CFD analysis of an expansion process using different real gas models

Lazhar Abdelli

Supervisors: Prof. dr. ir. Joris Degroote, Prof. dr. ir. Jan Vierendeels
Counsellor: Iva Papes

Master's dissertation submitted in order to obtain the academic degree of
Master of Science in Electromechanical Engineering

Department of Flow, Heat and Combustion Mechanics
Chairman: Prof. dr. ir. Jan Vierendeels
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Preface

Once upon a time, a professor from Ghent University came to the last year of high school and explained his vision on how to become an engineer. This person said to me: "First, you have to become an industrial engineer, which will give you lots of practical experience. Then, you have to study for civil engineer, which will strengthen the foundations of what you already saw in industrial engineering. When combining both, you will become more knowledgeable than either of them."

Two years ago when I achieved the degree of industrial engineer, I followed his advice so I started my adventure in civil engineering. With the goal in mind of having a better theoretical foundation, I started my studies with no idea on what to really expect. The fact remains that although the content of my courses changed, I was still using the same approach of being curious. In all these years, my desire for knowing technology, how to contribute to a better future and how to interpret the world around me are still the principal driving forces to become a better engineer by learning new things and by improving what I already know.

In the meantime, I started appreciating the fact that both my industrial and civil engineer personae started blending together into who I am today. Studying for civil engineer is not only the integral sum of all the achieved knowledge and experience, but it is also the perfect way to ameliorate my personality. By pushing the envelope and going well beyond my comfort zone, I managed to discover new strengths and weaknesses which I would never have discovered without continuing my studies.

The choice for this particular thesis was an easy one. I knew the general outlines of the ORCNext project via prof. dr. Martijn van den Broek and the supervisors of my bachelors’ dissertation, ing. Bruno Vanslambrouck and ir. Sergei Gusev. Since attending the defense of the Master’s dissertation of ing. Marcio Verhulst, my interest grew to contribute to the ORCNext project. The combination of fluid dynamics, thermodynamics and CFD provided a really interesting challenge, which is why I chose for this particular thesis subject. The beautiful part of all this work is the way how every little fact builds upon
the other. Within due time, the different aspects of this thesis started clicking together and forming a finely tuned machine of knowledge. Each chapter of this dissertation cannot stand on its own, although together they form relations and bonds which explain the problem and the solution as a whole. The results published in this thesis will hopefully lead to further improvements in ORC technology, which will certainly play an important role in supporting the future energy requirements of our civilization.

Before starting with the technical part of this Master’s dissertation, I would like to thank all the involved persons for their unique contribution to this thesis. First of all, I would like to praise my counselor ir. Iva Papeš, along with my supervisors prof. dr. ir. Joris Degroote and prof. dr. ir. Jan Vierendeels for sharing their extensive knowledge and professional advice on how to properly formulate a concise solution for the given flow problem. Furthermore, this thesis would not even exist without the knowledge and support provided by all my teachers, my friends and my family. More specifically, I would like to thank Marcio Verhulst and Björn Deprest for their immense mental support and for giving me the daily courage necessary to complete this thesis. Furthermore, I would like to thank Emanuel De Peuter and Wouter Staessens, who joined and accompanied me on this quest to become a ‘Master of Science in Electromechanical Engineering’. And last but not least, I would like to thank you, the reader, for taking the time to read my dissertation.

Ghent, 22 May 2015

Lazhar Abdelli
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De auteur geeft de toelating deze masterproef voor consultatie beschikbaar te stellen en delen van de masterproef te kopiëren voor persoonlijk gebruik. Elk ander gebruik valt onder de bepalingen van het auteursrecht, in het bijzonder met betrekking tot de verplichting de bron uitdrukkelijk te vermelden bij het aanhalen van resultaten uit deze masterproef.

Ghent, 22 May 2015

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Abstract

With the increasing importance of minimizing primary energy usage and complying with emission restrictions, a significant interest has been developed towards waste heat recovery from industrial processes using organic Rankine cycles (ORCs). Twin screw expanders are used as an alternative to turbines with their cheap production costs and well proven efficiencies. 3D computational fluid dynamics (CFD) simulations will be performed on the original twin screw expander geometry and a simplified expansion model using R245fa as the working fluid. Since the ideal gas equation of state (EoS) provides inaccurate results for these calculations, the main goal of this research is to study the influence of different fluid property models on the presented geometries and simulation cases. For these calculations the ideal gas EoS, the Aungier Redlich-Kwong (ARK) EoS and the CoolProp database have been selected.

From the results of this study, it can be concluded that the ideal gas EoS shows big deviations near to the saturation vapor line, with a deviation in power output compared to the ARK EoS of around 8%. For this simulation case, the ARK EoS is the best choice since it presents more accurate results than ideal gas EoS and the calculation time is halved when compared to using the CoolProp database.

Keywords: Aungier Redlich-Kwong Equation Of State, CFD, CoolProp, Organic Rankine Cycle (ORC), R245fa, Real Gas Model, Twin Screw Expander
CFD analysis of an expansion process using different real gas models

Lazhar Abdelli

Supervisors: Joris Degroote, Jan Vierendeels, Iva Papes

This paper is submitted to the ASME IMECE2015 conference

Abstract—With the increasing importance of minimizing primary energy usage and complying with emission restrictions, a significant interest has been developed towards waste heat recovery from industrial processes. A large portion of this energy is available at low temperatures (350K-400K) but it can be relatively efficiently converted into mechanical power using an Organic Rankine Cycle (ORC). Twin screw expanders can be used as an alternative to turbines with their cheap production costs and well proven efficiencies. In this paper, 3D CFD simulations of a twin screw expander using R245fa as the working fluid are performed.

Since the fluid properties show big deviations when using the ideal gas equation of state (EoS), the flow problem has been evaluated using different real gas models. Thermodynamic parameters for the ideal gas EoS, the cubic Aungier Redlich-Kwong EoS and the CoolProp fluid database (open source) were compared in a preliminary study. After that, the models have been included through user-defined functions (UDFs) in ANSYS Fluent and were tested on 3D CFD calculations of a twin screw expander and a simplified expansion model.

Several performance indicators such as mass flow rates, pressure-volume diagrams and power output are used to compare different fluid models for R245fa. From the results of this study, it can be concluded that the ideal gas EoS shows big deviations going closer to the saturation vapor line and the deviation in power comparing to the Aungier Redlich-Kwong EoS is around 8%. Conversely, the Aungier Redlich-Kwong EoS and the CoolProp database present very similar results for this case.

Keywords—Aungier Redlich-Kwong Equation Of State, CFD, CoolProp, Organic Rankine Cycle (ORC), R245fa, Real Gas Model, Twin Screw Expander

I. INTRODUCTION

In times of diminishing fossil fuel reserves and an ever increasing importance of environmental awareness, the recuperation of low grade waste heat via Organic Rankine Cycle (ORC) technology provides significant benefits for the industry. Where conventional methods are economically infeasible, an ORC can operate efficiently with low temperature heat sources by using an organic working fluid. In modern implementations of these systems, significant efforts are made to maximize the power output and system efficiency while keeping investment costs to a minimum. This will result in ORC becoming a more economically viable technology due to a more extended range of low temperature applications.

One of the major steps towards higher efficiency is the optimization of the energy conversion process. The main characteristics of the organic working fluid are low saturation temperatures and a positive slope in the saturation vapor line of the T-s diagram. Due to these properties, volumetric expanders can be applied successfully to small scale ORC technology. Lemort et al. [1] showed that screw expanders are exceptionally suitable for ORC implementation. The current generation of screw expanders is in fact designed as compressors used the other way around [2], [3], [4]. The type of expander investigated in this paper is a twin screw expander, where two helical rotor screws counter rotate inside two overlapping cylindrical cavities. The working chambers are formed by the meshing rotor surfaces and by the cylinder wall sealing. Selecting the optimal working conditions and screw expander geometry is essential to optimize the ORC system performance.

Under typical ORC working conditions, the ideal gas law shows significant deviations from the real fluid properties. To increase simulation accuracy, more complex real gas models are required. One of the more commonly applied real gas models is the Redlich-Kwong Equation of State (EoS). This is an empirical third-order model which improves upon the ideal gas law, especially for high temperatures and pressures. Several expansions of the basic Redlich-Kwong EoS have been proposed to increase the accuracy for specific applications. The most accurate way of modeling fluid properties is by using databases such as NIST REFPROP [5] and CoolProp [6].

The main goal of this paper is to study the influence of different models for fluid properties on a twin screw expander using R245fa as the working fluid. 3D CFD simulations will be performed on the original twin screw expander geometry and a simplified expansion model. Both geometries will be analyzed using ideal Gas EoS, Aungier Redlich-Kwong (ARK) EoS and CoolProp fluid database (reference simulation). These differences will be evaluated using comparisons in mass flow rates, pressure-volume diagrams and power output. The models will be analyzed for differences during each phase of the expansion process.

II. EXPANSION PROCESS

A twin screw expander is a positive displacement machine. The expander consists of two counter-rotating screw rotors with opposing threads which are contained inside a double cylindrical casing. Multiple working chambers are formed by the screw lobes.

The ideal expansion process consists of three main phases (Fig. 1). An isobaric filling occurs up to the initial volume \( V_1 \). The working chamber will then undergo an isentropic expansion until the outlet port connects to the working chamber, which occurs when the maximum volume \( V_2 \) is reached. Finally, the working fluid is expelled from the screw expander during the isobaric discharge.

This study is based on an expander with a 4/6 (male/female) lobe arrangement. The diameter of the screw rotors is approximately 70 mm, with an L/D ratio of 1.9 and a wrap angle of 302° for the male rotor. The nominal operating speed of this
expander is 6000 rpm.

The expansion chamber volume is solely a function of the rotation angle (Fig. 2). The creation of a working chamber starts at the reference position $\theta = 0^\circ$. As the screws rotate, this working chamber gets connected to the inlet port at $\theta = 7^\circ$. A further increase of the rotor angle results in a simultaneous increase of the surface inlet area and the working chamber volume. An underpressure is created and the filling process takes place. As the inlet area reaches its maximum and starts to diminish, the working chamber volume keeps increasing. This causes the working fluid to undergo a pre-expansion. The working chamber is isolated when the inlet surface area reaches zero around $\theta = 126^\circ$. A further rotation of the screws will cause a volume increase and the accompanied expansion of the working fluid. As the volume inside the working chamber reaches its maximum $V_2$ ($\theta = 387^\circ$), the outlet port connects to the working chamber and the discharge process begins. Any further increase of the rotor angle will reduce the volume while maintaining the discharge process until the volume disappears.

The selected screw geometry combined with the inlet and outlet ports results in a (fixed) volume ratio $v$, which is defined as the relation between the discharge volume $V_2$ and the inlet closure volume $V_1$. This volume ratio has to be optimized according to the ORC operating conditions. If the volume ratio is too low, the fluid inside the working chamber has a higher pressure than the discharge pressure (under-expansion). If the volume ratio is too high, fluid from the outlet will flow into the working chamber and cause over-expansion.

### III. SIMPLIFIED GEOMETRY

The main goal of this paper is to characterize the performance of ideal gas EoS, ARK EoS and NIST and CoolProp databases with CFD simulations using the stated twin screw expander geometry. To analyze the behavior of the different real gas models inside a CFD simulation, it is also worthwhile to perform a pre-study using a simplified geometry, namely a piston expander. This will allow to gauge the model performance without including effects originating from the screw expander geometry.

Fig. 3 shows that part of the expansion process in the twin screw expander can be simplified to a quasi-linear process. Due to this, the moving wall velocity of the piston expander model is defined as being constant. This simplified CFD simulation is based on a square piston expander model. As shown in Fig. 4, a cuboid fluid domain (blue) with one moving face (green) will represent the volume increase during expansion. This working chamber is subdivided into a cell stack which is aligned with the piston motion. The cell thickness of the initial volume is chosen according to the moving wall velocity and the time-step size. The mesh growth is controlled by dynamic mesh layering and is constrained to one new cell per simulation time-step. The moving wall velocity is made equal to the axial velocity of the working fluid in the twin screw expander.

---

**Fig. 1.** Working principle of a twin screw expander

**Fig. 2.** Volume curve with inlet and outlet surface area as a function of the male rotation angle

**Fig. 3.** Comparison of the original and simplified volume curves
IV. GRID GENERATION FOR TWIN SCREW EXPANDER

The flow within a screw expander is complex due to the rotor geometry. A time-dependent solution is necessary to analyze the expansion process. Due to this, transient calculations require a specialized grid generator to manipulate the meshing of the flow domain. In 1999, Kovacevic et al. [7] presented the first grid generation algorithm in screw machines. In that paper, a block-structured grid was generated using analytical rack generation. An implementation of this algorithm was recently applied in a twin screw expander simulation using air as working fluid. A different approach has been proposed by Vande Voorde et al. [8], where a block-structured grid is generated from the solution of a Laplace problem. An unstructured grid of the same fluid domain serves as the input of the grid generator algorithm. In this paper, the grid generation is based on the same approach as [8].

As seen in Fig. 5, the expander can be divided into four main domains. The static parts (inlet, outlet and additional ports) and moving rotors’ domain. The stationary parts are meshed using an unstructured tetrahedral grid.

The grid in the casing is built by stacking two-dimensional structured (rectangular) grids in slices of the casing (Fig. 5, left). Before the CFD simulation, 2D structured meshes are constructed in slices corresponding with different rotation of the profiles, with steps of 1.5 degrees of the male rotor. These 2D meshes are generated using the Laplace potential equation \( \nabla^2 \phi = 0 \) as described in [9]. During the entire simulation the cells definitions are the same (the same faces and nodes). So, the nodes of the grid are moved in the housing (ALE, Arbitrary Langrangian-Eulerian method). For each time step in the calculation, a new position of the grid nodes can be found by interpolating between two supplied grids. The size of the gaps between the rotors and between the rotors and the casing are extremely small (order tens of microns versus a rotor diameter of about 70 mm).

All blocks are joined together by using sliding interfaces between the inlet, outlet, the injection ports and the casing. The complete 3D mesh of the twin screw expander consists of 2060515 cells.

V. REAL GAS MODELS FOR R245FA

R245fa is a hydrofluorocarbon which is typically applied as the working fluid in ORC systems. The T-s diagram features a positive slope of the saturation vapor line. This prevents the existence of a two-phase state at the outlet port of the screw expander.

TABLE I

<table>
<thead>
<tr>
<th>Property</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Critical temperature</td>
<td>( T_c )</td>
<td>427.2K</td>
</tr>
<tr>
<td>Critical pressure</td>
<td>( P_c )</td>
<td>3.64 MPa</td>
</tr>
<tr>
<td>Critical density</td>
<td>( \rho_c )</td>
<td>517 m³/kg</td>
</tr>
<tr>
<td>Acentric factor</td>
<td>( \omega )</td>
<td>0.3724</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>( M )</td>
<td>134.0482 g/mol</td>
</tr>
</tbody>
</table>
In 1949, O. Redlich and J.N.S. Kwong [10] proposed an empirical derivative of the Van der Waals equation. The main goal was to provide an overall more accurate model, notably in the region above the critical temperature and near to the saturation vapor line.

\[ p = \frac{RT}{v-b} - \frac{a}{\sqrt{T}v(v+b)} \]  
(1)

where:

\[ a = \frac{0.4275R^2T^5/2}{p_c} \]  
(2)

\[ b = \frac{0.08664RT_c}{p_c} \]  
(3)

In 1995, Aungier presented a modified form of the Redlich-Kwong EoS [11] which has been optimized for numerical applications. In these equations, the compressibility factor and the acentric factor have been added as additional parameters. The main reason of this expansion is to make the results more accurate while keeping the EoS simple to implement and calculate.

\[ p = \frac{RT}{v-b} - \frac{a(T)}{v^2 + b_0v} \]  
(4)

where:

\[ a(T) = a_0 \left( \frac{T_c}{T} \right)^n, \quad a_0 = \frac{0.42747R^2T_c^2}{p_c} \]  
(5)

\[ b_0 = \frac{0.08664RT_c}{p_c} \]  
(6)

\[ c_0 = \frac{RT_c}{p_c} + \frac{a_0}{v_c^2 + b_0v_c} + b_0 - v_c \]  
(7)

Before extending the CFD simulations to include real gas behavior, it is interesting to evaluate the differences between different models. To do this, the CoolProp fluid property database has been used as the principal reference to compare the performance of the ideal gas EoS and the ARK EoS. CoolProp is an open source solution which implements correlations based on physics experiments and was developed by Bell et al. [6].

Fig. 6 and Fig. 7 show the relative deviation of the ideal gas EoS and ARK EoS compared to the Coolprop database. Due to the simplicity of the ideal gas EoS, big deviations from the real fluid properties will be present at higher pressures and lower temperatures. To improve the simulation accuracy, it is necessary to use a more complex real gas model. The region of interest for this paper is the operating range of 350-400 K and 1-7 bar. It can be seen that the ARK EoS (max. 15%) is more accurate than the ideal gas EoS (max. 100%) for a large selection of working conditions. However, these deviations in fluid properties have varying influence on the simulation depending on the thermodynamic process involved. If we take for example an isentropic expansion process starting from 7 bar and 400 K, the maximum deviation for the ideal gas EoS is approximately 50% while for the ARK EoS is around 3% difference.

VI. CFD ANALYSIS

In this paper, all CFD simulations were performed using Ansys Fluent. The authors have already performed previous calculations in [12]. Any custom functionality such as real gas models and dynamic mesh behaviour are handled by user-defined functions (UDFs). The NIST database (included in Fluent) cannot work with multiphase fluids. To solve this, CoolProp can be integrated into Fluent using a custom defined real gas via UDF. Since CoolProp is open source, the code has been compiled and included into the UDF library. The CFD model consists of solving the mass conservation, momentum and energy equations in the fluid domain. The fluid domain is spatially discretized using second-order upwind for the comparison between ARK EoS and ideal gas EoS. The CoolProp database integrated in Fluent is currently working only with the first-order discretization. Therefore, the ARK EoS was additionally cal-
TABLE II  
PISTON EXPANDER RESULTS

<table>
<thead>
<tr>
<th>Initial operating point</th>
<th>Work on moving wall (J)</th>
<th>Work output relative to NIST (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Ideal gas</td>
<td>ARK</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>Temperature (K)</td>
<td>7.64</td>
</tr>
<tr>
<td>B</td>
<td>6</td>
<td>355</td>
</tr>
<tr>
<td>C</td>
<td>6</td>
<td>400</td>
</tr>
<tr>
<td>D</td>
<td>12</td>
<td>385</td>
</tr>
</tbody>
</table>

calculated also with the first-order discretization and compared to the CoolProp database. In that way any difference between the ARK EoS and the CoolProp database due to different discretization is avoided. The temporal discretization in all calculations is first-order fully implicit. The k-ε turbulence model is used to predict the effects of the turbulent regime inside the expander.

For the twin screw expander geometry, some further simplifications were applied. The thermal expansion of the rotors and the casing due to the working fluid has been neglected. The performance analysis will be done with the expander operating in oil-free mode. The inlet and outlet boundary conditions were specified as pressure inlet/outlet. In all calculations the inlet pressure was set to 6 bar with an inlet temperature of 400 K. The outlet pressure was set to 1 bar. The expander casing is configured as adiabatic wall. This assumption is valid due to the short residence time of the working fluid.

In the piston expander model, the system is considered to be a thermodynamically closed system. To achieve this, all walls of the fluid domain are considered to be adiabatic. Furthermore, to limit the influence of any boundary layer effects on the working fluid, the shear stress at the wall is constrained to zero. Due to these conditions, the sole cause of an entropy increase is due to energy dissipation in the working fluid. Before starting the expansion process, the complete fluid domain is initialized to the required inlet conditions.

VII. RESULTS AND DISCUSSION

In this section comparison for ideal gas EoS, ARK EoS and CoolProp and NIST databases has been done. The calculations were performed on a simplified expansion model and a real 3D geometry of the twin screw expander. For the simple geometry, calculations were performed with constant \( c_p \) of 1004 J/kgK when using the ideal gas EoS. For the 3D screw expander model, \( c_p \) is 1045 J/kgK when using the ideal gas EoS, which is the average value between the inlet and outlet conditions.

A. Simplified geometry

Simulations were performed for different operating points with the ideal gas EoS, ARK EoS, Coolprop and NIST fluid property databases. Table II shows the resulting work on the moving wall and the work output relative to NIST. The differences between NIST and Coolprop are in the order of 0.0001%. It can be concluded that NIST and Coolprop produce the same results.

From these results, it can be seen that ideal gas EoS shows 2-8% smaller power output compared to NIST. For the chosen operating points, the ARK EoS shows a maximum of 0.2% deviation from the NIST reference. Overall, the error terms in power output are significantly lower than the deviation of the individual fluid properties. This is to be expected, since the expansion process is not concentrated in one point of the T-s diagram. Furthermore, not every fluid property has the same influence on the expander power output.

The influence of the varying inlet conditions on the model accuracy is clearly visible. Points B and D show the biggest deviation for ideal gas EoS. These operating points are closer to the saturation vapor line and correspond to larger fluid property differences between the ideal gas EoS and the NIST/Coolprop databases. For the ARK EoS, the absolute deviations are significantly smaller.

B. Twin screw expander geometry

From the results of 3D CFD analysis, the overall performance parameters like mass flow rates and power outputs are calculated.

One of the parameters to be compared between the ideal gas EoS, ARK EoS and CoolProp database is the P-V indicator diagram of the screw expander. The P-V diagram shows how the pressure in every moment is changing with the instantaneous volume. It will also show the difference in calculated power between the models. Additional parameters like mass flow rates and leakage flows are also checked.

A first comparison is made between the ideal gas EoS and the ARK EoS. In Fig. 8 the difference in P-V curve can be seen. In Table III, the differences in mass flow rates and power output are presented. It can be seen that the power output for R245fa with the use of the ideal gas EoS is around 8% smaller than with the use of the ARK EoS.

A second comparison has been made between the ARK EoS and the CoolProp database. The difference in power output is less than 0.2%. Since this difference is so small, P-V curves for the ARK EoS and the CoolProp database are on a top of each other. Although the difference in power output is small, the calculation time between these two models is big. In Fig. 9 calculation times for one revolution of the male rotor for the ARK

<table>
<thead>
<tr>
<th>Inlet (kg/s)</th>
<th>Ports (kg/s)</th>
<th>Power (kW)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ideal gas:R245fa</td>
<td>0.1368</td>
<td>0.112</td>
</tr>
<tr>
<td>ARK:R245fa</td>
<td>0.1462</td>
<td>0.1445</td>
</tr>
</tbody>
</table>
were performed for several expansion processes with a piston expander and a simplified piston expander model have been successfully carried out. In these simulations, the working fluid R245fa has been modeled with the ideal gas EoS, the ARK EoS and the CoolProp database.

The choice of the fluid property model mainly depends on the working conditions according to the required accuracy and calculation time constraints. It has been shown that in the ORC working conditions (0.1-2 MPa and 300-450 K), the ARK EoS shows maximal pressure deviations of 15% comparing to CoolProp database. These deviations are low compared with the ideal gas EoS whose deviations are above 100%. Also, it can be concluded that the accuracy of the NIST and the CoolProp databases will be identical.

In order to analyze the proposed models, CFD calculations were performed for several expansion processes with a piston expander geometry. Table II is a summary that shows their maximum deviations in work output. The 3D CFD calculations of a twin screw expander were performed for a typical expansion process from 0.6 MPa - 0.1 MPa and 400 K - 350 K. In these calculations, the ideal gas EoS shows a difference of 8% in the work output compared to the ARK EoS. The ARK EoS shows a smaller maximum deviation of 0.2% compared to CoolProp. A slight improvement of 0.2% for CoolProp database compared to the ARK EoS results in doubling of the required calculation time. Therefore, the ARK EoS is the optimal compromise for both simulation accuracy and calculation time.

ACKNOWLEDGEMENT

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\end{figure}

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List of Abbreviations and Symbols

Acronyms

**ALE** arbitrary Lagrangian-Eulerian
**ARK** Aungier Redlich-Kwong
**CFC** chlorofluorocarbon
**CFD** computational fluid dynamics
**CHP** combined heat and power
**CSP** concentrated solar power
**EoS** equation of state
**HCFC** hydrochlorofluorocarbon
**HVAC&R** heating, ventilation, air conditioning and refrigeration
**ICE** internal combustion engine
**IUPAC** International Union of Pure and Applied Chemistry
**NIST** National Institute of Standards and Technology
**OFC** organic flash cycle
**ORC** organic Rankine cycle
**RANS** Reynolds-averaged Navier Stokes
**RKS** Redlich-Kwong Soave
**TFC** trilateral flash cycle
**UDF** user-defined function
**VLE** vapor-liquid equilibrium
Symbols

- $a$ speed of sound
- $c_p$ specific heat capacity at constant pressure
- $c_v$ specific heat capacity at constant volume
- $h$ enthalpy
- $m$ mass
- $M_w$ molecular weight
- $n$ amount of substance
- $p$ pressure
- $R$ gas constant
- $s$ entropy
- $T$ temperature
- $t$ time
- $V$ volume
- $v$ specific volume

Greek letters

- $\gamma$ ratio of specific heat capacities
- $\omega$ acentric factor
- $\rho$ density

Subscripts

- $c$ critical
- $ref$ reference
- $s$ specific
- $u$ universal
Chapter 1

Introduction

Ever since the Industrial Revolution took place in the first half of the 18th century, electrical and thermal energy became the cornerstone of modern society. With the increasing importance of minimizing primary energy usage and complying with emission restrictions, big steps are being made to provide the future generations of mankind with a reasonable ecological heritage. Organic Rankine cycle (ORC) technology plays a significant role in recuperating energy from industrial waste heat and converting it into electricity. Since most of this energy is only available at lower temperatures, conventional methods for electricity generation are economically infeasible. By using an organic working fluid, the ORC can operate efficiently with low temperature heat sources [1]. While this technology has already proven significant benefits in the industry, significant efforts are made to maximize the power output and system efficiency while keeping the investment costs low. Due to this evolution, ORCs will become an economically more viable technology for an extended range of electricity generation applications using unconventional low temperature heat sources (Fig. 1.1). Recent strides have been made to apply this technology in renewable energy applications such as geothermal power plants and concentrated solar power (CSP) installations [2]. ORCs are also implemented in applications where an increase of the global system efficiency is required, such as biogas power plants [3].

The energy conversion process plays a significant role in defining the overall system efficiency. The main characteristics of the organic working fluid are a low saturation temperature and a positive slope in the saturation vapor line of the T-s diagram. Due to these properties, the technology used for expanding the working fluid is not limited to turbines. Volumetric expanders show significant benefits when applied to small scale ORC installations. Lemort et al. [4] concluded that positive displacement machines can handle two phase flow and have better efficiency at part load, all while showing a lower investment cost. Furthermore, the author noted that twin screw expanders were the most
mature technology compared to piston and scroll expanders. This technical maturity is attributed to the research in screw compressor technology, since the design process of the current generation of screw expanders is based on compressors working in the reverse direction [5, 6, 7].

Producing accurate results from computational fluid dynamics (CFD) calculations of the expansion process is mainly achieved by taking into account the interaction between the working conditions and the screw expander geometry. Fluid property modeling of the working fluid R245fa is essential to attain accurate simulation results. Under typical ORC working conditions, the ideal gas law shows significant deviations from the real fluid properties. To increase simulation accuracy, more complex real gas models are required. One of the commonly applied is the Redlich-Kwong equation of state (EoS) and it’s derivatives. This is a family of EoS which are easy to implement while keeping the calculation time short. The most accurate way of modeling fluid properties is by using high quality data from scientific experiments performed by institutions such as the National Institute of Standards and Technology (NIST). This data is then implemented inside fluid databases such as NIST REFPROP [12] and CoolProp [13].

Figure 1.1: Typical ORC applications [8, 9, 10, 11]
1.1 Aim & motivation

The main goal of this thesis is to study the influence of different fluid property models on the performance of a twin screw expander using the working fluid R245fa. The twin screw expander geometry is delivered by Atlas Copco and the achieved results will be used by the research group ORCNext (granted by IWT) to further optimize the internal flow and increase the efficiency for ORC applications. The ideal gas EoS, Aungier Redlich-Kwong (ARK) EoS and NIST and Coolprop fluid databases will form the basic models of this research. The deviations occurring between these models have been analyzed and compared to results given by Luján et al. [14] and Feng et al. [15]. These different models have also been analyzed in 3D Reynolds-averaged Navier Stokes (RANS) CFD calculations performed on the twin screw expander geometry and a simplified piston expander model. From these simulations, model differences were analyzed using mass flow rates, pressure-volume diagrams and power output. Model differences were evaluated for each phase of the expansion process.

1.2 Outline

Chapter 2 contains a brief overview of the ORC technology, how the thermal cycle works and how the working fluid and expander can be selected to suit the particular application of waste heat recuperation. To model the working fluid in the expander, chapter 3 will give an overview of the different fluid property models that are relevant. In chapter 4, these models are then analyzed in the range of typical ORC working conditions and are compared to results obtained by Luján et al. [14] and by Feng et al. [15]. Chapter 5 describes the ideal expansion process based on the geometry of the twin screw expander and how the grid generation algorithms are applied to this rotor geometry. The simplified square piston expander model is then derived from the described geometry. Finally, this chapter contains an overview of the simulation setup for both geometries in Fluent. Turbulence models, spatial and temporal discretization schemes and boundary conditions of the fluid domain are selected in the final part of this chapter. In chapter 6, the results of the CFD analysis are discussed for both the twin screw expander and the simplified model.
Chapter 2

ORC-Technology

2.1 Introduction

The Rankine cycle is one of the most commonly applied thermal cycles for producing mechanical work from an external heat source. Up to the present day, most of the large scale power plants still use this thermal process to support the daily electricity demand. In the ORC, the working fluid of the cycle is replaced by an organic substance with a higher molecular mass and a lower boiling point than water. The main goal of this replacement is to shift the phase change to lower temperatures.

This chapter will give a brief overview of the cycle topology, commonly applied ORC technology and how the expander and working fluid have been optimized to the application of waste heat recuperation.

2.2 Organic Rankine cycle (ORC) Technology

2.2.1 Cycle topology

Typical thermal cycles are the combination of heat addition, work output, heat subtraction and work input. For waste heat recovery applications, different cycle topologies exist. The ORC is one of the commonly applied thermal cycles which can accept external heat addition.
Different modifications can be performed on this basic cycle architecture. Their main focus is to increase the cycle thermal efficiency $\eta_{th}$ and increasing the heat addition $Q_{in}$ to the cycle. Typical modifications are:

- the usage of regenerators/recuperators
- reheating after partial expansion
- employing multiple pressure levels in the cycle
- using zeotropic mixtures as the working fluid
- pressurizing the working fluid to a supercritical state

Even more complex system topologies such as the organic flash cycle (OFC) and the trilateral flash cycle (TFC) can achieve even better performance, although the discussion and analysis of these architectures is beyond the scope of this thesis. In the case of the basic Rankine cycle and ORC, the cycle operates in a closed manner and the working fluid has to be circulated in a single loop. During the circulation, the working fluid undergoes a specific change each time it passes through a component of the cycle loop. Figure 2.1 shows the typical components present in a classic Rankine cycle and an ORC installation:

**Heat source**  This is the input for primary energy which drives the complete thermal cycle. In classic power plants, the primary energy carrier is often biomass, fossil fuels or nuclear fuel. ORCs are typically fueled by biomass, geothermal energy, solar energy or waste heat.

**Evaporator**  This is the two-phase heat exchanger where energy is extracted from the heat source by evaporating the working fluid.

**Turbine/Expander**  To convert the thermal energy into mechanical work, the working fluid has to be expanded to the discharge pressure using a turbine or a volumetric expander. The shaft of the turbine/expander is then linked to an electric generator, which converts the mechanical work into electricity. Turbines are typically applied in classic Rankine cycles, while volumetric expanders are commonplace in ORCs.

**Regenerator**  Organic working fluids which belong to the category of the dry fluids will remain superheated after the expansion process. Before condensation can occur, the excess heat has to be removed from the working fluid. The regenerator transfers the excess heat of the superheated vapor to the liquid working fluid before the evaporator.
**Condensor** Since the working fluid is artificially produced, the cycle is operated in a closed manner. By condensing the expanded vapor, the working fluid can be reused in the evaporator.

**Pump** The pump is used to circulate the working fluid and to bridge the operating pressure difference between the condensor and the evaporator.

**Heat sink** To be able to condense the working fluid, heat needs to be extracted from the vapor. This is often achieved by circulating cooling fluid in a secondary loop to the heat sink.

![Figure 2.1: Cycle topology](image)

![Figure 2.2: T-s diagram](image)
2.2.2 T-s diagram and cycle efficiency

To better understand the process happening inside the ORC, a visual representation of the cycle is necessary. Any thermodynamic cycle can be visually represented by plotting two variables of the process. By choosing the temperature and the entropy (a measure for the usefulness of the energy), the area circumscribed by the curve represents the mechanical work extracted from the cycle. Figure 2.2 shows the T-s diagram for a classic Rankine cycle and an ORC. When the working fluid passes through a component, the working fluid undergoes a process which changes the temperature and the entropy. The following processes can be discerned in Fig. 2.2a:

1-2: Ideal isentropic pressure increase in the pump
2-3: Heating of the liquid working fluid, followed by evaporation and superheating of the vapor
3-4: Ideal isentropic expansion over the turbine
4-1: Condensation of the working fluid

Isentropic processes are the combination of being adiabatic and reversible. In reality, the points 2 and 4 are not reachable due to irreversibilities occurring in the pump and turbine/expander. This means that the pump will perform the process 1-2’ and the turbine will perform the process 3-4’ instead.

These same steps can be repeated for the ORC, which is in essence the same process as the classic Rankine cycle. The only additional component which is often applied is the regenerator. By generating a link between two points in the cycle, the liquid after the pump is preheated by using the excess heat of the superheated vapor after expansion. By doing this, the energy available in the superheated vapor is applied in a useful way.

The maximum obtainable thermal cycle efficiency is defined by the theoretical Carnot cycle [17]. This is a lossless thermal process which operates between two (constant) temperature reservoirs. Since this is the most efficient way of converting thermal energy into mechanical work, the Carnot efficiency $\eta_{th,Carnot}$ is used as a benchmark to compare real system efficiencies. The Carnot efficiency is defined as follows:

$$\eta_{th,Carnot} = \frac{T_{\text{high}} - T_{\text{low}}}{T_{\text{high}}}$$

(2.1)

$$= 1 - \frac{T_{\text{low}}}{T_{\text{high}}}$$

(2.2)
Assuming the lower temperature reservoir is the atmosphere, $T_{\text{low}}$ can be assumed to be quasi-constant. If $T_{\text{high}}$ becomes larger, the ratio $\frac{T_{\text{low}}}{T_{\text{high}}}$ becomes smaller and a higher efficiency is achieved. This means that the classic Rankine cycle, which works with high temperature steam, will show a higher efficiency than the ORC.

### 2.3 Working fluid

The only theoretical difference between a classic Rankine cycle and the ORC is the replacement of the steam with an organic working fluid. By making this change, the working fluid can evaporate at a lower temperature, which benefits the ORCs’ capability of operating with heat sources that are unsuitable for classic Rankine cycles. Several aspects of the heat source have to be taken into account, such as temperature range, thermal power range and heat modulation. Table 2.1 shows the principal differences between the classic Rankine cycle and the ORC.

<table>
<thead>
<tr>
<th>Working fluid</th>
<th>Water</th>
<th>Organic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemistry</td>
<td>stable</td>
<td>reactive</td>
</tr>
<tr>
<td>Operating pressure/temperature</td>
<td>high</td>
<td>low</td>
</tr>
<tr>
<td>Health &amp; environment</td>
<td>safe</td>
<td>hazard</td>
</tr>
<tr>
<td>Turbine expansion</td>
<td>wet</td>
<td>dry</td>
</tr>
<tr>
<td>Thermal efficiency</td>
<td>high</td>
<td>low</td>
</tr>
<tr>
<td>Heat source requirements</td>
<td>stringent</td>
<td>flexible</td>
</tr>
<tr>
<td>Material cost</td>
<td>high</td>
<td>low</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Applications</th>
<th>Rankine Cycle</th>
<th>ORC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biomass</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>CHP</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>Fossil fuels</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>Geothermal</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>Nuclear</td>
<td>✓</td>
<td></td>
</tr>
<tr>
<td>Solar</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>Waste heat recovery</td>
<td></td>
<td>✓</td>
</tr>
</tbody>
</table>
The high specific enthalpy (heat content per mass/volume unit) of steam dictates that it is a very compact energy carrier. The negative aspect of the high specific enthalpy is that steam is difficult to use when applied to relatively low power applications. Due to this, the turbine of a classic Rankine cycle is unsuitable for small scale ORC applications due to reduced part load efficiency (low mass flow rate). A solution to this problem is to only provide partial steam admission to the turbine. This will keep the efficiency at a reasonable level, but fringe effects of this admission type will result in a lower efficiency than for a full admission turbine.

Since steam is unsuitable for low temperature operation, another thermal cycle energy carrier is required. The most commonly used replacements are synthetic coolant fluids which originate from the cooling industry and are specifically selected to have a higher density than steam and to be a dry fluid (right slanting saturation vapor line in the T-s diagram). These working fluids are commonly derived from crude oil products, which gives the ‘organic’ Rankine cycle it’s name. Since the fluid properties can now be freely chosen, the selection procedure includes several criteria which optimize the working fluid for a specific application. The selection of the correct substance is mainly dependent on it’s interaction with the type of heat source. The following fluid properties can be optimized before additional technical improvements are implemented [1, 18]:

- Saturation vapor line
- Condensor pressure
- Evaporator pressure
- Specific & latent heat
- Critical temperature
- Density
- Production cost & distribution
- Health & environmental hazard
- Chemical reactivity
2.3.1 Saturation vapor line

Figure 2.3 shows the different saturation vapor lines occurring in the T-s diagram of the working fluid. The type of saturation vapor line can also be evaluated using the slope factor $\xi = \frac{d\alpha}{dT}$, which is the rate of change in entropy with respect to temperature [19]. Since this slope factor is temperature dependent, this indicator is typically calculated at the normal boiling point (atmospheric pressure). The following types of saturation vapor lines are distinguished:

- $\xi < 0$: wet fluid
- $\xi = 0$: isentropic fluid
- $\xi > 0$: dry fluid

Substances such as water and R22 are known as wet expansion working fluids (Fig. 2.3a). If the working fluid is expanded immediately after complete evaporation is achieved, the end of the expansion is situated in the two-phase region. This can lead to increased wear due to droplet erosion in the expander, which decreases the expander lifetime and increases the maintenance costs. This problem can be solved by adequately superheating the working fluid after the evaporation process.

By selecting a working fluid with a right slanting saturated vapor line (rising temperature with rising entropy), a dry expansion is obtained (Fig. 2.3c). This ensures that the end point of the expansion is situated outside of the two-phase region. This also means that little to no additional superheating is necessary to prevent droplet erosion. After the expansion, the working fluid remains in a highly superheated dry vapor state. As already seen in Section 2.2, the regenerator functions as a preheater for the working fluid entering the evaporator while removing the excess heat after the expansion has occurred. Although this helps to maximise the thermal efficiency $\eta_h$, the heat addition to the cycle $Q_m$ will be lowered.

The regenerator can be removed from the ORC cycle if the fluid has a quasi-vertical saturated vapor line (Fig. 2.3b). This is referred to as being an isentropic fluid, named after the isentropic expansion process which is also a vertical line in the T-s diagram. Due to this, the superheating before and after the expansion is limited and can be integrated into the evaporator and condenser design.
Chapter 2. ORC-Technology

(a) Wet fluid \((\xi < 0)\)

(b) Isentropic fluid \((\xi = 0)\)

(c) Dry fluid \((\xi > 0)\)

Figure 2.3: Categorization of working fluids by saturation vapor line [16]
2.3.2 Condensor pressure

If the condensor pressure is selected to be slightly above the atmospheric pressure, no additional measures (deaerator) need to be taken to prevent non-condensible gases from entering the cycle. The disadvantage of this positively pressurized system is that leakages to the environment are possible. The selection of the condensor pressure is therefore a trade off between leakage prevention and system maintenance.

2.3.3 Evaporator pressure

The highest pressure in an ORC installation is the evaporation pressure. When selecting component materials for these parts of the cycle, higher pressures and temperatures will result in higher system costs and more stringent safety measures for safe operation of the installation.

2.3.4 Specific & latent heat

To make the condensor and evaporator operate in a more effective way, heat addition during phase change can be promoted by selecting a working fluid with high latent heat and liquid specific heat [20, 21]. By doing this, the mass flow rates occurring in the system will also be reduced, which results in less circulation losses. On the other hand, some authors suggest that a lower specific heat means that the working fluid is more suitable to be used as a heat carrier [22].

2.3.5 Critical temperature

The critical temperature of the selected working fluid has to be tailored to the evaporation temperature. Quoilin et al. [23] suggests that proximity of the evaporation temperature to the fluid critical temperature is required to keep the vapor density sufficiently high. If the evaporation process occurs too far away from the critical point, larger components and pressure drops due to the low vapor density will result in lower system efficiency and higher system costs.

2.3.6 Density

The density of the working fluid dictates the volumetric flow rate of the system and therefore the compactness of the components in the installation.
2.3.7 Production cost & distribution

The production process of the working fluid must be both technically and economically feasible. Adequate distribution is also required to allow for applications in remote sites and system maintenance.

2.3.8 Health & environmental hazard

The organic fluid can have a detrimental effect on the ozone depletion, the greenhouse gas effect and the human health. The production of organic compounds affecting the ozone layer, such as chlorofluorocarbons (CFCs) and hydrochlorofluorocarbons (HCFCs), has ceased since the Montreal Protocol was enforced in May 1989. The working fluid should preferably be in the liquid phase when exposed to typical atmospheric conditions. This will ensure safer transport and handling of the substance. Working fluids which are in the gas phase in typical atmospheric conditions must be pressurized and/or cooled, which leads to higher transport costs. Furthermore, special care and safety measures have to be taken to prevent any leaks during the machine’s lifecycle (including installation decommissioning). To account for these hazards, proper detection systems are required, which adds to the cost of implementing an installation using these working fluids [24].

2.3.9 Chemical reactivity

If chemical corrosion is triggered by the working fluid, more resistant and therefore more costly materials will be necessary to keep the system functional.

2.3.10 Typical organic working fluids

Typical technical fluids used in ORC technology include HDR-14, R132a, R1234yf, R134a, R152a, R245fa, R600a, R601, SES36 (Solkatherm), octamethyltrisiloxane and toluene [25, 26, 27]. R245fa (1,1,1,3,3-Pentafluoropropane) has been selected as the working fluid to be applied in this research. The main reasons of choosing this specific refrigerant is because R245fa is a dry fluid and it is a commonly applied working fluid in the waste heat recovery industry [25]. The main fluid properties of R245fa are shown in Table 2.2.
Table 2.2: Properties of R245fa (1,1,1,3,3-Pentafluoropropane)

<table>
<thead>
<tr>
<th>Property</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Critical temperature</td>
<td>$T_c$</td>
<td>427.2 °C</td>
</tr>
<tr>
<td>Critical pressure</td>
<td>$P_c$</td>
<td>3.64 MPa</td>
</tr>
<tr>
<td>Critical density</td>
<td>$\rho_c$</td>
<td>517 m$^3$/kg</td>
</tr>
<tr>
<td>Acentric factor</td>
<td>$\omega$</td>
<td>0.3724 –</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>$M_w$</td>
<td>134.0482 kg/kmol</td>
</tr>
</tbody>
</table>

2.4 Expander technology

The target output power range of an ORC is a lot lower than for a classic Rankine cycle. Since the specific flow rate of the system is reduced at lower power ranges, alternative types of expanders can be applied that are better suited for the ORC operating conditions. This has been confirmed in experimental research performed on small scale ORC test setups, which show that volumetric expanders are better suitable for these applications. The key advantages of volumetric expanders are lower rotational speeds, better robustness (fewer moving parts), higher pressure ratios, wider power range (part-load performance), market availability and high isentropic efficiency [4, 28, 29].

2.4.1 Turbine

This type of turbomachine works by letting the working fluid act on the turbine blades. In this way, energy in the vapor is extracted and converted into mechanical work. Turbines are typically applied in scenarios where the highest efficiency is required, although this technology only becomes economically viable when being implemented in larger installations which work at a stationary regime. Due to the sensitivity of the turbine to droplet erosion, the working fluid has to be superheated to prevent wear of the last turbine stage. Another disadvantage is that turbines have increasing rotational speed for lower power, which means that specialized generators are required. Sealings at high operating speeds show increased wear, although this problem can be solved by making the turbine-generator combination hermetically sealed.
Turbines are typically subdivided in impulse and reaction types. The impulse turbines produce mechanical work by the turning of the flow by the blades. This means that the flow pressure in the rotor stays constant, while the direction of the flow velocity changes. In the reaction turbine, the flow in the rotor undergoes an expansion, which generates an additional lift force on the turbine blades and a resulting torque on the turbine output axis. One of the most commonly applied reaction turbine types consists of a number of consecutive expansion stages which are combined in an axial configuration. Due to the high specific enthalpy of steam (1000 kJ/kg), this pressure compounded configuration (Fig. 2.4) is typically applied in modern steam turbines, where the expansion is spread over multiple stages to limit the operating speeds.

Figure 2.4: Working principle of a pressure compounded reaction turbine [30]


2.4.2 Piston expander

Reciprocating piston expanders were historically the first type of expanders to be applied during the Industrial Revolution. Current day niche applications are small scale combined heat and power (CHP) installations and waste heat recovery on internal combustion engines (ICEs).

The valves used in compressors and expanders are passive check valves. Since these valves need a pressure differential to open, one of the main benefits is the automatic compensation for over- and under-expansion. This means that the expander automatically adapts to small variations in working conditions. The inlet and discharge valves are situated on the same side of the working chamber, which means that thermal short circuiting needs to be taken into account to prevent extra losses. Another disadvantage of this construction is the limited flow area, which can lead to a lower volumetric efficiency $\eta_v$ due to pressure drops during the filling phase of the expansion process. Of the available configurations, axial piston expanders are commonly applied due to low vibrations and compactness.

Figure 2.5 shows the working principle of an axial piston expander. In this configuration, the generator, consisting of a solenoid coil and a permanent magnet, is combined together with a piston in the housing. The suspension of the piston by resonant springs together with a periodic inflow of the working fluid forms a periodic mechanical vibration. The result is a reciprocating movement where the energy can be extracted by the generator.
2.4.3 Scroll expander

Orbiting scroll technology has been commonly applied for heating, ventilation, air conditioning and refrigeration (HVAC&R) compressors, vacuum pumps and automobile superchargers. The main advantages are low noise and vibrations. The disadvantage is that this type of expander is only available in a limited power range. If the scrolls are too small, excessive leakage flows occur which limits the volumetric efficiency $\eta_v$. When the scrolls are increased in size to account for the high power ranges, the centrifugal forces increase due to the added weight of a bigger and heavier orbiting scroll. Another reason of the limited power range is the availability and the niche applications of the compressor counterpart in the HVAC&R industry. Due to this, new research is necessary to adapt the scroll expander to ORC applications. Oralli et al. [32] states that especially the built-in volume ratio of converted scroll compressors needs to be adapted to the optimal operation conditions of the ORC.

Figure 2.6 shows the working principle of an orbiting scroll expander. The scroll expander is configured with one inlet port in the center and two outlet ports at the outer perimeter of the spiral shaped scrolls. One scroll is fixed while the orbiting scroll is rotated by 180°. The orbiting movement can be translated into a pure rotation by using an eccentric drive. The crescent-shape working chambers (red) are created by the eccentricity of the moving rotor compared to the fixed rotor. As the moving rotor orbits around the fixed rotor, the working chambers (orange-yellow) are displaced towards the outer part of the scroll while the volume increases. The working chambers (green) starts to disappear again when the working fluid is being discharged through the outlet ports.

Figure 2.6: Working principle of an orbiting scroll expander
2.4.4 Screw expander

Screw expanders are available in a wide power range of 20 kWe - 1 MWe. Due to their low rotational speed, these expanders can be directly coupled to the electric generator. Smith et al. [33] states that screw expanders are beneficial for small scale geothermal ORC applications (up to 3 MWe, 100-140°C) and have a lower cost than radial inflow turbines while allowing for two phase expansion. The author also states that a TFC cycle using the right operating conditions would have an even lower cost while increasing the efficiency.

The current generation of screw expanders are mainly derived from the already extensive knowledge and research of screw compressor technology. In essence, the screw expander is one of the most simply constructed volumetric machines, where two meshing helical screw rotors are contained in a double cylindrical casing. The rotors and the casing are precision machined to keep the clearances small. To synchronize the movement of the rotors, an external synchronization gear set can be implemented (synchronized screws). The screw lobes can also be used as a synchronization mechanism (unsynchronized screws), although the maximum operating speed will be lower to limit rotor wear.

![Figure 2.7: Twin screw expander with synchronized gear set [34]](image_url)
2.5 Conclusion

The optimization process of the ORC consists of different aspects. The first step is to tailor the component selection to the heat source. Since the ORC is not limited to using steam, the best choice can be made from a variety of organic working fluids. These substances show a whole range of different fluid properties and characteristics, which can be tuned to the specific project requirements. It is often so that different types of working fluids are applied in different branches of the industry. The selection procedure of the most appropriate working fluid is often correlated to the type of heat source. For the research presented in this thesis, R245fa has been selected as the working fluid for the 3D CFD calculations. This is a refrigerant which finds common application in waste heat recovery and has a positive slope in the T-s diagram which enables dry expansion. To adapt the ORC cycle for this expansion process, a regenerator is used to transfer excess heat from the superheated vapor after the expander to the working fluid before the evaporator. By doing this, the energy is being recycled internally instead of being evacuated by the heat sink. The result is a smaller cooling circuit and a better thermal efficiency of the cycle.

A second optimization can be applied to the expander. Since the main applications of ORC cycles are varying over a wide power range, it is necessary to invest research into the most effective and scalable expander technologies. Since the target output power of a typical ORC installation is a lot lower than for classic Rankine cycles, the specific flow rate of the expander will be lower and will allow reciprocating and volumetric expanders to be implemented. When comparing piston, scroll and screw expanders, it can be seen that the former two types are mainly used in niche HVAC&R applications. The twin screw expander, which is analyzed in this thesis, presents the most mature technology since it is applicable over a broad power range and major research has already been performed for screw compressors.
Chapter 3

Fluid property models for R245fa
Literature review

3.1 Introduction

This chapter will give a brief overview of the fluid property models which are relevant to 3D CFD simulations for expanders in ORC technology. The fluid properties of a certain working fluid can be fully derived from the so-called thermodynamic state. The system state is controlled by the state variables, which are in this case a limited set of thermodynamic properties. A commonly used triad of state variables are the pressure, temperature and density.

The first (and most basic) fluid property model that came into existence was the ideal gas law. It originated from several individual laws which applied to a theoretically perfect gas. Several experimental relationships have been analyzed and empirical laws were proposed by R. Boyle, J. Charles and A. Avogadro. These individual relations were then combined in what is now known as the ideal gas law.

Although the precision of the ideal gas law is acceptable for many gases and working points (including standard atmosphere), the model soon proved to be inadequate for certain applications. It was shown that systems which work with two phase flow, near to the saturation line and/or the critical point will exhibit significant deviations from the ideal gas law. Since the ORC working conditions are situated inside this region, more refined real gas models are necessary to better approximate the observed phenomena of real gases.
Propositions were made to make expansions or derivations of the ideal gas law to better approximate the real behavior of these gases. Since the increased use of computer-aided engineering in the industry, there is also a growing need for digital modeling of fluids and systems. The most accurate way of modeling a fluid is by using fluid property databases.

### 3.2 Ideal gas law

In its commonly written form, the ideal gas law can be formulated as:

\[ pV = nR_uT \]  \hspace{1cm} (3.1)

where:

- \( p \) = pressure
- \( V \) = volume
- \( n \) = amount of substance
- \( R \) = gas constant
- \( u \) = universal
- \( T \) = temperature

To get a more practical formula, the amount of substance can be substituted for the mass using the molecular weight \( M_w \) and the specific gas constant \( R_s \). To make the formula even more flexible, the volume \( V \) is substituted for the specific volume \( v \).

\[ m = nM_w \]  \hspace{1cm} (3.2)

\[ R_s = \frac{R_u}{M_w} \]  \hspace{1cm} (3.3)

\[ v = \frac{1}{\rho} = \frac{V}{m} \]  \hspace{1cm} (3.4)

\[ pv = R_sT \]  \hspace{1cm} (3.5)
where:

\[ m = \text{mass} \]
\[ M_w = \text{molecular weight} \]
\[ s = \text{specific} \]
\[ v = \text{specific volume} \]
\[ \rho = \text{density} \]

The ideal gas law can then be rewritten into the following EoS form, where the pressure is a function of the specific volume \( (p = f(v)) \):

\[
p = \frac{R_s T}{v} \tag{3.6}
\]

### 3.2.1 Further derivation of fluid properties

To allow for an easy computation, the EoS is solved for the specific volume using the pressure and temperature as input parameters. Further calculations are required to derive the required fluid properties from the solution of the EoS.

The density \( \rho \) can be found by combining the definition of the specific volume with the EoS.

\[
\rho = \frac{1}{v} \tag{3.7}
\]

\[
\rho = \frac{p}{R_s T} \tag{3.8}
\]

A reference state is defined to facilitate the derivation of some properties. This reference state can be defined in any arbitrary point where all the fluid properties are known, although this is typically chosen in conditions where accurate measurements on fluid properties are possible. The International Union of Pure and Applied Chemistry (IUPAC) defines the standard pressure as \( 10^5 \) Pa [35]. According to the authors, the standard temperature is typically chosen as 273.15 K or 298.15 K since most thermodynamic tables are compiled using these values.
The enthalpy $h$ can therefore be written as follows:

$$h = h_{ref} + c_p(T - T_{ref}) \quad (3.9)$$

where:

$h = \text{enthalpy}$

$ref = \text{reference}$

$c_p = \text{specific heat capacity at constant pressure}$

The entropy $s$ can be written as follows:

$$s = s_{ref} + c_p \cdot \ln\left(\frac{T}{T_{ref}}\right) - R_s \cdot \ln\left(\frac{p}{p_{ref}}\right) \quad (3.10)$$

where:

$s = \text{entropy}$

To find the speed of sound $a$, the definitions of the specific heat are used.

$$R_s = C_p - C_v \quad (3.11)$$

$$\gamma = \frac{C_p}{C_v} \quad (3.12)$$

$$a = \sqrt{\gamma R_s T} \quad (3.13)$$

$$a = \sqrt{\frac{C_p}{C_p - R_s T}} \quad (3.14)$$

where:

$a = \text{speed of sound}$

$c_v = \text{specific heat capacity at constant volume}$

$\gamma = \text{ratio of specific heat capacities}$
3.3 Real gas models

To further approximate real gases, the ideal gas law can be enhanced using one or more expansion coefficients. The pressure then has an n\textsuperscript{th} order behavior w.r.t. the specific volume (n = 1, 3,\ldots). This will result in an overall more accurate model, especially closer to the saturation line and the critical point.

3.3.1 Van der Waals

The Van der Waals equation can be assumed to be the first enhancement made to the ideal gas law. The equation of state is given by:

\[ p = \frac{R_s T}{v - b} - \frac{a}{v^2} \]  

where:

- \( a = \) attraction term (measure of the attraction between particles)
- \( v - b = \) reduced specific volume

The extra coefficients a and b are theoretically derived from the molecule dimensions, the intermolecular forces and other physically relevant parameters.

3.3.2 Redlich-Kwong

In 1949, O. Redlich and J.N.S. Kwong [17, 36] proposed an empirical derivative of the Van der Waals equation. The main goal was to provide an overall more accurate model, notably in the region above the critical temperature. Up to the present day, the Redlich-Kwong model and its variants are commonly applied due to the relatively simple to use equations. The original EoS can be written as:

\[ p = \frac{R_s T}{v - b} - \frac{a}{\sqrt{T}v(v + b)} \]  

(3.16)
where:

\[ a = 0.42748 \frac{R^2 \sigma^{5/2}}{p} \]

(3.17)

\[ b = 0.08664 \frac{R \sigma}{p} \]

(3.18)

\[ c = \text{critical} \]

The main difference between this model and the Van der Waals equation is the empirical approach to the reduced specific volume and the expansion coefficient. By making these coefficients dependent on the critical pressure and temperature, the model remains accurate for a large range of working points. More specifically, the following criterion should be fulfilled to obtain the maximum model performance:

\[ \frac{p}{p_c} < \frac{T}{2T_c} \]

(3.19)

Several enhancements have been made to the original model with the purpose to:

- improve the overall accuracy
- include the two-phase region into the model
- increase the model flexibility by accounting for highly acentric gases
- increase the model flexibility by integrating fluid/gas mixtures and compounds

**Soave expansion**

The Soave expansion [37] is a three-parameter EoS and is one of the more commonly applied variants of the Redlich-Kwong model. By making the attraction term a function of the acentric factor \( \omega \), the model can also be applied to fluids with highly asymmetric molecules (e.g. hydrocarbons). This model has therefore been commonly applied in the petrochemical industry. The attractive term \( \alpha \) is also made temperature dependent. Due to these modifications, accurate modeling of fluids in the vapor-liquid equilibrium (VLE) and near to the saturation vapor line can be obtained. A drawback is an increased error near to the critical point. The Redlich-Kwong Soave (RKS) model is mostly applied for liquids and subcritical/supercritical vapors.
Chapter 3. Fluid property models for R245fa - literature review

Equation of state:

\[ p = \frac{R_s T}{v - b} - \frac{\alpha(T) \cdot a}{v(v + b)} \]  

(3.20)

where:

\[ a = 0.42747 \frac{R^2_s T^2}{p_c} \]  

(3.21)

\[ b = 0.08664 \frac{R_s T_c}{p_c} \]  

(3.22)

\[ \alpha(T) = \left( 1 + \alpha_{RKS} \left( 1 - \sqrt{\frac{T}{T_c}} \right) \right)^2 \]  

(3.23)

\[ \alpha_{RKS} = 0.48 + 1.574\omega - 0.176\omega^2 \]  

(3.24)

\( \omega = \) acentric factor

**Peng-Robinson expansion**

To study pure substances, another useful addition to the RKS model has been done by Peng-Robinson [38]. This EoS can still be configured using three parameters. The main advantage for this model is the improved density accuracy near to the critical point.

\[ p = \frac{R_s T}{v - b} - \frac{\alpha(T)a}{v^2 + 2bv - b^2} \]  

(3.25)

where:

\[ a = 0.45274 \frac{R^2_s T^2}{p_c} \]  

(3.26)

\[ b = 0.07780 \frac{R_s T_c}{p_c} \]  

(3.27)

\[ \alpha(T) = \left( 1 + \alpha_{PR} \left( 1 - \sqrt{\frac{T}{T_c}} \right) \right)^2 \]  

(3.28)

\[ \alpha_{PR} = 0.37464 + 1.54226\omega - 0.26992\omega^2 \]  

(3.29)
Aungier expansion

In 1995, Aungier presented a modified form of the Redlich-Kwong EoS [39] which has been optimized for numerical applications. In this four-parameter model, the additional parameter is the critical specific volume $v_c$ in addition to the critical pressure $p_c$, the critical temperature $T_c$ and the acentric factor $\omega$ used in the previous models. The main reason for this expansion is to make the results more accurate near to the critical point while keeping the EoS simple to implement and calculate. This EoS is mainly applied for improved accuracy of subcritical and supercritical vapors (especially near to the critical point), as well as for fluids with a negative acentric factor.

Equation of state:

$$p = \frac{R_s T}{v - \tilde{b}} - \frac{a(T)}{v^2 + b_0 v} \quad (3.30)$$

where:

$$a(T) = a_0 \left( \frac{T_c}{T} \right)^n \quad (3.31)$$

$$a_0 = 0.42747 \frac{R^2 T_c^2}{p_c} \quad (3.32)$$

$$b_0 = 0.08664 \frac{R_s T_c}{p_c} \quad (3.33)$$

$$c_0 = \frac{R_s T_c}{p_c + \frac{a_0}{v^2 + b_0 v_c}} + b_0 - v_c \quad (3.34)$$

$$\tilde{b} = b_0 - c_0 \quad (3.35)$$

In this research, the ARK EoS has been implemented in Fluent using a user-defined function (UDF). This specific real gas model has been selected since it is optimized for CFD calculations.
3.4 Conclusion

A certain working fluid can be modeled by using the thermodynamic state together with fluid-specific properties such as the molecular weight, the critical point and the acentric factor. The ideal gas EoS is commonly applied in a large variety of applications. For calculations in ORC operating conditions, more complex models are necessary to cope with the variation of the fluid properties in proximity of the saturation vapor line.

One of the more commonly applied real gas models is the Redlich-Kwong EoS. Since this is an empirical model, it can be tailored to the specific requirements of the application. Several other real gas models for applications in niche industries have been based on modifications of the original Redlich-Kwong model. The Aungier Redlich-Kwong EoS has been selected to be implemented in this research, based on the fact that this model has been optimized for CFD calculations.
Chapter 4

Comparison of ideal gas EoS, ARK EoS & CoolProp

4.1 Introduction

To give a better understanding of how the different models perform in typical ORC working conditions, a comparison will be made between the ideal gas EoS, ARK EoS and CoolProp fluid database. To verify the fluid property models used in the 3D CFD simulations, the comparison is made with the results attained by Luján et al. [14] and by Feng et al. [15]. The results published in these papers can be reconstructed with the models presented in Chapter 3. By attempting to reconstruct several diagrams, a direct comparison can be made of the accuracy between these different fluid property models.

4.2 p-T diagram

The p-T diagram can be used to analyze how a fluid property changes according to a specific value of pressure and temperature for the different models. The range of interest for this comparison is from 1-7 bar and 350-400 K. In Fig. 4.1 the variation of different fluid properties is shown for ideal gas EoS, ARK EoS and CoolProp.

Figure 4.1a shows the density variation for the different models in Matlab. It can be seen that the density in the region of interest is mainly a function of the pressure. In the low pressure region (1 bar), the density of the ideal gas EoS matches the ARK EoS and CoolProp database. Differences start to be visible at high pressures (7 bar) and low temperatures (350 K), which is the region near to the saturation vapor line. Here the
ARK EoS and the CoolProp database show slight variations in density. The ideal gas EoS shows a much lower density compared to the ARK EoS. If the temperature is increased to 400 K, the differences between the models start to become smaller again.

In Fig. 4.2a the density of the different models are compared at a temperature of 80°C. In the visualized range, the density in the ideal gas EoS shows the biggest changes when varying the operating pressure. The ideal gas EoS shows larger deviations (compared to CoolProp) than the ARK EoS. These same trends are noticed in Fig. 4.2b. The main difference between these figures are the slight differences between the respective Redlich-Kwong and CoolProp/real gas reference models. In Fig. 4.2a, the density for CoolProp is larger than the ARK EoS, while in Fig. 4.2b the Redlich-Kwong model has a slightly larger density than the real gas reference.

Figure 4.1b shows the variation of the enthalpy $h$ for the fluid property models. It can be seen that the enthalpy is a function of the pressure in the ideal gas EoS. At lower pressures and higher temperatures, model differences become smaller. In this region, the ARK EoS and CoolProp values are on top of each other. It is noted that the ideal gas EoS has the highest enthalpy of all the models. As the pressure is increased and the temperature is decreased, the enthalpy of the ARK EoS and the CoolProp database is visibly becoming lower than the ideal gas EoS. In this region, CoolProp values are slightly smaller than ARK EoS values.

In Fig. 4.1c, the differences in speed of sound $a$ are shown for the Matlab calculations. The speed of sound, which is a function of the temperature in the ideal gas EoS, shows a decrease with lower temperature. The ARK EoS and the CoolProp database are similar and are a function of both the pressure and the temperature. At low pressures (1 bar), the difference between the ideal gas EoS and the ARK EoS remains constant over the temperature range 350-400 K. When increasing the pressure to 7 bar, the differences become bigger and at lower temperatures large deviations occur between ideal gas EoS and ARK EoS.

The change of specific heat $c_p$ for ideal gas EoS, ARK EoS and CoolProp is shown in Fig. 4.1d. In the region of interest, the $c_p$ shows large differences with both the pressure and temperature. It can be seen that the ideal gas EoS was configured with a constant $c_p$ of 1004 J/kgK. The ARK EoS shows a varying $c_p$ in function of the pressure and temperature. CoolProp generates similar values at low pressures (1 bar) and high temperatures (400 K). At higher pressures and lower temperatures, the ARK EoS starts to deviate from the CoolProp results.
Figure 4.1: p-T diagrams of different fluid properties to show model differences (Matlab)
Chapter 4. Comparison of ideal gas EoS, ARK EoS & CoolProp

Figure 4.1: p-T diagrams of different fluid properties to show model differences (Matlab)

(continued)
Chapter 4. Comparison of ideal gas EoS, ARK EoS & CoolProp

Figure 4.2: Pressure diagram of density $\rho$ at $T = 80\,^\circ C$
4.3 T-s diagram

To generate a T-s diagram, the data for the entropy p-T diagram was used to generate a transformation script. By using this conversion, every fluid property which can be written as function of temperature and pressure can be converted into the T-s equivalent. The region of interest for the simulation case presented in this thesis is from 350-400 K and 1-7 bar. Figures 4.3 and 4.4 shows the relative deviation of the pressure and the \( c_p \) for the ideal gas EoS and Redlich-Kwong EoS compared to the reference database.

In Fig. 4.3a, the ideal gas EoS shows big deviations from the real fluid properties at higher operating pressures and lower temperatures. Figure 4.3b show the same trends in increasing deviation with higher pressures and lower temperatures. The Redlich-Kwong EoS (Fig. 4.3c) shows overall higher accuracy (max. 15%) than the ideal gas EoS (max. 100%). It can be seen that the area of high deviations in the Redlich-Kwong EoS is more concentrated near to the saturation vapor line, while the deviations for the ideal gas EoS are more spread out across higher entropy values. This means that the Redlich-Kwong EoS will show an increased accuracy for a wider range of operating points.

The effect of the fluid property model on the \( c_p \) is shown in Fig. 4.4. For the ideal gas EoS (Fig. 4.4a), the deviation is more constant with the same operating pressure. It can be seen that when following the isobaric line of 7 bar, the deviation varies between 5-10%. At operating pressures nearing the critical point of R245fa, the deviation shows a sudden increase to 80%. For the ARK EoS (Fig. 4.4c), the overall deviation is lower at temperatures higher than 400 K. When nearing the saturation vapor line, the ideal gas EoS performs better than the ARK EoS, which attains deviations of up to 10%. It is again noted that Fig. 4.4b and 4.4d visualize the same trends in \( c_p \) variation. The overall deviation of the respective models is higher for the pressure than for the \( c_p \).

It is noted that deviations in fluid properties have a varying influence on the overall simulation accuracy, since the expansion process is composed of a range of operating points along a T-s line. If we take for example an isentropic expansion process starting from 7 bar and 355 K, the maximum deviation in pressure for ideal gas EoS is approximately 95% while ARK EoS is around 10%. When the temperature is increased to 400 K, the maximum deviation for ideal gas EoS is lowered to 50% while the accuracy for ARK EoS is around 3%. When selecting an appropriate fluid property model for a simulation case, it is a necessity to analyze the working conditions occurring during the expansion process.
Chapter 4. Comparison of ideal gas EoS, ARK EoS & CoolProp

![Graphs showing pressure deviation of R245fa comparing to the reference (%)](image)

**Figure 4.3:** Pressure deviation of R245fa comparing to the reference (%)
Chapter 4. Comparison of ideal gas EoS, ARK EoS & CoolProp

Figure 4.4: $c_p$ deviation of R245fa comparing to the reference (%)
4.4 Conclusion

The choice of the fluid property model mainly depends on the working conditions of the system. Depending on the required accuracy and calculation speed, different models can be chosen and parametrized to achieve adequate performance. A detailed analysis of the ORC operating points is necessary to select the most appropriate model for a specific flow problem. A valuable tool for simplifying this selection procedure is to use deviation graphs as shown in Fig. 4.3 and Fig. 4.4.

For typical ORC working conditions (1-20 bar and 300-450 K), the ARK EoS shows maximal pressure deviations of 15% comparing to the CoolProp database. These deviations are low compared with the ideal gas EoS, whose pressure deviations are above 100%. For the specific heat $c_p$, the deviations have a maximum of 10% for the ARK EoS compared to the reference, while the ideal gas EoS shows a maximum of 30%.
Chapter 5

3D CFD analysis
Geometry, mesh & simulation setup

5.1 Introduction

In this chapter, the geometry of the twin screw expander will be analyzed to show what effects occur that make the real expansion process deviate from the ideal expansion process. Since the twin screw expander has a complex geometry, it is useful to construct a simplified square piston expander model. By doing this, a brief comparison of the different fluid property models is possible while minimizing the calculation time. In this way, effects originating from the twin screw expander geometry will be excluded from this simulation case.

Before 3D CFD calculations are possible, it is necessary to chose the most suitable simulation options to properly model the fluid domain in the expander. To do this, the space discretization, time discretization, turbulence model and boundary conditions have to be selected to model the real situation as accurate as possible.

Before this thesis was initiated, preliminary simulations were already performed on the twin screw expander geometry in Fluent using the ideal gas EoS and the ARK EoS [40]. Since CoolProp is open-source, the code will be compiled inside the UDF library of Fluent. By doing this, the calculation time is minimized while the simulation accuracy is maximized. The performance of other EoS can then be compared to the CoolProp simulation results. Other custom functionality such as dynamic mesh is also included into the UDF library.
5.2 Expansion process

The screw expander is part of the positive displacement machines. This family of machines can be further subdivided according to the number of screws involved. In this research, the twin screw expander consists of two counter-rotating screw rotors with opposing threads. These screws are contained inside a double cylindrical casing, where multiple working chambers are formed by the screw lobes.

The ideal expansion process consists of three main phases, which are shown in Fig. 5.1. Before the expansion starts, the working chamber is isobarically filled to the initial volume $V_1$. After that, the screws will rotate and expand the working fluid in an isentropic manner to the end volume $V_2$. This maximum volume is reached when the outlet port connects to the working chamber. Any further rotation will result in the working fluid being isobarically discharged through the outlet.

<table>
<thead>
<tr>
<th>Phase</th>
<th>Male rotor angle</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference position</td>
<td>0°</td>
</tr>
<tr>
<td>Filling</td>
<td>7-126°</td>
</tr>
<tr>
<td>Expansion</td>
<td>126-387°</td>
</tr>
<tr>
<td>Discharge</td>
<td>387-720°</td>
</tr>
</tbody>
</table>

The inlet port is connected to the cylinder end face, while the outlet and auxiliary inlet ports are connected to the cylinder mantle. The inlet area, the outlet area and the working chamber volume will change according to the rotor angle, which is due to the geometry of the screws and the ports. This relationship results in the different phases of the expansion process, which can be seen in Fig. 5.2 and Table 5.1. The start of the filling process begins at $\theta = 7^\circ$, when the inlet port makes connection with the working chamber. As the rotor angle increases, the inlet area enlarges and reaches a maximum. Any further rotation results in a decrease of the inlet area while the working chamber volume keeps increasing.
This results in a **pre-expansion** of the working fluid. As the filling ends at $\theta = 126^\circ$ with an inlet closure volume $V_1$, the **expansion** phase starts and increases the volume of the working chamber. When the maximum volume $V_2$ is reached at $\theta = 387^\circ$, the outlet area is connected and the **discharge** process begins. This discharge phase will continue until the working chamber volume is reduced to zero.

![Volume curve with inlet and outlet surface area as a function of the male rotation angle](image)

**Figure 5.2:** Volume curve with inlet and outlet surface area as a function of the male rotation angle

Table 5.2 shows the configuration of the selected screw geometry. One of the essential design parameters of the screw expander is the volume ratio $v$, which is defined as the relation between the discharge volume $V_2$ and the inlet closure volume $V_1$. Since this ratio is fixed by the geometry, each expander has to be optimized to the selected operating pressure of the system. If the volume ratio is too high, the working fluid pressure will be lower than the discharge pressure (over-expansion). If the volume ratio is too low, the pressure in the working chamber is higher than the discharge pressure when the outlet port starts to open (under-expansion).

**Table 5.2: Twin screw expander design parameters**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lobe configuration</td>
<td>4/6 (male/female)</td>
</tr>
<tr>
<td>Nominal speed</td>
<td>6000 rpm</td>
</tr>
<tr>
<td>Rotor diameter</td>
<td>70 mm</td>
</tr>
<tr>
<td>L/D ratio</td>
<td>1.9</td>
</tr>
<tr>
<td>Male rotor wrap angle</td>
<td>302 °</td>
</tr>
</tbody>
</table>
5.3 Simplified geometry

To maintain similarity between the original geometry and the simplified model, the simulation will be performed in 3D. This simplified CFD model is based on a square piston expander model and is shown in Fig. 5.3. The cuboid fluid domain (blue) with one moving face (green) represents the volume increase during the expansion of the working fluid.

![Figure 5.3: Piston expander geometry](image)

Fig. 5.4 shows that part of the expansion process in the twin screw expander can be simplified to a quasi-linear process. This means that the moving wall velocity $v_{mw}$ can be defined as a constant. To achieve further similarity between the twin screw expander and the simplified piston expander model, the moving wall velocity $v_{mw}$ is made equal to the axial velocity $v_a$ of the working fluid.

![Figure 5.4: Comparison of the original and simplified volume curves](image)
Chapter 5. 3D CFD analysis

The mesh for the working chamber will be composed of a cell stack which is aligned with the piston motion. By doing this, the gas velocity in the directions not aligned to the piston motion will be constrained to zero. The cell width equals the domain width and can be found as follows:

\[ w_{\text{domain}} = w_{\text{cell}} = \sqrt{\frac{\Delta V}{\Delta t} \frac{1}{v_{mw}}} \]  

(5.1)

where:

- \( w_{\text{domain}} \) = domain width
- \( w_{\text{cell}} \) = cell width
- \( \Delta V \) = change in volume
- \( \Delta t \) = change in time
- \( v_{mw} \) = moving wall velocity

The cell thickness \( h_{\text{cell}} \) of the initial volume \( V_1 \) is chosen in such a way that these are equal to the cells created by the expansion process. To achieve this, the cell thickness is defined as the change in volume in one time-step \( dt \):

\[ h_{\text{cell}} = v_{mw} dt \]  

(5.2)

where:

- \( h_{\text{cell}} \) = cell thickness
- \( dt \) = time-step size

**Table 5.3:** Dynamic mesh zone configuration

<table>
<thead>
<tr>
<th>Zone</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fixed wall</td>
<td>Stationary</td>
</tr>
<tr>
<td>Side walls</td>
<td>Deforming</td>
</tr>
<tr>
<td>Moving wall</td>
<td>Rigid body</td>
</tr>
<tr>
<td>Fluid domain</td>
<td>Deforming</td>
</tr>
</tbody>
</table>
The mesh growth is controlled by dynamic mesh layering. The goal is to achieve a growth of exactly one cell per simulation time-step. To trigger the layering process during each time-step, the layering is based on the cell height with a split factor of one. To achieve proper mesh growth, the dynamic mesh zones are configured as shown in Table 5.3.

5.4 Grid generation for twin screw expander

As shown in Fig. 5.5, the expander geometry can be subdivided into four main components. The inlet, the outlet and the additional ports belong to the static parts, whereas rotor domain is considered as the moving part of the geometry.

![Twin screw expander geometry](image)

**Figure 5.5:** Twin screw expander geometry

The stationary part of the fluid domain is meshed using an unstructured tetrahedral grid. The number of cells in each part of the fluid domain is shown in Table 5.4.

<table>
<thead>
<tr>
<th>Rotors</th>
<th>Inlet</th>
<th>Outlet</th>
<th>Ports</th>
</tr>
</thead>
<tbody>
<tr>
<td>570000</td>
<td>51789</td>
<td>1420688</td>
<td>18038</td>
</tr>
</tbody>
</table>

**Table 5.4:** Number of cells in different parts of expander domain
Chapter 5. 3D CFD analysis

The flow within the twin screw expander is complex due to the screw lobe geometry. Since transient calculations are required for this simulation case, a specialized grid generator is used to manipulate the meshing of the flow domain. The first grid generation algorithm for screw machines was presented in 1999 by Kovacevic et al. [41]. In this paper, a block-structured grid was generated via analytical rack-generation of the complex rotor geometry. This algorithm was recently applied in a twin screw expander simulation using air as the working fluid [6]. Vande Voorde et al. [42] proposes a different approach to grid generation, where the rotor geometry is first meshed using an unstructured tetrahedral grid. The block-structured grid is then generated from the solution of the Laplace problem and the unstructured grid. The algorithm presented in that paper uses the differential method [43], which is suitable for complex geometries such as screw machines. This grid generation algorithm was recently tested on a twin screw compressor geometry and showed good agreement with the experimental results [44]. In this thesis, the grid generation is based on the same approach as [42].

The rotor grid is constructed by stacking two-dimensional block-structured (rectangular) grids in axial slices of the expander casing. Before the CFD simulation was initiated, 2D structured meshes of the rotor profiles were generated in correspondence with the rotation (one step per 1.5° male rotor angle). To achieve a finer angular resolution, the mesh at a certain simulation time-step can be interpolated from the two adjacent generated grids. This method is known as the arbitrary Lagrangian-Eulerian (ALE) method, where a pure rotation of the grid in the housing is performed without any cell deformation during the transient calculations. The 2D meshes are generated from the solution of the Laplace potential equation $\nabla^2 \phi = 0$, as already stated in [44]. This solution was generated from an unstructured triangular grid in the rotor domain. Since the casing has a double cylindrical shape, the grid is divided into two blocks (male and female rotor) by the division line. The size of the gaps between the rotors and between the rotors and the casing are extremely small (order tens of microns versus a rotor diameter of about 70 mm). The interaction between the stationary and rotating parts of the fluid domain is achieved by using sliding interfaces.
5.5 Mathematical flow models

The turbulent regime inside the twin screw expander is modeled by using the two equation
$k-\epsilon$ model. The flow field of the simulation is solved using the conservation of mass, mo-
mentum and energy equations. The fluid domain was spatially discretized using second-
order upwind for the comparison between ideal gas EoS and ARK EoS [40]. The CoolProp
database integrated into Fluent is currently only operational using the first-order spatial
discretization. Therefore, the ARK EoS was additionally calculated with the first-order
discretization to allow for a proper comparison to the CoolProp fluid database. In that
way, any difference in calculations between the ARK EoS and the CoolProp database
due to dissimilar discretization schemes is avoided. The temporal discretization in all
calculations is configured as first-order fully implicit. The pressure-based solver is also
configured to calculate the pressure and flow velocity simultaneously. These settings in
the twin screw expander setup have been duplicated and applied to the simplified model
as well. This decision is made to maintain maximum similarity between the simulations
while still simplifying the geometry and shortening the required calculation time.
5.6 Boundary conditions

5.6.1 Simplified geometry

The simplified piston expander model is a thermodynamically closed system, which can be achieved by configuring the walls of the fluid domain as being adiabatic. For the simplified model, only the expansion process is of importance. To neglect boundary layer effects due to the cuboid shape of the fluid domain, the shear stress on the walls is constrained to zero. The expansion process happening inside the simplified model is therefore quasi-isentropic, with the only increase in entropy originating from the internal energy dissipation in the working fluid. To initialize the mesh, a variety of initial conditions (including the inlet conditions of the twin screw expander simulation) are applied to the whole fluid domain.

5.6.2 Twin screw expander

The deformation of the rotors and the expander casing due to thermal expansion is not taken into account. The analysis presented in this thesis is made by operating the expander in oil-free mode, while still injecting working fluid through the auxiliary ports. The inlet and outlet faces of the fluid domain were defined as pressure based boundary conditions. For all simulations, the inlet was set to 6 bar and 400 K, while the outlet was set to 1 bar. The housing of the expander is considered to be adiabatic, which is a valid assumption due to the short residence time of the working fluid.
5.7 Conclusion

The expansion process occurring in the working chambers of a twin screw expander can be split up in multiple phases, namely the filling, expansion and discharge phases. Geometrical effects such as pre-expansion, under-expansion and over-expansion have to be taken into account when dimensioning the twin screw geometry.

Based on the expansion process of a working chamber in the twin screw expander, an equivalent square piston expander model can be constructed. Since most part of the expansion process is linear, the velocity of the moving wall in the simplified model can be kept constant. Since geometrical effects are neglected in this simplified geometry, the only difference in results will be caused by the selected fluid property model. In this way, the influence of a variety of fluid property models can be tested on the expansion process while keeping the calculation time low due to the simple geometry.

Due to the complex rotor geometry in the twin screw expander, a special grid generation algorithm is necessary to provide the optimal mesh for the rotor domain. The algorithm implemented in Fluent is based on the same approach as Vande Voorde et al. [42], which uses a solution of the Laplace potential equation to generate the grid. The domain of the rotors has been subdivided into a stack of 2D slices in axial direction. By generating the rotor grid for 60 different rotor positions and combining this with interpolation, a fine angular resolution can be achieved.

Simplifications are necessary to translate a flow problem into CFD simulations while still achieving results with adequate accuracy in a limited time frame. The flow field is resolved by solving the conservation of mass, momentum and energy equations using a pressure-based solver. To account for the energy dissipation due to the turbulent regime, the two equation $k-\epsilon$ model was chosen. Second-order spatial discretization was applied for ideal gas EoS, while first-order spatial discretization was applied for the CoolProp database. Calculations were performed with both first-order and second-order spatial discretization for ARK EoS. The temporal discretization was chosen as first-order implicit for all cases.

The simplified piston expander model was tested using a variety of initial operating conditions, of which one equals the inlet conditions of the twin screw expander simulation. This simplified model was configured to neglect boundary layer effects due to the geometry, which resulted in a quasi-isentropic model where the biggest differences occur due to the deviations in the fluid property models. Both geometries are considered to be rigid and the housing is configured as being adiabatic.
Chapter 6

Results and discussion

In this section, the results of the comparison of ideal gas EoS, ARK EoS, CoolProp and NIST databases are discussed. The specific heat $c_p$ for ideal gas EoS is configured as being constant and has a value of 1004 J/kgK for the simplified geometry. The value of 1045 J/kgK was chosen for the ideal gas EoS in the twin screw expander calculations, which is the average specific heat between the inlet and outlet.

6.1 Simplified geometry

The simplified piston expander model has been tested with ideal gas EoS, ARK EoS, CoolProp and NIST databases in a variety of operating conditions (Table 6.1). The work on the moving wall and the work output relative to NIST are shown in Table 6.2. Since CoolProp and NIST show differences in the order of 0.0001%, it can be concluded that both databases will produce the same simulation results.

<table>
<thead>
<tr>
<th>Pressure [bar]</th>
<th>Temperature [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>400</td>
</tr>
<tr>
<td>B</td>
<td>6</td>
</tr>
<tr>
<td></td>
<td>355</td>
</tr>
<tr>
<td>C</td>
<td>6</td>
</tr>
<tr>
<td></td>
<td>400</td>
</tr>
<tr>
<td>D</td>
<td>12</td>
</tr>
<tr>
<td></td>
<td>385</td>
</tr>
</tbody>
</table>

Table 6.1: Piston expander: initial operating points
Figure 6.1: Pressure deviation of R245fa compared to CoolProp for the operating points of the simplified piston expander model (%)
It can be seen that ideal gas EoS is the overall least accurate model, with a 2-8% smaller work output than the NIST reference. In comparison, the ARK EoS shows deviations in the order of 0.2% compared to NIST, which is a magnitude lower than for the ideal gas EoS. When comparing the individual fluid properties with the work output, it can be seen that error terms for the latter are significantly lower. Since the expansion process is spread out over a range of the T-s diagram, several deviations in fluid properties are occurring during different phases of the expansion process. Furthermore, every fluid property has a varying influence on the resulting work output. When combining these arguments, the more accurate results for work output are to be expected.

These results also show the influence of different expander inlet conditions on the model accuracy. Figure 6.1 shows the deviation of the pressure for ideal gas EoS and ARK EoS compared to CoolProp, together with the initial operating point for each of the simulation cases. Since the work output of a closed system is calculated using the $\int p\,dV$ integral, any significant deviation in pressure compared to the reference will contribute to an error in the work output of the simulation. Points B and D show the biggest deviation for ideal gas EoS. These operating points are situated near to the saturation vapor line, where the largest fluid property differences occur between ideal gas EoS and CoolProp/NIST databases. For the ARK EoS, the absolute deviations are an order of magnitude lower.

### Table 6.2: Piston expander: results

<table>
<thead>
<tr>
<th>Work on moving wall [J]</th>
<th>Ideal gas</th>
<th>ARK</th>
<th>CoolProp</th>
<th>NIST</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>7.64</td>
<td>7.79</td>
<td>7.78</td>
<td>7.78</td>
</tr>
<tr>
<td>B</td>
<td>11.46</td>
<td>11.96</td>
<td>11.95</td>
<td>11.95</td>
</tr>
<tr>
<td>C</td>
<td>11.46</td>
<td>11.80</td>
<td>11.78</td>
<td>11.78</td>
</tr>
<tr>
<td>D</td>
<td>22.91</td>
<td>24.75</td>
<td>24.72</td>
<td>24.72</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Work output relative to NIST [%]</th>
<th>Ideal gas</th>
<th>ARK</th>
<th>CoolProp</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>98.23</td>
<td>100.16</td>
<td>100.00</td>
</tr>
<tr>
<td>B</td>
<td>95.85</td>
<td>100.07</td>
<td>100.00</td>
</tr>
<tr>
<td>C</td>
<td>97.28</td>
<td>100.21</td>
<td>100.00</td>
</tr>
<tr>
<td>D</td>
<td>92.70</td>
<td>100.15</td>
<td>100.00</td>
</tr>
</tbody>
</table>
6.2 Twin screw expander geometry

6.2.1 Ideal gas EoS vs. ARK EoS

Figure 6.2 shows the results of the 3D CFD analysis for ideal gas EoS and ARK EoS. Performance indicators like mass flow rates (Fig. 6.2b) and power output (Fig. 6.2c) are calculated for ideal gas EoS and ARK EoS. The p-V indicator diagram of the twin screw expander (Fig. 6.2a) shows how the pressure changes during different phases of the expansion process. The area in the p-V curve is also a measure for the work output, which is used to compare the calculated power between the different models. Table 6.3 shows the calculated power and the mass flow rates at the inlet and auxiliary ports.

Figure 6.2b shows that the mass flow rate fluctuations for ARK EoS are larger than for the ideal gas model. For the given geometry and operating conditions (6 bar and 400 K), the ideal gas EoS has a mass flow rate which is 14.4% smaller than for the ARK EoS. The power fluctuations in Fig. 6.2c are approximately similar for both models, although it can be seen that the average power is lower for ideal gas EoS. The power output for ARK EoS is 8% larger compared to the ideal gas EoS, which is to be expected since the area of the p-V diagram is bigger for the ARK EoS.

<table>
<thead>
<tr>
<th></th>
<th>Ideal gas</th>
<th>ARK</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet mass flow rate</td>
<td>0.1368</td>
<td>0.1462 kg/s</td>
</tr>
<tr>
<td>Port mass flow rate</td>
<td>0.112</td>
<td>0.1445 kg/s</td>
</tr>
<tr>
<td>Outlet mass flow rate</td>
<td>0.2488</td>
<td>0.2907 kg/s</td>
</tr>
<tr>
<td>Average power</td>
<td>6.57</td>
<td>7.14 kW</td>
</tr>
</tbody>
</table>
Chapter 6. Results and discussion

Figure 6.2: Graphical comparison between ideal gas EoS and ARK EoS
In the p-V diagram (Fig. 6.2a), several effects can be seen which do not occur in the ideal expansion process. Figure 6.3 shows the real inlet flow pattern during the filling process. It can be seen that there is a pressure drop due to the throttling loss, which is significant compared to the theoretical isobaric filling. This means that the expander inlet has to be optimized to minimize the flow losses during the filling process. In Fig. 6.3a, it is shown that the lowest pressure is concentrated near to the connection of the expander inlet and the rotor domain. The small low pressure flow between the screws (blue) is the leakage flow through the blowhole of the expander. This means that a more detailed analysis is required to evaluate the influence of individual fluid properties and the operating conditions on the expander performance.

Figure 6.4 shows the pressure contour on the rotor wall. The orange/green high pressure region near the inlet shows the first working chamber which is undergoing the filling process through the inlet. Since there are auxiliary ports available which inject working fluid in the radial direction of the twin screw, an additional pressure peak can be seen in the p-V diagram. The effect of this injection can be seen in the aqua colored region of the pressure contour, where the working chamber is connected to the auxiliary ports (Fig. 6.4a). Compared to a normal expansion, this additional injection increases the area of the p-V diagram and results in an increase of the power output for a given geometry and operating conditions. Furthermore, it can be seen that the blue parts of the geometry are the working chambers that have established a connection with the outlet port and are in the discharging phase of the expansion process.
Figure 6.3: Inlet flow pattern during filling process for ARK EoS
Figure 6.4: Pressure contour on the rotor wall for ARK EoS
Figure 6.4: Pressure contour on the rotor wall for ARK EoS (continued)
6.2.2 ARK EoS vs. CoolProp

The second comparison is made between the ARK EoS and the CoolProp database. The power output difference between these models is about 0.2%, which makes the p-V diagrams overlay without any visible difference (Fig. 6.5). A larger calculation time is the penalty to achieve a 0.2% accuracy increase with the CoolProp database. Figure 6.6 shows the simulation time required to achieve one full rotation of the male rotor. Although the code for CoolProp has been natively compiled into the UDF library of Fluent, the calculation time for CoolProp is doubled compared to the ARK EoS.

![Figure 6.5: p-V diagram to compare ARK EoS with CoolProp](image)

![Figure 6.6: Difference in calculation time for ARK EoS and CoolProp database](image)
Chapter 7

Conclusions

In this thesis, 3D CFD simulations of a twin screw expander have been carried out where the working fluid R245fa was modeled using different fluid property models. The original geometry has been analyzed using the ideal gas EoS, ARK EoS and CoolProp database. The expansion process due to the twin screw geometry has been analyzed and a simplified square piston model has been constructed. By doing this, the expansion process has been approximated and was subsequently tested using the ideal gas EoS, ARK EoS, CoolProp and NIST databases. Since the screw expander geometry is complex, this simplification allows to test the implementation of the different fluid property models in Fluent, which was done using UDFs.

Before the simulations were performed, an analysis of the different models was required to predict the effects of the individual fluid properties on the CFD calculations. Since the ideal gas EoS was inadequately approximating the real life properties of R245fa in the vicinity of the saturation vapor line, a more complex real gas model was necessary. Previous calculations on this twin screw expander geometry have already been performed in [40] using the ARK EoS. This is a simple empirical third-order model which is relatively easy to implement and calculate. A comparison was made in Chapter 4 between the ideal gas EoS, ARK EoS and CoolProp database in the typical ORC working conditions (1-20 bar and 300-450 K) and the resulting trends were verified by research performed by Luján et al. [14] and by Feng et al. [15].

The ARK EoS shows a maximum pressure deviation of 15% compared to the CoolProp database. These deviations are relatively low, since the ideal gas EoS produced deviations in pressure well over 100%. When using an operating pressure of 7 bar, the ARK EoS has an overall better accuracy. The deviation in $c_p$ for the ideal gas EoS follows isobaric lines and increases to a maximum of 80% in the proximity of the critical point. The ARK EoS
shows increasing deviations when nearing the saturation vapor line and has a maximum deviation of 10% comparing to the CoolProp database. When using an operating pressure of 7 bar, the ideal gas EoS performs better at lower temperatures while the ARK EoS has an improved accuracy for the specific heat $c_p$ at high temperatures. The CoolProp and NIST fluid databases have also been compared and were considered to produce the same results for these simulation cases.

This comparison of the different fluid property models, together with Fig. 6.1 on p. 49, shows how the simulation accuracy is highly dependent on the selected model and the working conditions present in the complete fluid domain. This means that the fluid property model has to be evaluated on a case-by-case basis. Deviation graphs can therefore be used as a valuable selection tool to determine the most appropriate fluid property model based on project requirements such as model accuracy and calculation time constraints. From the results presented in Chapter 6, it has to be noted that not every fluid property has the same influence on the power output of the expander. Furthermore, the expansion process is not concentrated in one point but occurs on a line in the T-s diagram, which means that deviations in fluid properties will be changing constantly depending on the current phase of the expansion process.

Utilizing the simplified piston expander model, several inlet operating points were analyzed for the work on the moving wall during the expansion process. It was concluded that the ideal gas EoS shows a maximum of 8% smaller power output compared to CoolProp. On the other hand, the ARK EoS shows a maximum of 0.2% deviation from the CoolProp reference. In the twin screw expander simulations, it was seen that the power output for the different models was matching the results obtained by using the simplified geometry. Although the CoolProp database achieves 0.2% better accuracy, the drawback is the increased overhead due to the interaction between the CFD package and the fluid database. Despite the CoolProp library being compiled inside the UDF library of Fluent, the calculation time is doubled compared to the ARK EoS simulation.

When combining all the elements for this simulation case, the ARK EoS is considered to be the optimal compromise for both simulation accuracy and calculation time.
Future work

A more detailed analysis and optimization of this twin screw expander geometry will be performed using the presented models. From the results discussed in this thesis, it can be seen that the operating conditions have a large effect on the results of the CFD calculations due to the deviations of the different fluid property models. To predict this influence more accurately, a sensitivity analysis is required to estimate the exact effect of the deviations in fluid properties on the simulation results.

The p-V diagrams obtained by the CFD calculations show that the real filling process does not approximate the ideal isobaric line. To improve on the current design, the inlet port geometry of the expander has to be further optimized to minimize the throttling losses occurring due to the pressure drop during the filling process. Furthermore, the selected geometry will be tested using a range of pressure ratios and operating speeds to determine the optimal working range of the expander, as well as a detailed analysis of the leakage flows and how oil injection can improve the performance of the expander.

The conclusions presented in this thesis will be used by the ORCNext project as a basis to further improve twin screw expanders for the application of waste heat recuperation using ORC technology. From these results, more accurate lower order models can be constructed to optimize the performance of the ORC installation, as well as reduced order models for the further optimization of the twin screw expander itself.

Ghent, 22 May 2015

Lazhar Abdelli
Bibliography


