l=1}^{n_l} u_{S_{2,l}} \]  

(12)

\[ \frac{\partial (\alpha p H)}{\partial t} + \frac{\partial (\alpha p u_i H)}{\partial x_j} = -\alpha \frac{\partial p}{\partial t} + \frac{\partial (\alpha \tau_i)}{\partial x_j} + \frac{\partial (\alpha u_j r_{ij})}{\partial x_j} - \sum_{l=1}^{n_l} L_{S_{2,l}}. \]  

(13)

2.3. Numerical procedure

Commercial Navier-Stokes flow solver ANSYS CFX 17.0 [27] was used for the steady states simulations in this article. Furthermore, RANS equations were closed through the two-equation k – \omega SST turbulence model of Menter [28]. Convergence criteria of the simulation were based on the reduction of Root Mean Square (RMS) momentum, mass and energy residuals below \(10^{-4}\), reduction and stability of the imbalance (difference between inlet and outlet) of mass, volume, energy and momentum below \(10^{-3}\%), and constant volume fractions for both phases and droplet numbers at the outlet. Turbulence Intensity of 5% was prescribed at the inlet and reference pressure was set to zero. Total energy model, including the viscous work term was defined and all walls were assumed as non-slip. Total pressure and temperature were defined as the inlet boundary conditions and the static pressure was set as the outlet boundary condition. According to the different experimental measurements at the different boundary conditions, the closest inlet boundary condition to the critical point was selected to investigate the difficulty of the simulation and have a similar inlet boundary condition as one could have in a supercritical centrifugal compressor. Pressure and temperature at the inlet are 9 MPa and 40°C, respectively. Static pressure 3.89 MPa was set as the outlet boundary condition.

The structured 3D mesh was generated using a sufficiently fine grid for one fourth of the whole geometry. Grids were denser near the walls to ensure the values of \(y^+\) close to unity. The quality of the structured grid was tested by Jacobian and skewness factors and most of the cells had skewness below 0.11. Grid dependency test was carried out and it was seen that a number of grids around 300000 cells is sufficient to ensure the grid-independent pressure trend and drag coefficient on the walls.

Fluid near its critical point has non-linear behavior and properties change rapidly. Figure 2 shows the specific heat in constant pressure at different pressure and temperature near the critical point. Sharp variation of the fluid properties causes high instabilities in the simulation. In order to calculate with high accuracy, an external look-up table of properties is coupled with the flow solver. Real Gas Properties (RGP) table includes nine main properties of fluid such as entropy, enthalpy, speed of sound, specific heat in constant pressure and volume and their derivatives. Properties of both vapor and liquid components were defined in a single RGP table.
Among different real gas Equation of States (EOS) equations, Span and Wagner (SW) \[29\] has been proposed especially for CO$_2$. This EOS was previously tested for simulations near the critical point and shown to be more accurate compared to other EOSs \[2, 30\]. SW EOS is formed in terms of Helmholtz energy and covers thermodynamic properties of CO$_2$ from the triple point up to 1100 K and 800 MPa for temperature and pressure, respectively. Full details on SW EOS and its derivatives can be found in the Ref. \[31\]. The fluid properties for the external look-up tables were calculated using the multipurpose NIST REFPROP 9 \[31\] database. These data were stored in the separate tables includes, liquid, vapor, metastable and saturated regions. Range of the RGP table is from 0.7 MPa and 230 K to 50 MPa and 730 K for pressure and temperature, respectively. Range of the table was chosen wider than the operating condition to prevent extrapolating or clipping methods by the solver, which decreases the accuracy of the numerical simulation. RGP resolution dependency test was done previously by authors \[3\] and it was concluded that intervals of 0.26 K and 0.05 MPa for temperature and pressure, respectively, are sufficient to have a stable and accurate simulation.

The vapor properties in the metastable region, i.e. between the saturation and the upper spinodal curves in the Figure 3, are given from a bilinear cubic extrapolation of the saturation properties to the spinodal curve. The extrapolation procedure is done by an in-house FORTRAN code.

2.4. Numerical difficulties
In the non-equilibrium condensation model in Ansys CFX, critical radius is calculated according to the following equation \[32\],
\[ r^* = \frac{2\sigma}{\rho l \Delta G_v} \]  

(14)

where, \( \Delta G_v \) is Gibbs free energy change of the vapor. Therefore, by comparing the equation (14) with equation (1) it can be deduced that \( \Delta G_v \) in Ansys CFX must be calculated as

\[ \Delta G_v = \frac{L \Delta T}{T_s} \]  

(15)

The Gibbs free energy change of the vapor near the critical point is very small which leads the equation to have an infinite value and causes error in the solver. In order to prevent this numerical instability, the solver clips the critical radius to a certain amount, as a default 1 mm. This extremely large default clipping value decreases the accuracy of the simulation and results in non-realistic droplet sizes. The problem is that it is not possible to change or modify the formula in the Ansys CFX by the user. To sidestep this problem, the critical radius was calculated according to the equation (1) in the post processing stage. It was observed that the critical radius, see Figure 4, changes very moderately also in the nucleation zone. Therefore, the radius of one nano meter has been estimated to be realistic for the critical droplet size in this study and in the calculations the critical radius is clipped, by a CEL, to one nano meter.

![Figure 4. Critical radius distribution over the nozzle centerline.](image)

3. Results and discussion

In order to prevent shock waves inside the nozzle, shorter length (8.38 mm) of the diverging part of the nozzle was assumed in experimental pressure measurements [11]. Thermocouple channels were implemented into the drilled holes along the nozzle wall to measure the temperature profile. Through the nozzle, saturated pressures where obtained according to the measured temperature. In figure 5, experimental saturation pressure were connected using dash lines.
Saturation pressure in numerical calculation is in a good agreement with the experimental data in most of the locations, although near the outlet of the nozzle due to the droplet condensation, slight deviation has been observed. This is mostly because of lack of accuracy of the classical nucleation theory in supercritical region, experimental uncertainties and numerical errors.

Figure 6 shows liquid mass fraction, supercooling, surface tension and Mach number inside the nozzle. Maximum mass fraction of the liquid carbon dioxide is observed near the outlet of the nozzle. As mentioned in the experimental procedure, near the outlet, shock has been occurred which is in agreement with the numerical results. Furthermore, by investigating the Mach number inside the converging-diverging nozzle, it can be noticed that the onset of phase transition occurs near the outlet, but the flow becomes supersonic in the upstream region near the throat where the speed of sound is minimum in that region.

4. Conclusion
In this paper, non-equilibrium condensation of supercritical CO₂ has been modelled. An external look-up table of properties was coupled with the solver to accurately and efficiently calculate thermodynamic properties near the critical point. Bilinear cubic extrapolation of the saturation properties to the spinodal curves was done by an in-house FORTRAN code to calculate the fluid properties at the metastable region. In order to prevent clipping near the critical point, an external function was defined to estimate more accurate critical radius for CO₂. Shock was seen near the outlet of the nozzle in a same
location as mentioned in the experimental data. Around 5.7% mass fraction of the liquid was observed near the outlet and the flow becomes supersonic in upstream region near the throat where the speed of sound is minimum. Further investigations will be conducted by the authors to implement the same approach in turbomachines especially in the centrifugal compressors to predict the effect of the condensation on the blade loading and compressor performance. Also, more studies will be done in order to increase the accuracy of non-equilibrium condensation near the critical point by modifying the nucleation and droplet growth theories.

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References


Publication V

Ameli, A., Uusitalo, A., Turunen-Saaresti, T., and Backman, J.

**Numerical Sensitivity Analysis for Supercritical CO₂ Radial Turbine Performance and Flow Field**

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Numerical Sensitivity Analysis for Supercritical CO₂ Radial Turbine Performance and Flow Field

Alireza Ameli*, Antti Uusitalo, Teemu Turunen-Saaresti, Jari Backman

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Abstract

The predominant advantage of a supercritical CO₂ (SCCO₂) Brayton cycle is its diminished compression work when compared to an ideal working fluid such as helium, due to low compressibility factor. For flows where the density approaches the critical density, molecular interactions get stronger and the ideal gas assumption is no longer appropriate.

As a means to investigate the accuracy of real gas models and sensitivity of the performance of a turbomachine on the numerical accuracy in the supercritical region, numerous unsteady simulations of a radial turbine have been performed. Real Gas Properties (RGP) table has been generated to overcome difficulties of instabilities in simulations in the supercritical region. Four Equation of States (EOS) models with different RGP table resolutions have been studied and results are compared with the experimental measurement performed at the Sandia National Laboratory. The studied unshrouded radial impeller has 11 blades while the nozzle has 10 vanes. The unsteady simulation results show the dependency of the predicted radial turbine performance on the RGP table resolution as well as on the implemented EOS models. In general, the results indicate that by using appropriate EOS model and a look up table with high resolution, the CFD can predict turbine performance with high accuracy while the use of some EOS and low resolution look up tables lead to significant deviations between the simulated and measured results. As a result of this study, an appropriate EOS model and sufficient resolution of the look-up table for turbines operating at supercritical region are suggested.

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Keywords: Supercritical; real gas properties; critical point; radial turbine

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1. Introduction

Methodology for accurate simulations and improved design of supercritical CO$_2$ (SCO$_2$) turbomachines are at the forefront of many efforts in academia and industry. As SCO$_2$ cycle development and number of applications have accelerated over the next few years, the need for efficient and accurate methodology will increase dramatically.

Intractable variation of the thermophysical fluid properties in the supercritical region, especially in vicinity of the critical point, makes the simulations unstable. On the other hand, neglecting the real gas behavior of the fluid in the supercritical region decreases the accuracy of the simulation and strongly affects the calculation result. The specific features and characteristics of the turbomachine design in the supercritical region are addressed in the literature [1, 2, 3, 4, 5].

Due to high density of the supercritical fluid, small turbomachines are preferred in the supercritical Brayton cycle, and thus turbomachines of radial types are mainly used. Despite of significant progress in the design of turbomachinery operating with the ideal behaved fluid, there are few researches regarding the behavior and sensitivity of the turbomachine performance and flow field to the real gas model and numerical accuracy. Difficulties in the simulation and experimental measurements due to non-linear variation of the fluid thermophysical properties in the supercritical region are addressed in the literature [2, 6, 7, 8].

In the previous studies [7, 8], SCO$_2$ radial compressor operating in vicinity of the critical point were analyzed numerically and effects of the numerical accuracy and the real gas model on the compressor performance and flow field were investigated. In addition, the obtained numerical results were compared with the experimental data at the Sandia test loop facility [9] and strong sensitivity of the compressor performance to the real gas properties look-up table was identified. Despite some previous studies on compressors, there is a lack of studies in the literature examining the losses and fluid expansion in turbines operating with supercritical fluids. Increase the understanding of flow phenomena occurring during the fluid expansion with supercritical fluids will be one of the key issues in improving the efficiency and feasibility of SCO$_2$ cycles.

In this study, a radial turbine placed in the same shaft as the previously studied centrifugal compressor is analyzed numerically and the impact of the different real gas models as well as the accuracy of the look-up table on the turbine performance and flow fields are demonstrated. Results of the unsteady simulations are compared with the experimental measurements at the Sandia test loop facility.

<table>
<thead>
<tr>
<th>Nomenclature</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>d</td>
<td>diameter</td>
</tr>
<tr>
<td>h</td>
<td>enthalpy</td>
</tr>
<tr>
<td>( \dot{m} )</td>
<td>mass flow rate</td>
</tr>
<tr>
<td>( \eta )</td>
<td>efficiency</td>
</tr>
<tr>
<td>p</td>
<td>pressure</td>
</tr>
<tr>
<td>s</td>
<td>entropy/isentropic</td>
</tr>
<tr>
<td>t</td>
<td>total condition</td>
</tr>
<tr>
<td>T</td>
<td>temperature</td>
</tr>
<tr>
<td>( \pi )</td>
<td>pressure ratio</td>
</tr>
<tr>
<td>( \omega )</td>
<td>shaft rotational speed</td>
</tr>
<tr>
<td>Z</td>
<td>compressibility factor</td>
</tr>
<tr>
<td>1</td>
<td>nozzle inlet</td>
</tr>
<tr>
<td>2</td>
<td>nozzle outlet</td>
</tr>
<tr>
<td>3</td>
<td>rotor inlet</td>
</tr>
<tr>
<td>4</td>
<td>rotor outlet</td>
</tr>
</tbody>
</table>
2. Studied radial turbine and numerical methods

Studied turbine is a single-stage radial inflow turbine tested in the Sandia supercritical CO$_2$ test loop [9]. Main turbine dimensions are summarized in Table 1. The unshrouded impeller includes 11 blades while the nozzle possesses 10 vanes. Fully structured grid with sufficiently fine grids near the walls, to ensure the values of y$^+$ close to unity, was generated using Ansys Turbogrid [10]. Fig. 1 shows the studied computational domain and mesh. Due to lack of geometry information of the Sandia radial turbine impeller in the literature, the axial length of the rotor is estimated base on the Aungier’s correlation [11].

<table>
<thead>
<tr>
<th>Impeller diameter ratio $d_3/d_{sh}$</th>
<th>5.28</th>
</tr>
</thead>
<tbody>
<tr>
<td>Impeller inlet blade height</td>
<td>4.4 (mm)</td>
</tr>
<tr>
<td>Diameter of impeller at inlet</td>
<td>67.6 (mm)</td>
</tr>
<tr>
<td>Inlet diameter of nozzle</td>
<td>95.4 (mm)</td>
</tr>
<tr>
<td>Diameter at nozzle throat</td>
<td>73.2 (mm)</td>
</tr>
<tr>
<td>Diameter at nozzle outlet</td>
<td>69.8 (mm)</td>
</tr>
</tbody>
</table>

Different grids were examined in order to check the mesh dependency of the simulations. The mesh dependency was examined in steady states by calculating total to static isentropic efficiency obtained with different amounts of grids. The isentropic enthalpy is calculated by assuming the constant entropy at the inlet which is exported from the CFD result and calling the enthalpy as a function of entropy and outlet pressure from REFPROP [12]. The isentropic efficiency for the radial turbine is calculated according to Eq. 1. Fig. 2 shows the mesh dependency study. Different mesh resolutions with around 500k, 1000k, 1400k and 1800k cells were generated with the same mesh topology. By increasing the number of cells more than 1400k, no significant change in the turbine efficiency has been observed. Furthermore, the quality of mesh was tested by the Jacobian and skewness factors. Most of the cells has skewness below 0.77 and only a few cells had skewness around 0.82. Subsequently, the total number of 1400k cells was evaluated to be sufficient and used for all the simulations presented in this study.

$$\eta_s = \frac{h_3 - h_4}{h_1 - h_4s}$$  \hspace{1cm} (1)
The commercial Navier Stokes flow solver ANSYS CFX 17.1 [13] was used for the unsteady states simulations in this study. URANS equations were closed through the two equation $k-\omega$ SST turbulence model of Menter [14]. The transient blade row modeling with the Time Transformation interface [13] was set between the stationary and the rotating parts in the unsteady simulations. In this method, the unequal pitch problem between the zones is overcome by utilizing a time transformation to the equations of the flow. The Time Transformation method is valid when the pitch ratio does not deviate much from unity (valid between 0.6 - 1.5, in this study pitch ratio is 1.1). Moreover, second order discretization methods were applied and Total energy model, including the viscous work term, was set. All walls were assumed as non-slip. Total pressure and temperature were set at the inlet boundary conditions and constant mass flow rate was defined as the outlet boundary condition. Due to lack of geometry data, the volute have not been modeled in this study.

4. Real gas properties

In the supercritical region, especially near the critical point, the behavior of the fluid is very sensitive to temperature and pressure. Small changes in the boundary conditions can have a significant effect on the turbomachine performance. By getting far from the critical point, the sensitivity of the flow properties to the pressure and temperature decreases but still fluid behaves like a real gas during the expansion. In this study, different well-known equation of states (EOS) models are examined at different boundary conditions and results are compared to the experimental data.

Among the cubic equation of states models, improved cubic EOS models Peng-Robinson (PR) [15] and Soave-Redlich-Kwong (SRK) [16] are the most accurate and well-known models for the real gas simulations in industry and academic applications. The performance of SRK EOS and PR EOS are pretty close to each other but near the critical point, PR EOS has slightly better accuracy that makes the PR EOS better suited for the supercritical simulations. Furthermore, Span and Wagner [17] model is formed in terms of Helmholtz energy and covers the carbon dioxide properties from the triple point up to 800 MPa and 1100 K for pressure and temperature, respectively. SW model has been evaluated in the near critical point simulations and good agreement with the experimental data was observed [18, 7]. Details regarding each equation of states can be found in the literature [15, 16, 17]. These models in addition to an ideal gas assumption have been utilized to simulate a radial turbine in the supercritical region.

The fluid properties were taken from the multipurpose NIST REFPROP database [12] which employs SW and PR EOS models and stored in a real gas properties (RGP) table (look-up table with SRK model can be generated directly in the solver [13]). RGP tables include nine main properties of the fluid: specific entropy, specific enthalpy, speed of sound, specific volume, isobaric specific heat, thermal conductivity, dynamic viscosity, specific heat at constant volume, and partial derivative of pressure with respect to the specific volume at constant temperature. For each RGP table, three different resolutions have been generated to study the impact of the look-up table resolution on the turbine performance. For the ideal gas, the averaged properties (specific heat in constant pressure) have been implemented in the EOS according to the inlet and outlet boundary conditions. Mass flow averaging was used in all averaging procedures in this study.
5. Results and discussions

The design point and three-off design operating conditions of the radial turbine have been selected to perform the CFD simulations with different EOS models and RGP resolutions. The experimental boundary conditions and performance data in the T-s diagram are shown in the Fig 3 (points A, B, C and D). The data for case D (design point) was derived from the 1-D model provided at Barber-Nichols [19, 20].

![Fig. 3. Turbine experimental results and boundary conditions [19, 20]](image)

The RGP look-up table resolution for each real gas EOS model has been examined and effects of the look-up table resolution on the simulation accuracy have been investigated. According to the boundary conditions, range of the RGP tables for the design point is from 600 K and 6 MPa to 900 K and 15 MPa, and for the off-design points is from 350 K and 6 MPa to 650 K and 15 MPa for temperature and pressure, respectively. RGP ranges are selected wider than the boundary conditions to avoid extrapolating and clipping methods by the solver at the beginning of the iterations which decrease the accuracy of the simulation. Three RGP resolutions (100×100, 250×250 and 500×500 for temperature and pressure) for each real gas EOS model have been investigated in this study. The step sizes for the temperature and the pressure in the RGP tables are 3 K, 1.2 K, 0.6 K and 90 KPa 36 KPa, 18 KPa for RGP table size 100×100 to 500×500, respectively. Fig. 4 illustrates the accuracy of the different RGP tables with different EOS models. Enthalpy drops have been calculated based on the CFD simulation results with different RGP resolutions for each EOS model and the error is normalized with the experimental enthalpy drop values. Results with an ideal gas assumption cannot be performed with different table resolutions, but in the Fig. 4 it shows in different intervals in order to better compare between cases.

The operating condition of case D is relatively far from the critical point, but a significant deviation can be seen by comparing the 1-D data with the simulation results. There is no experimental measurements data available at the design point and according to the reference report [19], there is noticeable difference between the 1-D code results and the experimental off design measurements (from 51% to 33% error in the pressure drop accuracy from point A to C, respectively). Although the turbine is not supersonic, but the estimated static pressure at the outlet was used as a boundary condition in a CFD simulation to double check the accuracy of the simulation at the design point, but a noticeable difference in the mass flow rate and eventually velocity triangle and turbine performance was appeared. The aim of investigating the design point data in this study is only comparison the different EOS models with different resolutions in the supercritical region which is relatively far from the critical point. Boundary conditions of the case D
are far from the critical point, (reduced pressure and temperature by the critical point at the outlet are 1.07 and 2.46, respectively), and therefore there is no significant change in the simulation accuracy between different EOS models and RGP resolutions. The compressibility factor at the outlet boundary conditions of case D is 1.005 and the fluid behaves like an ideal gas even though the operating condition is in the supercritical region. At the maximum 2% error between ideal gas assumption and SW EOS model has been observed at the design point. Compressibility factors of all cases A to D, at the inlet and outlet are mentioned in the Fig. 3. Due to vicinity of the compressibility factor to the unity, in all cases there is not noticeable effect of the RGP resolution on the total enthalpy drop error.

The enthalpy drop error difference between the real gas EOS models at the off-design operating conditions (A to C) is not very significant (average 3% difference), but employing an ideal gas assumption can have a noticeable effect on the simulations accuracy. In most of the cases, maximum error of 1% is seen between RGP 100 and RGP 250, but there is not significant changes observed by increasing the look-table resolution from 250 to 500 points. Largest error between the real gas and the ideal gas assumption is occurred at case B, approximately 22%, due to the closer boundary conditions of case B to the critical point.

In order to compare the simulations cost and time, CPU time second per time step (0.33 degree of the rotor rotation) and per rotor rotation (360 degree) have been investigated and presented in Table 2. All simulations performed on 12 CPU cores with parallel simulation model and approximately 2 rotations of the rotor (720 degree) were seem to be enough to get the converge result in all simulations.

Table 2. Simulation time and cost

<table>
<thead>
<tr>
<th>Model</th>
<th>CPU time second per time step</th>
<th>CPU time second per rotor rotation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ideal gas</td>
<td>127</td>
<td>138545</td>
</tr>
<tr>
<td>RGP 100</td>
<td>827</td>
<td>902182</td>
</tr>
<tr>
<td>RGP 250</td>
<td>1082</td>
<td>1180364</td>
</tr>
<tr>
<td>RGP 500</td>
<td>1800</td>
<td>1963636</td>
</tr>
</tbody>
</table>

Numerical accuracy also affects the flow field inside the radial turbine. By comparing the Mach number in stationary frame between the ideal gas assumption and the real gas EOS models, difference in the Mach number contour especially near the rotor blade leading edge can be observed. Fig. 5 shows the Mach number in stationary
frame at 0.5 span for case B between the SW EOS model and the ideal gas model (due to the biggest difference in the accuracy at these cases). Differences in the Mach numbers emerge from the accuracy in calculation of speed of sound, as well as density which varies the velocity inside the passage. Difference in the velocities inside the studied turbine comes from calculation accuracy of the density, because the mass flow rate and the geometry are constant in all cases. Although, the same operating and boundary conditions were set for the all cases, but the calculation accuracy of the properties of the fluid especially the density can have an impact on velocity magnitude in different EOS models. Among all real gas models studied in this paper, there is no significant difference in the density calculation (below 0.2%), but the deviation between the ideal gas assumption density and the real gas model ones is around 12.3%. By using an ideal gas assumption, density is calculated smaller than the real gas models. By keeping the mass flow rate constant, higher velocity and subsequently higher Mach number are computed using the ideal gas model. Increasing the RGP look-up table resolution did not have a noticeable impact on the flow field in the different studied cases.

Furthermore, the accuracy tests for the total temperature drop for all cases have been done. At the operating condition B which has the biggest deviations in the calculation accuracy, SW model averaged error is 3.9%, PR and SRK almost have the same error around 5.4% and the ideal gas shows a significant deviation from the experimental data, 40.4%. Similar to the enthalpy drop and the flow field studies, there is no significant changes in the temperature drop accuracy test with the different RGP resolutions observed. Although, this conclusion is valid for the studied cases and operating conditions in this study which are relatively far from the critical point. Previous studies stated that in vicinity of the critical point, extremely small changes in the RGP resolution can have a significant effect on the compressor performance and flow fields [7, 8]. According to the numerical accuracy, time and cost of the simulations, SW EOS model with moderate resolution, (250), has been recommended for the supercritical applications in the mentioned operating conditions range.

![Mach number in stationary frame with the SW EOS (left) and the ideal gas (right) at the operating condition B.](image)

Fig. 5. Mach number in stationary frame with the SW EOS (left) and the ideal gas (right) at the operating condition B.

6. Conclusion

The effects of the accuracy of real gas and ideal gas models on the radial in-flow turbine in the supercritical region were investigated in this study. The design and three off-design operating conditions were studied with different EOS models and results were compared with the experimental measurements at the Sandia test loop facility. Data of the design point was achieved from the 1-D code and there is no experimental measurements at the design point, consequently there is a significant different between the CFD result and 1-D code. The design point boundary conditions were far enough from the critical point to minimize the impact of the different real and ideal gas models on the performance and flow fields. By getting closer to the critical point and off-design operating conditions, significant differences in the turbine total enthalpy drop and flow field were observed using the real and ideal gas EOS models. Among the different EOS models investigated in this study, Span and Wagner showed better accuracy compared to the Peng-Robinson, Soave-Redlich-Kwong and the ideal gas assumption. By studying the different resolutions of the look-up table for each EOS model (except the ideal gas assumption), a sufficient resolution and range were suggested. Moreover, by investigating the total temperature drop and the densities in different cases,
deviation in the velocity calculation and the Mach number contours in different EOS, due to density calculation accuracy, was observed. With an ideal gas EOS model, lower density at the same temperature and pressure was calculated which lead to higher velocity, while the mass flow rate kept constant. This study indicated that even though the boundary conditions of the turbine are relatively far from the critical point, but still a suitable real gas model with sufficient look-up table resolution is recommended to simulate and design a turbine with high accuracy. Although the differences between the studied real gas models were not significant, but in all cases SW model showed better agreement with the experimental measurements.

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References

Publication VI

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Pittsburgh, Pennsylvania, March 27-29, 2018
ABSTRACT

The supercritical CO$_2$ Brayton cycle has been recently attracting more attention compared to other common energy conversion cycles, chiefly due to its higher thermal efficiency with the relatively low temperature at the turbine inlet compared to its conventional counterparts. Centrifugal compressor operating conditions in the supercritical Brayton cycle are preferably located near the critical point to get advantage of low compressibility factor and eventually low compressor work. In this paper, the design of the compressor using the enthalpy loss models in the supercritical CO$_2$ region is investigated and the accuracy of the loss models near the critical using real gas is validated. Due to high density of the working fluid near the critical point, compressor size is relatively small. It is noticed that, the friction loss plays a significant role among all loss sources. Therefore, more attention is paid on the skin friction loss and friction coefficient estimations. Results are compared to the experimental measurements conducted at Sandia National Laboratories.

INTRODUCTION

Recently, there has been significant growing interest in the supercritical CO$_2$ (sCO$_2$) Brayton cycle as an alternative power conversion cycle, due to the relatively low maximum cycle temperature, high thermal efficiency and compactness. Chiefly due to high density and low specific volume of the fluid in the vicinity of the critical point, turbomachines and heat exchangers are compact compared to other Brayton cycles with different operating conditions [1]. According to a study by Angelino [2], the compressor operating condition near the critical point would improve the compressor performance and consequently cycle efficiency. Despite the enormous benefits of designing compressor in the proximity of the critical point, abrupt behavior of the thermophysical properties makes the design and simulation complicated. Figure 1 depicts the isobaric specific heat capacity variations near the critical point. Quite a few researchers have addressed the turbomachinery simulation and design challenges in the vicinity of the critical point [3]–[10]. One of the most used turbomachinery sizing methods is using the specific speed and specific diameter, $n_s - d_s$, diagram proposed by Balje [11]. However,
the predicted performance using the $n_s - d_s$ diagram in the supercritical region is imprecise due to real gas approximation and inconsistent behavior of thermodynamics properties [12]; consequently, a meticulous approach is needed to predict compressor performance through the one-dimensional analysis and computational fluid dynamic (CFD).

Many researchers have developed loss models for turbomachinery design such as Conrad et al. [13], Coppage et al. [14], Jansen [15], Aungier [16] and Rodgers [17]. Implementing the individual enthalpy loss models into the one dimensional design code was evaluated by Lee et al. [12] in the supercritical region; It was concluded that the future development of loss models are crucial to achieve more trustable designs.

In this paper, the authors have attempted to design and simulate the centrifugal compressor based on the individual enthalpy loss models. Due to the small size of the compressor, because of high density near the critical point, skin friction loss is found to play a noticeable role among the internal enthalpy loss models. To shed more light on this matter, the different skin friction loss models are compared and a general correlation for the skin friction loss and the skin friction factor are derived. Validation and verification have been carried out against the experimental measurements from the Sandia laboratory and time-dependent CFD simulations.

2. METHODOLOGY

The most practical and acceptable accuracy set of enthalpy loss models collected by Oh et al. [18] has been implemented in the in-house mean line code (AlFa CCD [19]) to design and evaluate centrifugal compressor performance. The studied set of loss models were evaluated in the supercritical applications previously [12] [18] [20].
Although, in all studied cases based on the loss models, skin friction factor has been assumed constant, or it has been calculated based on the pipe flow correlations. In the AlFa CCD code, the authors attempt to focus on the friction loss and derive a general correlation with acceptable accuracy for the near critical point applications.

Fluid properties have been derived from the NIST Reference Fluid Thermodynamic and Transport Properties Database 9.1 (REFPROP) [21] based on the Span and Wagner equation of state (SW EOS) model [22]. SW EOS covers the CO\(_2\) thermophysical properties from the triple point up to 1100 K and 800 MPa for temperature and pressure, respectively. This model has been employed and validated by considerable number of researchers in the near critical point applications and is been known as the most accurate EOS especially for CO\(_2\) in the supercritical region [8], [23]–[31].

### 2.1. MEAN LINE DESIGN

The inlet stagnation conditions, the mass flow rate, the rotor rotational speed and the inlet flow angle are the input variables. The velocity triangle definitions used in the study are illustrated in the figure 2.

![Figure 2. Velocity triangle definitions at the leading (left) and trailing (right) edges.](image)

The centrifugal compressor design is based on the two well-founded equations, Euler and continuity, as follows:

\[
\begin{align*}
(1) & \quad h_t - h_z = U_2C_w - U_1C_w \\
(2) & \quad \dot{m} = \rho A C_{a1}.
\end{align*}
\]

Where subscripts 1 and 2 stand for the inlet and outlet of the impeller, respectively. In the design code, velocity triangles are calculated at three different radii: hub, mean line and the shroud. Mean line radius is estimated as follows

\[
(3) \quad r_m = \sqrt{0.5(r_s^2 + r_h^2)}
\]
After calculating the velocity triangles at the mentioned locations by using the fluid properties derived from REFPROP, enthalpy loss models are estimated to update the compressor performance parameters.

The set of studied loss models can be classified into internal and external (parasitic) losses. Internal losses consist of incidence, blade loading, skin friction, tip clearance and mixing losses. After updating the compressor performance by considering the internal loss models, external loss models are calculated to take account the extra work of the rotor rotation. External losses are the leakage, the recirculation and the disc friction losses. Enthalpy loss models collected by Oh et al. [18] are summarized in table 1.

<table>
<thead>
<tr>
<th>Loss model</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Incidence loss</td>
<td>Conrad et al. [13]</td>
</tr>
<tr>
<td>Blade loading loss</td>
<td>Coppage et al. [14]</td>
</tr>
<tr>
<td>Skin friction loss</td>
<td>Jansen [15]</td>
</tr>
<tr>
<td>Tip clearance loss</td>
<td>Jansen [15]</td>
</tr>
<tr>
<td>Mixing loss</td>
<td>Johnston and Dean [32]</td>
</tr>
<tr>
<td>Leakage loss</td>
<td>Aungier [16]</td>
</tr>
<tr>
<td>Recirculation loss</td>
<td>Oh et al. [18]</td>
</tr>
<tr>
<td>Disc friction loss</td>
<td>Daily and Nece [33]</td>
</tr>
</tbody>
</table>

Details about the individual loss models can be found in the literature. In this study, only the details of skin friction loss and skin friction coefficient are investigating extensively. The skin friction loss occurs due to the viscous shear forces in the boundary layers at walls inside the impeller. The model proposed by Jansen [15] is defined as

\[ \Delta h_{SF} = 2c_f \frac{L_b}{d_{hb}} \bar{W}^2, \]

\[ \bar{W} = \frac{(2W_2 + W_{12} + W_{1b})}{4} \]

where \( \bar{W} \) stands for the mean relative velocity through the passage, \( d_{hb} \) is the average hydraulic diameter of the blade passage and \( c_f \) is the skin friction coefficient. The flow path length, \( L_b \) is estimated as

\[ L_b = \frac{\pi}{8} \left[ d_2 - \frac{d_1 + d_{1b}}{2} - b_2 + 2L_x \left( \frac{\cos \beta_{11} + \cos \beta_{1b} + 2 \cos \beta_2}{4} \right) \right] \]

and the axial length of the rotor, \( L_x \) is estimated by the modeled proposed by Aungier [16] as
\( L_z = d_2 \left( 0.014 + \frac{0.023d_1}{d_{1h}} + 1.58\emptyset \right) \)

Where \( \emptyset \) stands for flow coefficient. In order to calculate the skin friction factor, \( C_f \), Jansen [15] proposed a correlation which is based on the pipe flow friction calculation as follows

\[
(7) \quad C_f = 0.0412(Re)^{-0.1925}
\]

\[
(8) \quad Re = \frac{\bar{\rho} \bar{W} \bar{d}}{\mu}
\]

and the averaged hydraulic diameter of the rotor blade passage \( d_{hb} \) as follows

\[
(9) \quad d_{hb} = d_2 \left( \frac{\cos \beta_2}{\pi} \frac{d_{1h}}{d_2} \right) + \frac{0.5(d_{s1} - d_{h1}) \cos \beta_1}{2 \pi} \left( \frac{d_{s1} + d_{h1}}{2} \right) \cos \beta_2 \frac{d_{s1} + d_{h1}}{2} \left( \frac{d_{s1} + d_{h1}}{2} \right).
\]

Calculating the skin friction factor based on the pipe flow approximations may underestimate the actual value of friction loss due to curved shape of the blade passage. As suggested by Jansen [15], an average value of 0.006 results in a good agreement with the experimental data for the air compressors. However, due to the abrupt behavior of the viscosity and density in the vicinity of the critical point, employing this averaged value should be examined scrupulously.

Another well-established model for the skin friction factor in the turbulence flows was introduced by Schlichting [34] as follows

\[
(10) \quad \frac{1}{\sqrt{C_{f_s}}} = -2 \log\left( \frac{e}{3.71d} \right)
\]

\[
(11) \quad \frac{1}{\sqrt{C_{f_r}}} = -2 \log\left( \frac{2.51}{Re_{rb}/C_{f_r}} \right)
\]

Where \( e \) stands for the peak to valley surface roughness. \( C_{f_s} \) and \( C_{f_r} \) stand for the skin friction factors for fully smooth and rough surfaces, respectively. Centrifugal compressors operate in a wide range of the operating conditions, therefore a general statement for the skin friction loss and the skin friction factor is recommended to cover the laminar and turbulent flows as well as the influence of the surface finish. A weighted averaged model introduced by Aungier [16] can be used when the surface roughness becomes significant

\[
(12) \quad Re_e = (Re - 2000)e/d > 60
\]

Hence, the turbulent skin friction coefficient is defined as
\( \begin{align*} 
    c_f &= c_{f_s} + (c_{f_r} - c_{f_s})(1 - 60/\text{Re}_e) 
  \end{align*} \)

For a simple annular passage, hydraulic diameter can be assumed as the passage width, but for applying the generalized skin friction model to the compressor passage, the hydraulic diameter of the blade passage proposed by Jansen (equation 9) has been implemented into the weighted averaged model. In order to validate and examine the skin friction coefficient models, experimental data and unsteady CFD simulation over a wide range of operating conditions are needed.

2.2. NUMERICAL METHODS

To the best knowledge of the authors of this article, the only open access experimental data of a sCO\(_2\) centrifugal compressor can be derived from the Sandia National laboratories reports [35], [36]. The studied case is the main centrifugal compressor in the Sandia split-flow re-compression sCO\(_2\) Brayton cycle. The unshrouded impeller includes six main and six splitter blades, and the diffuser employs 17 wedge-shaped vanes. Main compressor dimensions are summarized in the table 2.

<table>
<thead>
<tr>
<th>Main compressor design dimensions [36]</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Impeller diameter ratio (d_2/d_1h)</td>
<td>1.993</td>
</tr>
<tr>
<td>Impeller tip diameter</td>
<td>37.36 (mm)</td>
</tr>
<tr>
<td>Exit blade height</td>
<td>1.712 (mm)</td>
</tr>
<tr>
<td>Blade tip angle (minus is backswept)</td>
<td>-50 (deg)</td>
</tr>
<tr>
<td>Blade thickness</td>
<td>0.762 (mm)</td>
</tr>
<tr>
<td>Inlet blade angle at tip</td>
<td>50 (deg)</td>
</tr>
<tr>
<td>Normal tip clearance (constant)</td>
<td>0.254 (mm)</td>
</tr>
<tr>
<td>Exit vaned diffuser angle</td>
<td>71.5 (deg)</td>
</tr>
</tbody>
</table>

The mesh dependency test was previously done and by authors [23] and the total amount of around 1.5 million cells found to be sufficient since the compressor performance remained constant by increasing the number of cells. The sufficient fine cells near the walls were generated to ensure the values of \(y^+\) close to unity. Figure 3 shows the Sandia centrifugal compressor geometry and structured mesh. The volute has not been modeled due to lack of geometrical data.

URANS equations were closed through the two equation \(k-\omega\) SST turbulence model of Menter [37]. Convergence criteria of the CFD simulations were based on reduction of Root Mean Square (RMS) momentum, mass and energy residuals below \(10^{-3}\%\), reduction and stability of the imbalances of (difference between inlet and outlet in each zone) mass flow rate, energy and momentum below \(10^{-3}\%\), and the stability in the stage isentropic efficiency. Transient sliding mesh Blade Row interface employing the Fourier
Transformation was defined between the impeller and the vaned diffuser to capture the losses occurring in the transient situation as the flow is mixed between the rotating and stationary zones.

Figure 3. Geometry and mesh of the Sandia centrifugal compressor.

An external real gas properties (RGP) look-up table has been coupled with the flow solver. RGP table resolution is gradually increased by getting closer to the critical density curve and sufficiency wide range has been used to prevent clipping or extrapolating methods by the flow solver during the simulations. RGP dependency tests have been done by the present authors near the critical point and the optimum resolution of the table was also examined [23], [38]. Boundary conditions at the inlet are defined as total pressure and total temperature, reduced values (normalized with the critical value) are 1.042 and 1.006 for pressure and temperature, respectively. The static back pressure was set as the outlet boundary condition (reduced values are from 1.16 to 1.33 with interval size of 0.2 MPa).

Skin friction coefficient can be calculated from the URANS simulations and is formulated as

\[ c_f = \frac{\tau_w}{\frac{1}{2} \rho \infty U_{\infty}^2} \]

where \( \tau_w \) is the wall shear stress and \( U_{\infty} \) is the free-stream velocity. In the complicated geometries like inside the compressor flow passage, defining the free-stream velocity is not straightforward. A method introduced by Tiainen et al. [39] estimates the boundary layer thickness as a distance between the impeller blade and the location where the stream velocity is 99.5% of the adjacent point velocity as follows

\[ \frac{dU}{dn} = 0.005 \]

\[ U_{n-1} = 0.995U_n \]

\[ U_{in} = U_n \]
where the subscript \( n \) denotes normal to the wall. The same method is used in the present study to estimate the boundary layer thickness from hub to shroud direction as well to increase the accuracy of the numerical calculation. After locating the boundary layer thickness from each wall inside the impeller, values are averaged at different meridional distances and consequently the skin friction coefficient is calculated.

**RESULTS AND DISSCUSION**

Based on the different calculation methods, various values of skin friction loss are found. Figure 4 shows the skin friction coefficient distribution along the meridional distance of the studied impeller at the peak efficiency among the studied off-design points. Skin friction coefficient based on the CFD simulation fluctuates along the impeller passage from inlet to outlet. Normalized distances of 0.2 and 0.6 are the locations of the leading edges of the main and splitter blades, respectively. Higher values of skin friction coefficient can be noticed at the leading edges compared to adjustment points.

![Figure 4. Comparison of skin friction coefficient.](image)

To validate the performances of the meanline code and the CFD simulation, figure 5 shows their comparison against measurements for the compressor isentropic efficiency along the off-design points at 50 KRPM rotor speed (using the weighed averaged model of skin friction loss). Although, the CFD simulation overestimates the efficiency which results from neglecting the external loss effects, real gas numerical errors and geometrical deviations acceptable trend of CFD simulation and meanline code can be observed.
The importance of skin friction loss can be highlighted by calculating the individual enthalpy loss models from Table 1 at the design point. Figure 6 shows that the skin friction loss plays the most important role among all loss sources with share of more than 50% of the total internal losses.
As it can be seen, the friction loss is not constant along the impeller, and constant values may reduce the design accuracy. The model proposed by Jansen for pipe flows (equation 7) shows biggest difference against the CFD averaged value. While the weighted averaged model by Aungier (equation 13) combined with the hydraulic diameter assumption proposed by Jansen (equation 9) predicts the smallest difference. By implementing the hydraulic diameter value of Jansen in to the model proposed by Aungier, the difference is reduced but still around 81.8 % difference appears. The difference between CFD averaged value and the weighted averaged method is around 1.01 %.

CONCLUSION AND FUTURE WORK

Centrifugal compressor design based on the individual enthalpy loss models in the near critical point applications was investigated in this study. Due to small size of the compressor near the critical point (because of high density and low specific volume of fluid), skin friction loss was found to be the most significant and effective loss inside the rotor. Different models for skin friction coefficient were investigated and the result was compared against the URANS CFD simulation. A weighted averaged method proposed by Aungier by implementing the hydraulic diameter of the impeller passage by Jansen showed the best agreement with the CFD result. Also, by comparing the compressor map at constant rotor speed with the experimental measurement conducted at Sandia national lab, acceptable agreement between the meanline code, CFD simulation and measurement was achieved.

Throughout this process, it was clear that further investigation and improvement of the enthalpy loss models are needed. Also, more validation against experimental measurement should be done in order to confirm the presented method as a general statement. Moreover, compressor operates near the critical point and there is possibility of condensation around the suction side of the blades. Further studies are needed to apply the effect of condensation and its loss on the compressor performance and design.

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