CO₂ COMPRESSOR-EXPANDER ANALYSIS

Final Report

Date Published – March 2003

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EXECUTIVE SUMMARY

Background
Carbon dioxide (CO₂) is a potential substitute for HCFC refrigerants with favorable environmental properties compared to other HCFC alternatives. One of the major challenges with CO₂ in air-conditioning applications is the low energy efficiency of systems at higher heat sink temperatures. The major loss in CO₂ cycles is the throttling loss associated with the expansion process. The availability lost during the expansion process can be recovered with a work-producing expansion device, an expander. Theoretical studies have estimated improvements of the basic CO₂ cycle in the range of 40% to 60% for outdoor temperatures of 27°C to 50°C, resulting in efficiencies competitive with or better than those of current conventional systems.

Objective
The overall objective of this project is to provide the HVAC industry with elements to understand the practical performance potential of CO₂ as an alternate refrigerant in residential air-conditioning applications through the implementation of an expander – compressor system. The work analytically defines the most promising approaches from a performance and feasibility standpoint. The work accounts for the requirements inherent in the integration of the selected types of expanders into CO₂ systems, in order to provide a realistic evaluation of the system performance.

System Performance with Expander, CO₂ vs. R22
The energy efficiency of a CO₂ air-conditioning system with conventional expansion valve and without suction line heat exchanger at an outdoor air temperature of 28°C is approximately 4% to 6% lower than the energy efficiency of a comparable R22 system. At outdoor air temperatures of 50°C, the energy efficiency of the CO₂ system is approximately 43% lower. A CO₂ system with an ideal expander performs 25% to 38% more efficiently at 28°C than an R22 system with a conventional expansion valve. At 50°C, the ideal CO₂ expander system is 4% to 7% more efficient than the R22 system. If the expander efficiency is 80%, the CO₂ system performs 16% to 27% better than the R22 system at 28°C and 7% to 11% worse at 50°C. At approximately 36°C, both systems perform with a similar efficiency. With an expander of 60% efficiency, the CO₂ system performs 7% to 18% better at 28°C and 18% to 21% worse at 50°C. At approximately 31°C, the performance of both systems is equal. If the expansion valve is replaced by an ideal work-recovering expander in both systems, the CO₂ system performs 19% to 31% more energy efficiently at outdoor air temperatures of 28°C. At 50°C, the CO₂ system performs approximately 9% to 12% worse than the R22 system. With an expander efficiency of 80%, the CO₂ system performs 10% to 21% better at 28°C and 19% to 22% worse at 50°C. If the efficiency of the expander is 60%, the energy efficiency of the CO₂ system is 4% to 14% higher than the R22 system at 28°C and 26% to 29% lower at 50°C.
outdoor air temperature. Table A lists the estimated coefficient of performance for the systems.

Table A: COP of CO₂ and R22 systems at ambient temperatures of 28°C and 50°C:

<table>
<thead>
<tr>
<th>Expander efficiency [%]</th>
<th>28°C</th>
<th></th>
<th></th>
<th>50°C</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CO₂</td>
<td>R22</td>
<td></td>
<td>CO₂</td>
<td>R22</td>
<td></td>
</tr>
<tr>
<td>100</td>
<td>6.9 – 7.6</td>
<td>5.8</td>
<td></td>
<td>2.9 - 3</td>
<td>3.3</td>
<td></td>
</tr>
<tr>
<td>80</td>
<td>6.4 – 7.0</td>
<td>5.8</td>
<td></td>
<td>2.5 – 2.6</td>
<td>3.2</td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>5.9 – 6.5</td>
<td>5.7</td>
<td></td>
<td>2.2 – 2.3</td>
<td>3.1</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>4.8 – 5.3</td>
<td>5.5</td>
<td></td>
<td>1.6</td>
<td>2.8</td>
<td></td>
</tr>
</tbody>
</table>

**Effect of Suction Line Heat Exchanger in Expander System**

At most operating conditions, a suction line heat exchanger does not improve the energy efficiency of an expander system. Only if a significant fraction (more than 70%) of the work extracted from the expansion process is lost during the energy conversion does the performance benefit from an internal heat exchanger. If more than 30% of the expander work can be recovered, the suction line heat exchanger reduces the energy efficiency of the system. This is due to the reduced work output at lower expander inlet enthalpy and the increased compressor work at higher super-heat. However, it should be noted that a suction line heat exchanger can have secondary benefits, such as protection of the compressor at operation with flooded evaporator, and should not be excluded from the system without careful consideration.

**Expander and Compressor Performance**

Three positive displacement mechanisms have been analyzed for their potential as expansion machines in a CO₂ system:

1. Reciprocating piston
2. Rotary piston
3. Scroll

Tables B and C summarize the expected performance for the devices as compressors and expanders at AHSRAE A test conditions for a range of machining tolerances (leakage gap size).

Table B: Compressor indicated, isentropic, and volumetric efficiency vs. leakage gap size

<table>
<thead>
<tr>
<th>Leakage gap size</th>
<th>5 µm</th>
<th></th>
<th></th>
<th>10 µm</th>
<th></th>
<th></th>
<th>15 µm</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>η_{ind}</td>
<td>η_{is}</td>
<td>η_{vol}</td>
<td>η_{ind}</td>
<td>η_{is}</td>
<td>η_{vol}</td>
<td>η_{ind}</td>
<td>η_{is}</td>
<td>η_{vol}</td>
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<tr>
<td>Recip. piston</td>
<td>0.93</td>
<td>0.77</td>
<td>0.88</td>
<td>0.91</td>
<td>0.76</td>
<td>0.84</td>
<td>0.85</td>
<td>0.72</td>
<td>0.79</td>
</tr>
<tr>
<td>Rotary piston</td>
<td>0.96</td>
<td>0.79</td>
<td>0.96</td>
<td>0.90</td>
<td>0.75</td>
<td>0.92</td>
<td>0.85</td>
<td>0.72</td>
<td>0.87</td>
</tr>
<tr>
<td>Scroll</td>
<td>0.87</td>
<td>0.73</td>
<td>0.88</td>
<td>0.64</td>
<td>0.56</td>
<td>0.65</td>
<td>0.39</td>
<td>0.36</td>
<td>0.38</td>
</tr>
</tbody>
</table>
Table C: Expander indicated and isentropic efficiency vs. leakage gap size

<table>
<thead>
<tr>
<th>Leakage Gap Size</th>
<th>5 µm</th>
<th>10 µm</th>
<th>15 µm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>η_\text{ind}</td>
<td>η_\text{is}</td>
<td>η_\text{ind}</td>
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<td>Recip. piston</td>
<td>0.90</td>
<td>0.75</td>
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<tr>
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<td>0.94</td>
<td>0.79</td>
<td>0.84</td>
</tr>
<tr>
<td>Scroll</td>
<td>0.93</td>
<td>0.78</td>
<td>0.75</td>
</tr>
</tbody>
</table>

The performance of the scroll mechanism is most dependent on the leakage gap size. At machining tolerances above 5 µm, the scroll mechanism performs significantly worse than the other mechanisms. The performance of the scroll mechanism is dominated by the leakage across the tips of the scroll wraps. If this leakage path is eliminated, the indicated efficiency of a scroll expander, for instance, is above 90% for a flank clearance of 15 µm. Experimental results of existing scroll compressors for conventional refrigerants show a high volumetric and compression efficiency, indicating that effective techniques for leakage reduction are available. The reciprocating piston and rotary piston mechanisms perform similarly at all leakage clearances. At small leakage gap sizes, the rotary piston performs slightly better than the reciprocating piston.

The reciprocating and rotary piston expanders require externally actuated valves. With externally activated and controlled valves, current technology limits the expander frequency to values on the order of 1 Hz. The scroll mechanism is not subject to this limitation. All mechanisms require some kind of valve controls to adjust the volume ratio. If the inlet valves of an expander are not controlled, the internal volume ratio is constant. If the internal volume ratio does not match the ideal volume ratio imposed by the operating conditions, over- or under-expansion reduces the expander efficiency. Performance simulation indicates that the ideal volume ratio in a CO₂ system with optimized high-side pressure changes by less than 25% over a wide range of operating conditions. The expander performance degradation due to over- or under-expansion is below 10%, indicating that expander valve control may not be necessary.

Due to the small change of the pressure ratio over a wide range of operating conditions in a CO₂ system, the compressor and expander indicated efficiencies are approximately constant at all operating conditions. The indicated efficiencies of a reciprocating piston compressor and a reciprocating piston expander with a leakage gap size of 10 µm are approximately 91% and 87%, respectively. With an effective isentropic efficiency 15% lower than the indicated efficiency (i.e. 76% and 72% for compressor and expander, respectively), the COP of an optimized CO₂ expander system is approximately 6.6 at 28°C outdoor air temperature and 2.4 at 50°C. Compared to a conventional R22 system, the CO₂ expander system performs 20% better at the low temperature conditions and approximately 14% worse at the high-temperature conditions. At approximately 34°C, both systems operate with the same energy efficiency.

**Integration Concepts**

For maximum efficiency, the mechanical work generated by the expander should be directly utilized. To reduce conversion and storage losses, the expander work can supply
part of the compressor shaft work, requiring the integration of the compressor and expander on a common shaft. With this design however, the optimization of the high-side pressure becomes a challenge, because the high-side pressure is no longer independent from the compressor speed (unless the expander displacement volume is variable). A number of control options have been analyzed. System simulations indicate that an expander cycle can be operated at or close to the optimum high-side pressure without variable expander displacement or additional control valves if the compressor and expander displacement volumes are designed appropriately.
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## LIST OF SYMBOLS

### Latin Symbols

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<thead>
<tr>
<th>Symbol</th>
<th>Unit</th>
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<tr>
<td>$A$</td>
<td>Area</td>
</tr>
<tr>
<td>$C_d$</td>
<td>Discharge coefficient</td>
</tr>
<tr>
<td>$COP$</td>
<td>Coefficient of performance</td>
</tr>
<tr>
<td>$d_h$</td>
<td>Hydraulic diameter</td>
</tr>
<tr>
<td>$F$</td>
<td>Field</td>
</tr>
<tr>
<td>$h$</td>
<td>Specific enthalpy</td>
</tr>
<tr>
<td>$\dot{H}$</td>
<td>Enthalpy flow rate</td>
</tr>
<tr>
<td>$k_m$</td>
<td>Coefficient for minor losses</td>
</tr>
<tr>
<td>$m$</td>
<td>mass</td>
</tr>
<tr>
<td>$\dot{m}$</td>
<td>Mass flow rate</td>
</tr>
<tr>
<td>$Nu$</td>
<td>Nusselt number</td>
</tr>
<tr>
<td>$P$</td>
<td>Pressure</td>
</tr>
<tr>
<td>$pr$</td>
<td>Pressure ratio</td>
</tr>
<tr>
<td>$Q$</td>
<td>Heat</td>
</tr>
<tr>
<td>$\dot{Q}$</td>
<td>Heat flow rate</td>
</tr>
<tr>
<td>$q$</td>
<td>Specific heat</td>
</tr>
<tr>
<td>$R$, $r$</td>
<td>Gas constant, Radius</td>
</tr>
<tr>
<td>$Re$</td>
<td>Reynolds number</td>
</tr>
<tr>
<td>$r_d$</td>
<td>Ratio of vapor density to liquid density</td>
</tr>
<tr>
<td>$Ref$</td>
<td>Refrigerant</td>
</tr>
<tr>
<td>$S$</td>
<td>Entropy</td>
</tr>
<tr>
<td>$s$</td>
<td>Specific entropy</td>
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<tr>
<td>$\dot{S}$</td>
<td>Entropy flow rate</td>
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<tr>
<td>$T$</td>
<td>Temperature</td>
</tr>
<tr>
<td>$TDC$</td>
<td>Top dead center, position of piston stop</td>
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<tr>
<td>$U$, $u$</td>
<td>Absolute, specific internal energy</td>
</tr>
<tr>
<td>$v$</td>
<td>Velocity</td>
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<tr>
<td>$V$</td>
<td>Volume</td>
</tr>
<tr>
<td>$w$</td>
<td>Specific work</td>
</tr>
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<td>$W$</td>
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<tr>
<td>$x$</td>
<td>Vapor quality</td>
</tr>
<tr>
<td>$y$</td>
<td>Entropy generation contribution</td>
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### Greek Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tr>
<td>$\beta$</td>
<td>Mismatch of volume ratio, volumetric expansion coefficient, velocity of approach factor $- / \text{K}^{-1}$</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>Isentropic expansion exponent</td>
</tr>
<tr>
<td>$\delta$</td>
<td>Leakage gap size</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Corrective coefficient for 2-phase orifice flow</td>
</tr>
</tbody>
</table>
\[ \mu \] Joule-Thomson coefficient, viscosity \quad \text{kg/m}^3, \text{kg/m\cdot s}

**Subscripts and Superscripts**

* Intermediate state  
\( C \) Cooling  
\( Comp \) Compressor  
\( Cond \) Condenser  
\( D \) Discharge  
\( Evap \) Evaporator  
\( Exp \) Expansion, expander, expansion valve  
\( G \) Gas phase  
\( GC \) Gas cooler  
\( is \) Isentropic reversible process  
\( j \) Iteration index  
\( L \) Liquid phase  
\( Leak \) Associated with leak flow  
\( Q \) Associated with heat transfer  
\( up \) Upstream  
\( Valve \) Associated with valve flow
1 INTRODUCTION

Background
Carbon dioxide (CO\textsubscript{2}) is a potential substitute for HCFC refrigerants with favorable environmental properties compared to other HCFC alternatives. One of the major challenges with CO\textsubscript{2} in air-conditioning applications is the low system energy efficiency at higher heat sink temperatures. The major loss in CO\textsubscript{2} cycles is the throttling loss associated with the expansion process. The availability lost during the expansion process can be recovered with a work-producing expansion device (expander). Theoretical studies have estimated improvements of the basic CO\textsubscript{2} cycle in the range of 40\% to 60\% for outdoor temperatures of 27\textdegree C to 50\textdegree C, resulting in efficiencies competitive with or better than those of current conventional system.

Objective
The overall objective of this project is to provide the HVAC industry with elements to understand the practical performance potential of CO\textsubscript{2} as an alternate refrigerant in residential air-conditioning applications through the implementation of an expander – compressor system. The work analytically defines the most promising approaches from a performance and feasibility standpoint. The work accounts for the requirements inherent in the integration of the selected types of expanders into CO\textsubscript{2} systems, in order to provide a realistic evaluation of the performance.

Overview
Following the definition of a baseline and review of the recent literature on CO\textsubscript{2} vapor compression systems with and without expanders, the performance potential of a CO\textsubscript{2} expander system depending on the expander efficiency is estimated and compared to a conventional, sub-critical system with and without expander. Section 5 presents the approach for the simulation of the compressor and expander efficiency in a CO\textsubscript{2} system. Results of the simulation for four compressor and expander mechanisms are presented and compared in Section 6. The potential for the compressor – expander integration and implications for the cycle control are discussed in Section 7. Section 8 summarizes and concludes the report.
2 BASELINE OF CONVENTIONAL AIR-CONDITIONING SYSTEMS

The baseline for the performance evaluation of the CO\textsubscript{2} transcritical vapor compression cycle is a 10 kW residential air-conditioning system with refrigerant R22. Extensive laboratory and field data is available to the industry, thus an experimental baseline is not established here. For the comparison between the CO\textsubscript{2} system and the R22 system, a simplified model is created. The modeling assumptions are given in Appendix A. The R22 and CO\textsubscript{2} systems with and without expander are briefly compared in Section 4.
3 REVIEW OF RECENT WORK ON CO₂ SYSTEMS

3.1 CO₂ Baseline Systems

The primary target application for transcritical CO₂ vapor compression system has been automotive air-conditioning. Consequently, most of the research has focused on automotive applications (e.g. Preissner 2001, Adiprasito 2000, Hirao et al. 2000, Ijima 2000, McEnaney et al. 1998). Work on residential size systems has been published among others by Cuttler (2000), Halozan and Rieberer (1999), Heyl (2000), Hwang and Radermacher (1998a), Neksa et al. (1998) and Rieberer et al. (1999).

For the comparison with a residential air-conditioning system, the work by Cuttler (2000) is the most appropriate option. The focus of Cuttler’s work was to develop and experimentally investigate a CO₂ air-conditioning system to replace a 12 kW environmental control unit with R22 as refrigerant. Experimental data are available at the CEEE of the University of Maryland. The system performance at ASHRAE A, B, and C test conditions is shown in Table 1.

Table 1: Performance data of 12 kW CO₂ air-conditioning system (Cuttler 2000)

<table>
<thead>
<tr>
<th>COP</th>
<th>ASHRAE A</th>
<th>ASHRAE B</th>
<th>ASHRAE C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cooling</td>
<td>2.9</td>
<td>3.5</td>
<td>3.4</td>
</tr>
<tr>
<td>capacity [kW]</td>
<td>12</td>
<td>12.2</td>
<td>11.6</td>
</tr>
</tbody>
</table>

3.2 Work Recovery Devices and Cycles with Work Recovery

Shortly after interest in CO₂ cycles was reinvigorated in the early 1990s, the expansion valve was identified as a major source of exergy loss and the use of work recovery machines began to be reconsidered theoretically (Lorentzen 1994 and later Robinson and Groll 1998, Heyl and Quack 2000, Preissner 2001, Fukuta et al. 2001). Depending on modeling assumptions, the researchers estimate the potential for improvement of energy efficiency to be 20% to 50%.

Heyl and Quack (2000) conducted experiments with a reciprocating piston expander and reported an isentropic efficiency of 51%. They investigated a system with two-stage compression where the second compressor stage was driven by the piston expander. The COP of the set-up was 30% higher than the COP of the two-stage system without expander. Maurer and Zinn (2000) conducted experiments with reciprocating piston type devices and gear pump type devices. The isentropic efficiency of the piston expander and the gear pump device were on the order of 50% and 55%, respectively. The energy efficiency of the refrigeration cycle was not measured. Preissner (2001) performed experiments with a modified R134a scroll compressor operating as an expander. Due to high internal leakage, the isentropic efficiency was lower than 30%. The advantage of scroll expanders pointed out by Preissner is the built-in volume ratio of the device. While piston expanders require active valves, the timing of suction and discharge in scroll expanders is purely determined be the geometry of the device. This reduces the level of
control complexity and still allows a large portion of the volume change work of the expansion process to be used. A reciprocating piston expander was built and tested by Baek et al. (2002). The measured isentropic efficiency was less than 10% and the improvement of the system COP was on the order of 10%. The system set-up was similar to that of Heyl and Quack (2000). Stosic et al. (2002) report test results from a twin screw combined compressor and expander in a low-temperature application for CO2. The isentropic efficiency of the expander section was on the order of 65%. The system was operated below the critical point. Similar to scroll expanders, screw devices have a built-in volume ratio and thus do not require control valves.

### 3.3 Other Cycle Improvements

In most of the investigations referenced in Section 3.1 the CO2 cycles were equipped with a suction line heat exchanger (SLHX), which accommodates internal heat transfer between gas cooler outlet and evaporator outlet. The effect of an SLHX is more pronounced at high temperatures of the heat sink (Preissner 2001). Preissner observed an improvement of the COP of 13% and of the capacity of 18% at gas cooler air inlet temperatures of 45°C and an insignificant effect on the performance at temperatures of 15°C.

Nippon Soken and Denso Corporation (1997) and Huff et al. (2002) investigated the potential for performance improvement by employing a two-stage compression process. They explored various options for the circuitry and reported a COP improvement in the order of 20% to 60% and an increase in cooling capacity of 10% to 35% for the most promising option. In addition to the basic components of a heat pump cycle and the modified compressor, this two-stage system requires two internal heat exchangers and one additional secondary fluid – refrigerant heat exchanger.

At the Center for Environmental Energy Engineering (CEEE) of the University of Maryland, the benefit of an evaporatively cooled gas cooler has been investigated (Preissner 2001, Preissner et al. 2000). Using liquid water drained from the evaporator, the air at the gas cooler inlet can be humidified and thereby cooled. A theoretical performance improvement of 40% in COP and capacity is predicted. In preliminary experiments, the COP improvement was 24% and the capacity increased by 8%. Problems encountered in the experiments included uneven distribution of the water over the gas cooler and incomplete evaporation. The power required for driving the pump, which was used to spray the water into the air-stream, was not included into the net work-input to the system.
4 PERFORMANCE POTENTIAL OF CO$_2$ EXPANDER SYSTEMS

Figure 1 shows the difference between a cycle with isenthalpic and isentropic expansion in a P-h diagram for CO$_2$. The cycle with isentropic expansion operates between the points 1 – 2 – 3 – 4 and the cycle with isenthalpic expansion between the points 1 – 2 – 3 – 4'.

In order for the expansion process to follow a line of constant entropy, the enthalpy difference $h_4' - h_4$ must be extracted in the form of expansion work. This means that the cycle with isentropic expansion must have a work-extracting expansion device. The work produced can reduce the net work-input to the cycle. At the same time, the capacity of the cycle is increased by the difference $h_4' - h_4$. Thus, the isentropic expansion reduces the net work-input to the cycle and increases the capacity.

An isentropic expansion process is technically impossible due to friction, leakage, and other unavoidable sources of irreversibility. In realistic applications, the process in a work-extracting expansion device, commonly referred to as an expander, will instead be a polytropic one, resulting in an evaporator inlet state between point 4 and 4' in Figure 1. The real process in an expander compared to the ideal isentropic process is usually characterized by the expander isentropic efficiency $\eta_{is}^{Exp}$

$$\eta_{is}^{Exp} = \frac{h(P_1, s_1) - h(P_0, s_0)}{h(P_1, s_1) - h(P_0', s_1)} = \frac{W_{real}^{Exp}}{W_{is}^{Exp}}.$$  

Equation 1
Similar to the isentropic efficiency of a compressor, this definition is only applicable if the process can be considered adiabatic. The isenthalpic throttling valve can be considered as an expander with isentropic efficiency of zero.

A first-law analysis allows estimating the potential for system performance improvement using an expander. The analysis has been carried out for both a transcritical CO\textsubscript{2} cycle and a subcritical R22 system. It is assumed that all of the work from the expansion process is recovered and contributes to the total system work-input. Detailed modeling assumptions are given in Appendix A.

Figure 2 graphs the result of the simulation over a range of ambient temperatures between 28°C and 50°C and expander efficiencies between 0% and 100%. Without expander, the R22 system performs better than or equal to the CO\textsubscript{2} system at all ambient temperatures (Figure 2 a). A CO\textsubscript{2} system with isentropic expansion performs better than the baseline R22 system with conventional expansion valve over the range of ambient temperatures considered. With an isentropic expander in both cycles, the CO\textsubscript{2} system performs better than the R22 system at ambient temperatures below 38°C (Figure 2 b).

![Figure 2: Performance potential of expander cycle for refrigerants CO\textsubscript{2} (a) and R22 (b)](image)

**Expander and Suction Line Heat Exchanger**

A suction line heat exchanger (SLHX) is a refrigerant to refrigerant heat exchanger, accommodating internal heat transfer between compressor suction line and gas cooler/condenser outlet. For CO\textsubscript{2} systems with isenthalpic expansion valves, an SLHX can improve the performance by up to 15% at high ambient temperatures. An SLHX is considered an integral component in these systems. In cycles with work-extracting expansion however, an SLHX does not always improve the system performance. An SLHX can be characterized by its effectiveness

\[
\varepsilon_{SLHX} = \frac{h(T_{low,\text{out}}, P_{low,\text{out}}) - h(T_{low,\text{in}}, P_{low,\text{in}})}{h(T_{high,\text{in}}, P_{low,\text{out}}) - h(T_{low,\text{in}}, P_{low,\text{in}})},
\]

Equation 2
where \textit{in} and \textit{out} refer to the inlet and outlet of the SLHX and \textit{low} and \textit{high} refer to the low-pressure and high-pressure sides, respectively.

The energy efficiency improvement of an SLHX depends on whether the work extracted in the expander can be recovered. If the expander work is not recovered, the system performance benefits from an SLHX at higher ambient temperatures. At an ambient temperature of 50°C (Figure 3 (a)). If the expander work is not recovered, the system performance benefits from an SLHX at higher ambient temperatures. At an ambient temperature of 50°C (Figure 3 (a)). If the expander work is not recovered, the system performance benefits from an SLHX at higher ambient temperatures.

Figure 3 shows the performance of four different cycle configurations over a range of ambient temperatures. Graph (a) presents the system with work recovery, graph (b) the system without work recovery. An isentropic efficiency \(\eta_{\text{Exp}}=0\) indicates a system without expander, \(\eta_{\text{Exp}}=1\) represents an isentropic expander. An SLHX effectiveness \(\varepsilon_{\text{SLHX}}=1\) indicates a system with ideal SLHX. The system without SLHX is represented by \(\varepsilon_{\text{SLHX}}=0\). No pressure drop in the SLHX is considered; thus the results represent a best-case scenario.

![Figure 3: Performance of CO2 system with expander and SLHX](image)

An SLHX does not improve the COP of an expander system with ideal work recovery (Figure 3 (a)). If the expander work is not recovered, the system performance benefits from an SLHX at higher ambient temperatures. At an ambient temperature of 50°C, the benefit of an additional SLHX is in the order of 5% compared to the COP of a cycle without an SLHX. At lower ambient temperatures, an additional SLHX has no effect on the COP. As the degree of work recovery increases, the benefit of an SLHX installed in addition to the expander decreases. If more than 30% of the expander work can be recovered, the SLHX does not improve the system performance in the temperature range considered in Figure 3. In order to investigate the optimum cycle configuration depending on the degree of work recovery, the cycle performance has been optimized numerically with the independent variables expander efficiency, SLHX effectiveness and high-side pressure. The ambient temperature was constant at 50°C and the degree of work recovery (\(\eta_{\text{Recovery}}\)) was varied from 0% to 100% in 10% increments. The results indicate an abrupt transition from an optimum configuration with SLHX to the optimum configuration without the heat exchanger (Table 2). This means that no “optimum SLHX
effectiveness” other than a perfect SLHX (at low degrees of work recovery) or no heat exchanger at all (at high degrees of work recovery) exists.

Table 2: Optimum expander efficiency and SLHX effectiveness vs. work recovery

<table>
<thead>
<tr>
<th>η_{Recovery} [%]</th>
<th>η_{Exp} [%]</th>
<th>ε_{SLHX} [%]</th>
<th>P_{high} [kPa]</th>
<th>COP</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>100</td>
<td>100</td>
<td>12371</td>
<td>2.05</td>
</tr>
<tr>
<td>10</td>
<td>100</td>
<td>100</td>
<td>12336</td>
<td>2.08</td>
</tr>
<tr>
<td>20</td>
<td>100</td>
<td>100</td>
<td>12298</td>
<td>2.11</td>
</tr>
<tr>
<td>30</td>
<td>100</td>
<td>0</td>
<td>13275</td>
<td>2.13</td>
</tr>
<tr>
<td>40</td>
<td>100</td>
<td>0</td>
<td>13163</td>
<td>2.21</td>
</tr>
<tr>
<td>50</td>
<td>100</td>
<td>0</td>
<td>13035</td>
<td>2.30</td>
</tr>
<tr>
<td>60</td>
<td>100</td>
<td>0</td>
<td>12895</td>
<td>2.4</td>
</tr>
<tr>
<td>70</td>
<td>100</td>
<td>0</td>
<td>12741</td>
<td>2.50</td>
</tr>
<tr>
<td>80</td>
<td>100</td>
<td>0</td>
<td>12568</td>
<td>2.62</td>
</tr>
<tr>
<td>90</td>
<td>100</td>
<td>0</td>
<td>12371</td>
<td>2.76</td>
</tr>
<tr>
<td>100</td>
<td>100</td>
<td>0</td>
<td>12142</td>
<td>2.91</td>
</tr>
</tbody>
</table>

As the expander efficiency of a realistic system deviates from 100%, the degree of work recovery from which an SLHX improves the cycle performance will shift towards higher values. Conversely, as the pressure drop in a realistic SLHX increases, the degree of work recovery from which the SLHX reduces the cycle performance will shift towards lower values.

In order to understand the effect of an SLHX on the system performance, it is helpful to compare the cycles in a P-h diagram (Figure 4). The indices C and E indicate compressor and expander, respectively. The indices 1 and 2 indicate the cycle without and with SLHX, respectively. Table 3 lists the specific work terms and cooling capacities presented in Figure 4.

Table 3: Specific work and cooling capacity for CO₂ cycle

<table>
<thead>
<tr>
<th></th>
<th>Without SLHX with expander</th>
<th>With SLHX with expander</th>
<th>Without SLHX, without expander</th>
</tr>
</thead>
<tbody>
<tr>
<td>q [kJ/kg]</td>
<td>116.6</td>
<td>163</td>
<td>117.4</td>
</tr>
<tr>
<td>w_C [kJ/kg]</td>
<td>39.4</td>
<td>54</td>
<td>42.5</td>
</tr>
<tr>
<td>w_E [kJ/kg]</td>
<td>11.9</td>
<td>7.5</td>
<td>0</td>
</tr>
<tr>
<td>mfr [kg/s]</td>
<td>0.04288</td>
<td>0.03062</td>
<td>0.0426</td>
</tr>
<tr>
<td>COP</td>
<td>4.24</td>
<td>3.51</td>
<td>2.76</td>
</tr>
</tbody>
</table>

The values indicate that the increase in specific cooling capacity is compensated by the decrease in expander work and the increase in compressor work. The SLHX shifts the expansion process towards the left in the P-h diagram and the compression process towards the right. Since the slope of the lines of constant entropy in the diagram increases from right to left, this results in an increase in compressor work and a decrease in expander work.
Figure 4: Expander work with and without SLHX
5 EXPANDER AND COMPRESSOR SIMULATION

In order to estimate the performance of realistic compressors and expanders, a general simulation of positive displacement machines has been developed. The algorithm calculates the performance of the devices accounting for valve losses, internal leakage, internal heat transfer, and unmatched volume ratio. Inputs to the program are the boundary conditions within which the compression/expansion takes place and geometric data of the positive displacement device. Outputs of the simulation are the thermodynamic state during the process, mass flow rate, work, and heat transfer to/from the fluid, and the gas forces and moments acting on the moving surfaces and the drive shaft. The algorithm is implemented in Matlab Release 12 and uses CEEEProps, an interface to Refprop 7, to calculate fluid properties. The program provides a graphical user interface for the simulation of single operating points and an interface to Microsoft Excel for batch operation.

5.1 Assumptions

Fluid Properties
The fluid properties in a control volume are average (bulk) properties. It is assumed that the properties are constant during each time step. The properties are calculated for thermodynamic equilibrium. Hence, the process is simulated as a quasi-steady-state process.

Valves
All valves are modeled as ideal valves. Pressure actuated (reed) valves are assumed to open fully and without any time delay. Position actuated valves, e.g. in scroll expanders, are assumed to open and close fully and instantaneously. Flow through the valves is simulated as flow through circular orifices.

All valves in expanders are simulated as position actuated valves. In expanders, it is not possible to use reed valves. For a valve to respond according to pocket and reservoir pressures, an external control is necessary. However, it is challenging to build an externally controlled valve that acts fast enough and has an acceptable flow resistance for typical residential AC applications (Maurer and Zinn 2000, Heyl 2000, Preissner 2001, Baek et al. 2002). With the timing of suction and discharge tied to the crankshaft angle, all expanders have built-in volume ratios. If the built-in (ideal) volume ratio does not match the volume ratio imposed on the expander by the boundary conditions (real volume ratio), the indicated efficiency decreases due to over- or under-expansion. The effect of over- and under-expansion is explained in Figure 5.
Oil
The presence of oil in the control volume is neglected, unless oil contributes significantly to refrigerant leakage (see \textit{Leak Flow} in Section 5.2.2). For the analysis of compressor and expander mechanisms in the report, only the rotary piston compressor was modeled with the effect of oil.

5.2 Modeling Approach
The algorithm is based on a discretization of the process into a number of time steps, following a control volume through the transient process from inlet to compression/expansion to discharge. At each time step, the irreversible processes of mass and heat flow are estimated. For each time step, a number of parallel control volumes can exist simultaneously. In a scroll compressor, for instance, two parallel control volumes are formed at the end of the suction process. These two control volumes are then compressed and finally merge into a single control volume at the center of the scroll.

The simulation of an expander starts at the intake process. At the beginning of the intake process, the crankshaft is at rotation angle zero. As the shaft turns, gas is flowing into the pocket and the crankshaft angle increases. At a specific angle, the pocket seals from the intake reservoir, and the gas is expanded. When the shaft reaches the discharge angle, the pocket opens to the low-pressure reservoir and the gas is expelled from the chamber. The crankshaft angle at which one cycle is completed depends on the type of expander. For a reciprocating piston expander, for instance, the process ends at crankshaft angle $2\pi$. For a rotary piston, the process ends at an angle of $4\pi$. For a scroll expander, the angle depends on the length of the wraps.

Figure 5: Effect of over- and under-expansion on indicated efficiency of expander
The process in a compressor is modeled as a reverse expansion process. The simulation starts with the suction process at the highest value of the crankshaft angle. As the suction pocket seals from the low-pressure reservoir and the gas is compressed and finally discharged, the value of the crankshaft angle decreases until it reaches zero when the cycle is completed.

5.2.1 Geometric Data

Geometric information about the device is required at each time step. These data are:

- Rotation angle of the crankshaft
- Control volume
- Projection of moving surfaces into x-, y-, and z-direction
- Position of moving surfaces with respect to coordinate system
- Leak paths: The data for the leak path contain topological information about the device, indicating the pockets adjacent to the control volume being followed
- Dimensions of each leak path

Additional information required:

- Device type
- Conversion factor of dimensions used to SI units
- Number of parallel control volumes
- Crankshaft angle at which discharge and suction port uncover
- Number of leak paths
- Type of each leak path

The geometric information is provided in an ASCII text file. For an expander, the tables are read from position 1 to end, for a compressor, the tables are read in reverse order. An example for a scroll device is offered in Appendix B.

5.2.2 Thermodynamic Simulation

Each time step is considered a sequence of two separate processes:

1. Isentropic change of volume at constant mass (process \(1 \rightarrow 2^*\))

\[
\begin{align*}
  s_2^* &= s_1 & \text{Equation 3} \\
  m_2^* &= m_1 & \text{Equation 4} \\
  \rho_2^* &= \frac{m_2^*}{V_2} & \text{Equation 5} \\
  u_2^* &= u(s_2^*, \rho_2^*) & \text{Equation 6}
\end{align*}
\]

2. Change of mass and internal energy due to mass and heat transfer at constant volume (process \(2^* \rightarrow 2\))
\[ m_2 = m_2^* + \sum m_{Valve} + \sum m_{Leak} \quad \text{Equation 7} \]
\[ U_2 = u_2^* \cdot m_2^* + \sum H_{Valve} + \sum H_{Leak} + \sum Q \quad \text{Equation 8} \]
\[ u_2 = \frac{U_2}{m_2} \quad \text{Equation 9} \]
\[ \rho_2 = \frac{m_2}{V_2} \quad \text{Equation 10} \]
\[ s_2 = s(u_2, \rho_2) \quad \text{Equation 11} \]

**Valve Flow**

The instantaneous mass flow rates through the valves are simulated as incompressible flow through an orifice.

(a) Single phase (White 1994)
\[ \dot{m}_{Valve}(t) = C_d \cdot A_{Valve} \cdot \sqrt{\frac{2\rho_{up} \Delta P}{1 - \beta^4}} \quad \text{Equation 12} \]
\[ C_d(t) = 0.5959 + 0.0312 \beta^{2.1} - 0.184 \beta^8 + \left(0.0029 \beta^{2.5}\right) \left(10^6 / Re(t)\right) \quad \text{Equation 13} \]
\[ \beta = 0.3 \quad \text{Equation 14} \]

(b) Two phase flow (Lin 1982)
\[ \dot{m}_{Valve}(t) = C_d(t) \cdot A_{Valve}(t) \cdot \sqrt{\frac{2\rho_{up}(t) \Delta P(t)}{(1 - \beta^4) + \sqrt{(1 - x_{up}) \Theta(t) + x_{up} \sqrt{\rho_L(t) / \rho_G(t)}}}} \quad \text{Equation 15} \]
\[ \Theta(t) = 1.48625 - 9.26541r_d(t) + 44.6954[r_d(t)]^2 - 60.615[r_d(t)]^3 - 5.12966[r_d(t)]^4 - 26.5743[r_d(t)]^5 \quad \text{Equation 16} \]

\( C_d \) and \( \beta \) as for single phase flow

The enthalpy flow rate through a valve is obtained by multiplying the mass flow rate with the upstream specific enthalpy. The valve flow is checked for choked flow by comparing the computed flow velocity against the speed of sound at the upstream conditions.

The effective flow area \( A_{Valve} \) is simply the cross sectional area of the port. Valve motion is not considered, clearly overestimating the valve performance. This simplification was made in order to obtain best-case results. Additional losses due to non-ideal valve motion can be simulated using smaller port diameters.
Heat Flow

The heat transfer in compressors has been studied by a number of researchers with contradicting results (Brok et al., 1980). Most research has focused on heat transfer in reciprocating piston compressors. Typically, the instantaneous heat flow rate is described by Newton’s approach

\[ \dot{Q}(t) = h(t) \cdot A(t) \cdot (T_{\text{wall}} - T(t)). \]  

Equation 17

The heat transfer coefficient \( h(t) \) is obtained from a function of the type

\[ Nu(t) = a \cdot [\text{Re}(t)]^b \cdot \text{Pr}^c. \]  

Equation 18

Various values for the coefficients and for the definition of the Reynolds number have been proposed. The effect of heat transfer on the performance of CO\(_2\) compressors and expanders is discussed in Section 6.3.

The temperature \( T_{\text{wall}} \) is the effective wall temperature of the control volume. In a realistic device, the wall temperature varies with location and time. In the simulation however, an average time-independent wall temperature is assumed. The effect of heat transfer on the performance of compressors and expanders in residential air-conditioning applications is discussed in Section 6.3.

Leak Flow

Although internal leakage has a significant effect on the performance of positive displacement compressors, little research has been undertaken to derive correlations for the instantaneous leakage mass flow rates that are dependent on geometry and driving pressure difference. In the open literature, isentropic compressible flow, adiabatic viscous compressible flow, and incompressible flow models are proposed (Fukuta et al., 2002). Most of the experimental research has been carried out on the leakage flow of air at room temperature and pressures below 1 MPa. Other researchers investigated leakage using conventional refrigerants (Ishii, 1996).

The instantaneous leak flow rates are computed assuming incompressible viscous flow and accounting for frictional losses and minor losses due to entrance and exit effects. The computed flow velocity is checked against the speed of sound and corrected for choked flow. In order to achieve a smooth transition from laminar to turbulent flow the leak flow rate is computed as

\[ \dot{m}_{\text{Leak}}(t) = \sqrt[20]{\left[ \dot{m}_{\text{Leak min ar}}(t) \right]^{20} + \left[ \dot{m}_{\text{Turbulent}}(t) \right]^{20}}, \]  

Equation 19

where

\[ \dot{m}_{\text{Leak min ar}}(t) = \frac{-4\mu wL}{k_m \delta} + \sqrt{\left(\frac{-4\mu wL}{k_m \delta}\right)^2 + \frac{\rho (w \delta)^2}{k_m} \Delta P} \]  

Equation 20
\[ m_{\text{Turbulent,Leak}}(t) = \sqrt{\frac{\rho (w \delta)^2}{0.01875 \cdot L/d + k_m}} \Delta P. \] \text{Equation 21}

The effective diameter is 2/3 of the hydraulic diameter (White 1994), the friction factor for turbulent flow is 0.075 (fully rough flow channel), and the coefficient for minor losses is 1.5, assuming a coefficient of 0.5 for the entrance losses and 1 for the exit losses.

There are two different types of leak paths in the compressors and expanders investigated: the tip leak and the flank leak. The tip leak is a flow passage of small height and large width. This type of leak is found, for example, in a scroll device between the top of the wall and the base plate of the other scroll or in a piston device between the piston and the cylinder wall. The flank leak is a flow passage between two curved walls and is found in a scroll device between two adjacent wraps or in a rotary piston machine between the roller and the cylinder wall. Preissner (2001) showed that the length of the flank leak path can be expressed as the curvature difference \( cd \)

\[ cd = 1/r - 1/R, \] \text{Equation 22}

where \( r \) and \( R \) are the radii of the channel wall with the greater and smaller curvature, respectively.

In some compressors (e.g. rotary piston), oil is used to improve sealing. In this case, refrigerant may leak from a high-pressure control volume to a low-pressure control volume via a so-called oil-leak. Refrigerant from the high-pressure pocket dissolves in oil and evaporates from the oil as the mixture enters the low-pressure pocket. In this case, the leakage mass flow rate of CO\(_2\) is estimated to be 10\% of the oil mass flow rate. The mass flow rate of oil is computed using Equation 19 through Equation 22 using a constant viscosity of 20 mPas (Hauk, Weidner, 2000), assuming a saturated PAG oil-CO\(_2\) mixture at 100°C and 10 MPa.

5.2.3 Solution Scheme
The simulation of the compression/expansion process consists of two problems:
(1) Numerical integration transient process from suction to discharge
(2) Numerical solution of the leakage flow rates to satisfy conservation of mass and energy

The numerical integration solves the problem

\[ f(t) = f_0 + \int y(f, t) dt, \] \text{Equation 23}

where \( f(t) \) is the mass or energy contained in the control volume, \( f_0 \) is an initial condition, \( y(f, t) \) is the mass or energy flow rate, and \( t \) is time. For the valve and heat flow rates, a fourth order Runge-Kutta method is used.
Using a step-by-step method, such as Runge-Kutta, for the leak flow rates may result in violation of conservation of mass or energy. The difference between the valve and heat flow and the leak flow is that the valve and heat flow only affects the control volume in question, while the leak flow also affects control volumes of previous or future time steps. This is especially apparent in devices with several pockets interacting with each other, for example in a scroll compressor. Shortly after a control volume has been formed in the suction process, it may be connected via a leak with a pocket closer to the center of the scroll and some amount of mass may leak to into the control volume, resulting in a pressure increase. After one rotation of the crankshaft, the control volume may be exactly at the point where the high-pressure pocket was. The control volume communicates now with a pocket closer to the perimeter of the scroll, which has a higher pressure than at the previous instance. Thus, the pressure difference and hence the mass flow rate is smaller. Consequently, the control volume and the low-pressure pocket contain more mass than there was before, resulting in a violation of the conservation of mass and energy, as well as in the destruction of entropy.

In order to avoid this type of problem, the leak flow rates are computed simultaneously for all time steps. Starting with an initial guess for the leak flow rates at all time steps (for instance, all flow rates are zero), the integration is carried out, producing a mass and internal energy profile in the device for the time interval from suction to discharge. Based on this pressure profile, the leak flow rates are computed. In order for the solution to represent the compressor/expander at steady operation, the pressure and enthalpy field must not change when the newly computed leak flow rates are reapplied. Conversely, the leak flow rates of two subsequent iterations must be equal. This means the leak flow rates must produce the same pressure and enthalpy field from which they were computed

\[
\dot{m}_{\text{Leak}} = F(\dot{m}_{\text{Leak}}) \quad \text{and} \quad \dot{H}_{\text{Leak}} = F(\dot{H}_{\text{Leak}}),
\]

Equation 24

where \( F \) is a system of equations consisting of **Equation 19** through **Equation 21** with the mass and energy field in the compressor/expander as variables. Mathematically, this can be interpreted as the flow rates being the eigenvector to the linear map \( F \). This means that the solution flow rates are fixed points to the system of equations \( F \). Following these observations, **Equation 24** is solved using a fixed-point iteration scheme

\[
\begin{align*}
\dot{m}_{\text{Leak}}^{j+1} &= F(\dot{m}_{\text{Leak}}^j) \\
\dot{H}_{\text{Leak}}^{j+1} &= F(\dot{H}_{\text{Leak}}^j)
\end{align*}
\]

Equation 25

Convergence is reached when

\[
|\dot{m}_{\text{Leak}}^j - \dot{m}_{\text{Leak}}^{j+1}| < \varepsilon, \quad \text{or} \quad |\dot{P}_j - \dot{P}_{j-1}| < \varepsilon
\]

Equation 26

where \( \dot{P} \) indicates the pressure field.
5.2.4 Step Size Adaptation

The error in the numerical integration depends strongly on the size of the time intervals. In order to reduce the error while keeping the computational time within limits, the step size is refined only where the error is large. The step size is reduced if the dependency of mass and internal energy on mass flow and heat transfer is strong

\[ \left| \frac{\partial f_j}{\partial y_j} \right| \Delta t_n > \epsilon , \]

Equation 27

where the criterion \( \epsilon \) can be determined by the user.

5.2.5 Boundary Conditions

The performance of a compressor or expander depends on the boundary conditions within which it operates. For the simulation developed in this project, the following boundary conditions are considered:

- Angular speed
- Pressure and density of the fresh suction gas, entering the suction reservoir from the evaporator (compressor simulation) or gas cooler (expander simulation)
- Pressure in the discharge reservoir
- Control volume wall temperature

Further parameters affecting the performance are:

- Leakage gap size (machining tolerances)
- Inlet and outlet port area
6 SIMULATION RESULTS

Section 6.1 defines the performance characteristics of compressors and expanders used in this report. With the boundary conditions (inlet pressure, inlet density, wall temperature) and the machining tolerance (leakage gap size) as independent variables, the compressor and expander performance is a function of four variables. If any of the variables can be neglected in the generation of performance maps, the computational time can be reduced significantly. In Sections 6.2 and 6.3, the superheat at the compressor inlet and the internal heat transfer in compressor and expander are demonstrated to produce an insignificant effect on the performance. Hence, the compressor inlet density and the wall temperature for compressor and expander can be neglected. In Section 6.4, the geometric design of possible candidates for compressors and expanders in residential CO2 air-conditioning systems is optimized. Section 6.5 discusses the results of the optimization.

By convention, an expansion process is modeled with increasing crankshaft angle from intake to discharge. A compression process is modeled with decreasing shaft angle from suction to discharge (see Section 5.2). All angles are given in radians.

6.1 Performance Characteristics

The indicated and volumetric efficiencies are used to characterize the performance of the analyzed compressors. The expanders are characterized by the indicated efficiency and the volumetric flow rate coefficient. Knowing the displacement volume and the boundary conditions (inlet state, discharge pressure, and possibly wall temperature), these parameters can be translated into the mass flow rate delivered and the work input or output. The indicated efficiency is defined as

\[
\eta_{\text{ind}} = \begin{cases} 
\frac{W_{\text{is}}}{W_{\text{real}}} = \frac{h(s_{\text{in}}, P_{\text{out}}) - h(s_{\text{in}}, P_{\text{in}})}{h(s_{\text{out}}, P_{\text{out}}) - h(s_{\text{in}}, P_{\text{in}})} & \text{Compressor} \\
\frac{W_{\text{real}}}{W_{\text{is}}} = \frac{h(s_{\text{in}}, P_{\text{out}}) - h(s_{\text{in}}, P_{\text{in}})}{h(s_{\text{out}}, P_{\text{out}}) - h(s_{\text{in}}, P_{\text{in}})} & \text{Expander} 
\end{cases}
\]

Equation 28

The volumetric efficiency \( \eta_{\text{vol}} \) and the volumetric flow rate coefficient \( \varepsilon_{\text{vol}} \) are defined as

\[
\eta_{\text{vol}} = \frac{m_{\text{real}}}{\rho_{\text{in}} \cdot V_{\text{displ}}} \quad \text{Compressor}
\]

\[
\varepsilon_{\text{vol}} = \frac{m_{\text{real}}}{\rho_{\text{in}} \cdot V_{\text{max}}} \quad \text{Expander}
\]

Equation 29

where \( V_{\text{displ}} \) is the compressor displacement volume and \( V_{\text{max}} \) is the maximum volume during the course of a control volume from inlet to outlet (e.g. the geometric cylinder volume in a piston expander or the volume of the two most outer pockets in a scroll expander). An ideal expander has a volumetric flow rate coefficient equal to the inverse
of its optimum volume ratio. This characterization parameter for the expander is chosen because it bases the inlet volume purely on the geometry of the device and eliminates any effect of the operating conditions on the definition of the suction volume. The volumetric flow rate coefficient can be understood as a dimensionless volume flow rate through the expander per revolution. In an expander, the direction of the flow though the expander is in the same direction as the pressure gradient, preventing the definition of a volumetric efficiency with the same significance as that of a compressor.

6.2 Effect of Inlet Density on CO₂ Compressor Performance

The effect of inlet density is studied on the example of a reciprocating piston compressor. The piston mechanism has losses due to internal leakage and valve losses. Internal heat transfer is not considered in this analysis. It is assumed that the results for the reciprocating piston can be transferred to other mechanisms.

Figure 6 shows the indicated and volumetric efficiency of a piston compressor over a range of values for the suction density at constant suction and discharge pressures. The range of the inlet density represents a degree of suction superheat from 0 K to 20 K. The indicated and volumetric efficiencies change by less than 2% over the range of super heat considered. Therefore, the effect of super heat on the compressor performance is neglected in the simulation.

The effect of inlet density on the performance of an expander cannot be neglected since it affects the volume ratio and hence the indicated efficiency.
6.3 Effect of Heat Transfer on CO₂ Compressor and Expander Performance

Heat transfer between the fluid contained in a control volume and the wall of the control volume depends on the surface area of the wall, wall and fluid temperatures, and the heat transfer coefficient between wall and fluid. The surface area is given by the geometry of the device. The wall temperature is given as a boundary condition, and the fluid temperature is solved for. The heat transfer coefficient depends on the fluid state and the fluid movement in the control volume. The fluid movement varies with time and depends strongly on the geometry of the control volume.

Compressor

Adair et al. (1972) proposed a correlation for the instantaneous heat transfer in a piston compressor, which is intended to reflect the effect of the transient velocity field in the pocket and yet does not require detailed flow simulations. In the correlation the Reynolds number $Re$ is based on the swirl velocity $\omega_s(t)$ in the pocket, which itself is a function of compressor angular velocity $\omega$ and the crankshaft angle $\varphi(t)$:

$$\omega_s(t) = \begin{cases} 2\omega[1.04 + \cos(2\varphi)] & \pi/2 < \varphi < 3\pi/2 \\ \omega[1.04 + \cos(2\varphi)] & \varphi < \pi/2 \text{ or } \varphi > 3\pi/2 \end{cases}$$

Equation 30

$$Re(t) = \frac{\rho(t)[D_e(t)]^2 \omega_s(t)}{2\mu(t)}$$

Equation 31

$$D_e(t) = \frac{6 \cdot Volume(t)}{Area} = \frac{3/2 D \cdot S(t)}{S(t) + D/2}$$

Equation 32

with $S(t)$ the stroke length, $D$ the piston diameter, and $\rho$ the fluid density. The heat transfer coefficient is then obtained from the Nusselt number given by

$$Nu(t) = 0.053[Re(t)]^{0.8}[Pr(t)]^{0.6}$$

Equation 33

$$Nu(t) = \frac{h(t)D_e(t)}{k(t)}$$

Equation 34

The correlation was used to study the effect of heat transfer on the performance of CO₂ piston compressor. Figure 7 is a plot of the Nusselt number for CO₂ at different angular velocities. The plot shows one complete piston stroke from top dead center at $2\pi$ over bottom dead center at $\pi$ and back to top dead center at $0$. The points of discontinuity at angles of $\pi/2$ and $3\pi/2$ are due to the discontinuous function for the swirl velocity (see Equation 30). The swirl velocity undergoes a sudden change when the piston movement changes from acceleration to deceleration.
Figure 7: Instantaneous heat transfer coefficient in piston compressor

Figure 8 and Figure 9 show the isentropic and volumetric efficiency ratios versus the pocket wall temperature for different values of the angular speed. The efficiency ratio is the ratio of the efficiency with heat transfer compared to the appropriate efficiency without heat transfer. The adiabatic operating points designate the wall temperatures at which the sum heat transfer into and out of the fluid is zero (~23°C for all angular speeds). The graphs show that the change in efficiency is less than 1% in the significant range of operating conditions.

Figure 8: Isentropic efficiency versus piston compressor wall temperature
The small effect of internal heat transfer is due to the short time interval that the gas is in contact with the compressor wall and to the reversal of the direction of the heat transfer during the compression.

In order to support the assumption that internal heat transfer in a compressor for the current application is insignificant, the effect of heat transfer in a scroll compressor is investigated. Research on the gas to wall heat transfer in scroll compressors could not be found in the open literature. Therefore, an approach for turbulent pipe flow is used. The heat transfer coefficient is given by a Nusselt number relationship

$$Nu_{turb} = 0.023 \cdot Re^{4/5} \cdot Pr^{2/5}$$  \hspace{1cm} \text{Equation 35}

where the Reynolds number is based on the rate of volume change in the device

$$Re = \left( \frac{\left[ V_{prev} / V \right]^{1/3} - 1}{\Delta t} \right) \left( \frac{3V}{4\pi} \right)^{2/3} \frac{\rho}{\mu}.$$  \hspace{1cm} \text{Equation 36}

Figure 10 shows the instantaneous Nusselt number in a scroll compressor. The plot follows a compression chamber from the position where the pocket is just sealed from the suction reservoir at approximately 10.5 rad to complete discharge with pocket volume equal to zero at crankshaft angle 0. With increasing pocket pressure and density, the Nusselt number increases. As the two pockets merge at $2\pi$, the pocket volume increases suddenly, resulting in an increase of the Nusselt number. During most of the discharge process ($2\pi$ to 0), the Nusselt number is approximately constant, reflecting the constant fluid properties during this process. At the end of the discharge process, the rate of change of the pocket volume decreases, resulting in a decreasing Nusselt number.
Figure 10: Instantaneous heat transfer coefficient in scroll compressor

Figure 11 is a plot of the instantaneous heat flow rate in the scroll compressor over a range of wall temperatures between 5°C and 100°C. The effect on the compressor performance is shown in Figure 12.

Figure 11: Instantaneous heat flow rate in scroll compressor
The plot shows that the compressor performance is affected by less than 1% over the range of wall temperatures considered. Hence, it seems safe to neglect internal heat transfer in the simulation of scroll compressors. These results support the conclusion that internal heat transfer in compressors can be neglected for residential CO₂ air-conditioning applications.

**Expander**

Little attention has been paid in the literature to internal heat transfer in positive displacement expanders. In the absence of experimental correlations for the heat transfer coefficient, modified correlations for the heat transfer coefficient in compressors are used. In addition to convection, the heat transfer in expanders is enhanced by evaporation of liquid refrigerant at the wall of the pocket. In turbulent pipe flow, the heat transfer coefficient is typically increased by a factor of five in the presence of evaporation. Therefore, the heat transfer coefficients obtained with Equation 33 are multiplied by five for expander simulations.

Figure 13 shows a plot of the instantaneous heat transfer coefficient in a piston expander, obtained using Equation 30 through Equation 34 versus the crankshaft angle. The expansion proceeds from angle $\theta$ to $2\pi$. 
The sudden increase of the heat transfer coefficient at crankshaft angle 1.25 is due to the change of fluid properties as the fluid enters the two-phase region. Figure 14 shows the heat transfer between fluid and wall for wall temperatures between 5°C and 110°C. The wall temperature at which the net heat transfer is equal to zero, approximately 30°C, represents the boundary condition for adiabatic operation.

The performance of the expander is shown in Figure 15. The volumetric and isentropic efficiencies are approximately constant for all wall temperatures considered (the isentropic efficiency changes with expander speed due to valve losses). This implies that the effect of internal heat transfer on the performance of a piston expander is negligible.
Figure 15: Piston expander performance versus wall temperature

Figure 16 shows the instantaneous Nusselt number in a scroll expander and the pressure in the expander pocket. At a crankshaft angle of approximately 6.3, the refrigerant enters the two-phase region and evaporation occurs, causing a sharp peak in the heat transfer coefficient due to changes in the fluid properties.

Figure 16: Instantaneous heat transfer coefficient in scroll expander

Figure 17 shows the instantaneous heat flow rates in the scroll expander. Comparing Figure 17 with Figure 11 shows that the flow rates in the expander have increased significantly. The adiabatic operating point of the expander is found where the net heat flow rate between the refrigerant and wall is zero. The device operates adiabatically at a wall temperature of approximately 25°C.
Figure 17: Instantaneous heat flow rate in scroll expander

Figure 18 shows the effect of heat transfer on the expander performance over a range of wall temperatures. The expander efficiency changes by up to 20%.

Figure 18: Volumetric and isentropic efficiency in scroll expander with heat transfer

Figure 19 compares the efficiency of the expander including heat transfer to the efficiency with no heat transfer between the wall and refrigerant. It is found that heat transfer affects the performance at adiabatic operating conditions (zero net heat transfer) by less than 3%.
If compressor and expander are combined in an integrated device, the two components are coupled through internal heat transfer. Assuming an insignificant heat resistance between compressor and expander, such that the temperature of the expander wall is equal to the wall temperature of the compressor, the integrated device operates adiabatically if the net heat transfer between expander and compressor is zero, according to

\[ \dot{Q}_{\text{Compressor}} = -\dot{Q}_{\text{Expander}} \quad \text{and} \quad T_{\text{Compressor}}^{\text{Wall}} = T_{\text{Expander}}^{\text{Wall}}. \]

Figure 20 shows the heat flow rates of the compressor and the negative flow rate in the expander. The adiabatic operating point of the integrated device is found where the two curves intersect. The process is dominated by the heat transfer of the expander due to the high heat transfer coefficient during evaporation. The adiabatic operating point of the integrated device is close to that of the expander alone. Therefore, the performance is not strongly affected by internal heat transfer (Figure 12 and Figure 19).

Considering the uncertainty in the correlation for the heat transfer coefficient and the small effect of heat transfer on the performance, it seems justified to neglect heat transfer in the simulation of scroll compressors and expanders.
Figure 20: Heat flow rates in integrated scroll compressor-expander device

Thus far only heat transfer between the fluid and the pocket wall has been considered. However, a fluid also exchanges heat inside the compressor/expander before entering the compression/expansion compartment. This process is referred to as suction heating. The fluid in the suction reservoir is at suction pressure and close to suction temperature. The fluid heats up when it is in thermal contact with the reservoir wall. Suction heating reduces isentropic and volumetric efficiency. Since the direction of the heat transfer is never reversed in this process (as it is in internal heat transfer), the effect on performance is greater than the effect of internal heat transfer. The heat transfer coefficient for suction heating is obtained from a correlation for heat transfer in circular tube with turbulent flow. Caillat et al. (1988) and Lee and Kim (2001) used this method for the simulation of scroll compressors and found good agreement with experimental results.

6.4 Optimization of Compressor and Expander Geometry for Residential Air-Conditioning Applications

The performance of the following compressor and expander mechanisms has been analyzed:
- Reciprocating piston
- Rotary piston
- Scroll

In order to make a fair comparison, the geometry of each individual mechanism has been optimized for use as compressor and expander under constant boundary conditions. The

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1 During the project meeting in January 2002, it was agreed to not consider the option of an expander based on the gear pump mechanism due to the limited indicated efficiency of the constant pressure expansion.
boundary conditions are given in Table 4. The values are chosen for a 10 kW CO₂ expander cycle at AHRAE A conditions with an assumed compressor and expander isentropic efficiency of approximately 75%. The approach temperature in the gas cooler is on the order of 3 K and the evaporating temperature is approximately 7°C. The cycle does not include an SLHX. The valve timing of the devices, which have a built-in volume ratio (all expanders and the scroll compressors), has been optimized for the individual operating conditions.

Table 4: Boundary conditions for compressor and expander optimization

<table>
<thead>
<tr>
<th></th>
<th>Compressor</th>
<th>Expander</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{\text{inlet}}$ [MPa]</td>
<td>4.126</td>
<td>8.563</td>
</tr>
<tr>
<td>$\rho_{\text{inlet}}$ [kg/m³]</td>
<td>120.2</td>
<td>524.2</td>
</tr>
<tr>
<td>$P_{\text{outlet}}$ [MPa]</td>
<td>8.676</td>
<td>4.174</td>
</tr>
<tr>
<td>Heat transfer</td>
<td>neglected</td>
<td>neglected</td>
</tr>
</tbody>
</table>

The compressor displacement volume is 18.46 cm³; the expander displacement volume is 7.93 cm³ at 3300 RPM for both devices.

The individual optimization is reported in Sections 6.4.1 to 6.4.3. The optimum designs of all mechanisms are compared in Section 6.4.4.

6.4.1 Reciprocating Piston

The reciprocating piston compressor and expander are assumed to each have two cylinders. The clearance volume is approximated by a distance between the piston and cylinder head of 1 mm at TDC. Given a fixed displacement volume, the geometry of a cylinder is a function of one variable, for instance the ratio of cylinder height to diameter. In addition to the aspect ratio of the cylinder, the performance is also affected by the cross sectional area of the inlet and outlet ports. It is assumed that a given fraction of the bore area is available as valve area. The area of the valve connecting to the high-pressure reservoir is 2/3 of the area of the low-pressure valve.

Sealing is provided by piston rings. The flow resistance of the piston rings is assumed equivalent to a flow passage of 3 mm length and 10 µm height per unit width. The shell pressure in both the compressor and expander simulation is the low-side pressure.

Compressor

Figure 21 shows the indicated and volumetric efficiency of a reciprocating piston compressor over a range of aspect ratios. The graphs show the effect of valve area on the performance. The indicated efficiency increases sharply from small aspect ratios, undergoes a maximum at aspect ratios on the order of 0.5 and reduces slowly at ratios greater than 0.5 to 1. This curve reflects the effects of leakage and valve losses on performance. At small aspect ratios, the area available for valves is small, so that the process is dominated by valve losses. As the bore area increases, the valve losses become
less important, but the sealing length around the piston increases, resulting in higher leak flow rates.

![Graph showing indicated efficiency and volumetric efficiency for different port areas.](image)

Figure 21: Performance of reciprocating piston compressor

In a realistic machine, the effective port area is probably in the range of 50% of the bore area. For this design, the optimum aspect ratio is in the order of 1. The resulting indicated efficiency is approximately 91% and the volumetric efficiency 84%. The bore and stroke of each cylinder are approximately 2.3 cm.
Expander

Figure 21 shows the indicated efficiency of a reciprocating piston over a range of aspect ratios. The graphs show the effect of valve area on the performance. The volumetric efficiency is not shown because it cannot be used to characterize the performance.

![Graph of indicated efficiency vs aspect ratio for different valve areas.]

Figure 22: Performance of reciprocating piston expander

Assuming a port area in a realistic expander in the order of 50% of the bore area, the optimum aspect ratio is approximately 1. The resulting indicated efficiency is approximately 88%. The bore and stroke of each cylinder are approximately 1.7 cm.

6.4.2 Rotary Piston

With a given displacement volume and assuming a constant vane thickness of 4 mm, the design of a rotary piston device is a function of two independent variables. The displacement volume can be expressed in terms of the ratio of cylinder height to cylinder diameter and of cylinder diameter to piston diameter. In the simulations, the gap height of the leak between piston and vane is 3 µm. The leakage gap height between roller and cylinder side and between roller and cylinder end plates is 10 µm. It is assumed that the inlet and outlet ports can be designed large enough that valve losses can be neglected. The diameters of both ports were set to 12 mm. The clearance volumes introduced by the ports are estimated as half the volume of a cone with cylindrical cross section. The diameter of the cross sections and the heights of the cones are given by the diameter of the ports. The fluid trapped in the clearance volumes is assumed to undergo sudden expansion or compression when the clearance volume opens to the control volume. The shell pressure of the compressor is set to the pressure in the discharge reservoir. The leakage mechanism is via oil (see Section 5.2.2). The shell pressure in the expander is the discharge (low-side) pressure of the expander. The leakage mechanism is refrigerant leakage.
Compressor

The indicated and volumetric efficiencies of a range of design for rotary piston compressors are shown in Figure 23. The maximum performance is found for a ratio of cylinder height to diameter of 0.4 and for the ratio of piston diameter to cylinder diameter as small as possible. The theoretical limit for this ratio is 0.5. However, in a realistic machine, the oscillating motion of the vane is often a limiting factor, so that the piston diameter should not be smaller than 70% of the cylinder diameter (following the design of existing rotary piston compressors for conventional refrigerants). With this limitation, optimum ratio of cylinder height to cylinder diameter is approximately 0.5. The indicated and volumetric efficiency of this design is approximately 90% and 92%.

Figure 23: Performance of rotary piston compressor

The optimum cylinder diameter and height are approximately 4.9 cm and 1.9 cm, respectively. The piston diameter is approximately 3.4 cm.
**Expander**

The indicated efficiency of a rotary piston expander is shown in Figure 24 for a range of possible designs. The maximum performance is found at a ratio cylinder height to cylinder diameter of 0.3 and at a ratio cylinder diameter to piston diameter as small as possible. Choosing a minimum for the piston diameter of 70% of the cylinder diameter, the maximum indicated efficiency is approximately 87%. The resulting cylinder diameter and height are approximately 4.0 cm and 1.2 cm, respectively. The piston diameter is approximately 2.8 cm.

![Figure 24: Performance of rotary piston expander](image)

**6.4.3 Scroll**

The geometry of a scroll device is more complex than that of the piston devices discussed above. The milling tool method developed at CEEE (Lindsay and Radermacher 2000) allows an efficient and flexible description of the scroll geometry. The geometry is defined by the path of a circular milling tool through a block of material. The two scroll wraps are formed by the material remaining after the tool has moved from the side of the block to the center and outwards again (Figure 25 (a)). For simplification, the path of the milling tool is limited to an involute, and the tips of the scroll wraps are circular arcs in this project (Figure 25 (b)). The path of the milling tool at the center of the scroll is a straight line and the path outwards from the center is symmetrical to the first half of the path.

![Figure 25: Scroll geometry](image)
The scroll design is constrained by a given displacement volume and a given built-in volume ratio (for the compressor a minimum volume ratio is applied to avoid over-compression). The ratio of wall height to wall thickness should not exceed a value of 3.5 for material strength reasons (Preissner 2001) and the ratio of wall height and gap between two walls should be smaller than 2 in order to avoid deflection of the milling tool during machining. It is assumed that inlet and outlet ports can be designed large enough so that valve losses are insignificant. The leakage gap height for flank and tip leak was set to 10 µm.

With these limitations, the geometry of the scroll is a function of 6 variables with 4 constraints, for instance:

- Wall thickness
- Wall height
- Orbiting radius
- Tip radius
- Location of tip center
- String length of involute

Two constraints are equality constraints (displacement volume and volume ratio). The wall height and the length of the string of the involute are used to satisfy these constraints. The other two constraints are inequality constraints. A simple gradient search method is used to locate optimum designs. Starting from an initial design, the gradient of the performance as a function of the four independent variables is approximated. The method follows the direction of this gradient until either the performance decreases or a constraint is violated. If the performance decreases, a new gradient is approximated. If a constraint is violated, the method searches along this constraint in the direction of increasing performance. It is not guaranteed that this method finds a global maximum; therefore, the optimum design found may represent a local maximum.

It is assumed for both the compressor and expander simulation that suction and discharge are constant pressure processes. The shell pressure for both devices is the low-side pressure. The leakage mechanism is pure refrigerant leakage.

Table 5 lists the parameter of the optimum compressor and expander design. The indicated and volumetric efficiencies of the scroll compressor are 64% and 65%,
respectively. The indicated efficiency of the scroll expander is 75%. Figure 26 shows the shape of the wraps for optimum compressor and expander designs.

Table 5: Parameters of optimum scroll compressor and expander design

<table>
<thead>
<tr>
<th></th>
<th>Displacement volume [cm³]</th>
<th>Volume ratio</th>
<th>Wall thickness [mm]</th>
<th>Wall height [mm]</th>
<th>Orbiting radius [mm]</th>
<th>Tip x-coordinate [mm]</th>
<th>Tip radius [mm]</th>
<th>Overall diameter [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compressor</td>
<td>18.46</td>
<td>1.91</td>
<td>3.87</td>
<td>14.1</td>
<td>4312</td>
<td>5.2</td>
<td>3.83</td>
<td>82.5</td>
</tr>
<tr>
<td>Expander</td>
<td>7.3</td>
<td>2.42</td>
<td>2.7</td>
<td>9.3</td>
<td>2</td>
<td>-7.5</td>
<td>4.5</td>
<td>86.6</td>
</tr>
</tbody>
</table>

The performance of the expander is significantly better than the performance of the compressor. The reason is that the expander has a higher volume ratio, resulting in a longer wrap and more chambers in the scroll. Consequently, the pressure differences between chambers communicating through leaks, and hence the leak flow rates, are smaller.

6.4.4 Comparison

The performance of the compressors and expanders over the pressure ratio is shown in Figure 27 to Figure 29. The leakage gap size for all devices is 10 μm. The boundary conditions (pressures and inlet densities) are in the range of expected values for an optimized expander cycle operating at ambient conditions from 32°C to 55°C. The cycle was simulated using constant values for the expander and compressor efficiencies. The built-in volume ratios of the expanders are not adjusted for the pressure ratio.

---

2 The y-coordinate is determined by the milling tool method when reflecting the path of the tool at the center of the scroll.
Figure 27: Compressor indicated efficiency vs. pressure ratio (leakage gap 10 µm)

Figure 28: Compressor volumetric efficiency vs. pressure ratio (leakage gap 10 µm)
As found in the previous section, the scroll compressor performs significantly worse than the other mechanisms if no additional tip seal is used. Up to a pressure ratio of approximately 2.5, all compressors (except the scroll) have a similar performance. Above pressure ratios of 2.5, the performance of the rotary piston compressor falls behind that of the reciprocating. The reciprocating and rotary piston expanders perform similarly for all pressure ratios considered. The scroll expander performs 15% to 20% worse than the other expander mechanisms.

The performance of the devices has been evaluated for a range of machining tolerances. The results are shown in Table 6 and Table 7 and are plotted in Figure 30 through Figure 32. The reciprocating piston and rotary piston mechanisms perform similarly at all leakage gap sizes in the compressor and expander applications with the performance of the reciprocating piston dropping more with leakage gap size. The performance of the scroll compressor and expander drops sharply as the leakage gap size increases due to the large sealing length across the tip of the scroll wraps. For almost all conditions, the scroll performs worse than the other mechanisms analyzed. Only at very tight machining tolerances does the scroll expander perform better than the reciprocating piston expander.

Table 6: Compressor indicated and volumetric efficiency vs. leakage gap size

<table>
<thead>
<tr>
<th>Leakage Gap Size</th>
<th>5 µm</th>
<th>10 µm</th>
<th>15 µm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\eta_{\text{ind}}$</td>
<td>$\eta_{\text{vol}}$</td>
<td>$\eta_{\text{ind}}$</td>
</tr>
<tr>
<td>Recip piston</td>
<td>0.93</td>
<td>0.88</td>
<td>0.91</td>
</tr>
<tr>
<td>Rotary piston</td>
<td>0.96</td>
<td>0.96</td>
<td>0.90</td>
</tr>
<tr>
<td>Scroll</td>
<td>0.87</td>
<td>0.88</td>
<td>0.64</td>
</tr>
</tbody>
</table>
Table 7: Expander indicated efficiency vs. leakage gap size

<table>
<thead>
<tr>
<th></th>
<th>5 µm</th>
<th>10 µm</th>
<th>15 µm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Recip piston</td>
<td>0.90</td>
<td>0.87</td>
<td>0.81</td>
</tr>
<tr>
<td>Rotary piston</td>
<td>0.94</td>
<td>0.84</td>
<td>0.78</td>
</tr>
<tr>
<td>Scroll</td>
<td>0.93</td>
<td>0.75</td>
<td>0.47</td>
</tr>
</tbody>
</table>

Figure 30: Compressor indicated efficiency vs. leakage gap size

Figure 31: Compressor volumetric efficiency vs. leakage gap size
6.5 Discussion

The low performance of the scroll compressor and expander at higher leakage gap sizes implies a strong disadvantage of this mechanism compared to the others. This strong disadvantage is not found in scroll compressors for conventional refrigerants, due to smaller pressure differences compared to CO₂ and good sealing methods available. In order to fully explore the potential of the scroll mechanism as compressor and expander in a CO₂ system, accurate data about the effective leakage gap size as well as experimental investigations are necessary.

When analyzing the results of the expander optimization, it must be considered that all devices were simulated with ideal valve actuation. The assumption is not critical for the scroll expander, because opening and closing of the ports in these devices is purely dependent on the crankshaft angle. In the reciprocating and rotary piston expander however, the expansion compartment is permanently connected to the inlet and/or outlet port. Therefore, the timing of the port openings must be controlled externally.

For the reciprocating piston, both the inlet and the outlet port must be controlled. Heyl (2000) used valves actuated by pressurized air and Beak et al. (2002) used solenoid valves in CO₂ reciprocating piston expanders. In both of these projects, the expander speed was limited to approximately 60 RPM due to valve timing. Heideleck and Kruse (2000) investigated rotating disc with slots as control mechanisms, borrowed from hydraulics applications. It has the advantage of the valve control depending only on the shaft speed and not on external means. Heideleck and Kruse report that a first prototype showed problems with leakage through the valves.
For the rotary piston expander, only the inlet port needs to be controlled. When operated at the same shaft speed, the inlet port of a rotary piston expander is open twice as long as the port of a reciprocating piston expander, potentially reducing the problems with externally controlled valves. It may also be possible to adopt the concept of a rotating disc as valve control for the rotary piston expander.

The small variation of the expander indicated efficiency over the pressure ratio (Figure 29) indicates that it may not be necessary to adjust the built-in volume ratio to the operating conditions over the range considered here. The volume ratio over the range of ambient conditions between 32°C and 55°C changes from approximately 2.3 to 2.9. The performance degradation for a volume ratio mismatch on the order of 25% can be estimated from Figure 5. The indicated efficiency drops by approximately 5%.

The gas trapped in the clearance of the reciprocating and rotary piston compressors undergoes re-expansion until the pocket pressure is close to the pressure in the suction line. In the reciprocating and rotary piston expanders however, the inlet valve opens when the pocket volume begins to increase. The gas in the clearance volume is at low pressure and low density. The incoming gas is high-pressure, high-density gas. In the first instants after the inlet valve opens, the suction gas undergoes sudden, irreversible expansion until the pressure level in the pocket reaches the pressure in the high-pressure line. This process introduces additional losses in the expansion process in the piston devices. It is theoretically possible to eliminate these losses with accurate valve timing.

The inlet and outlet ports of the scroll compressor uncover at specific angles of the crankshaft without need of external actuators. However, without additional control, a scroll expander operates with constant volume ratio, which does not necessarily match the optimum volume ratio imposed by the boundary conditions. The volume ratio of a scroll compressor is usually adjusted by a reed valve after the discharge port, so that the center pocket of the scroll opens to the discharge reservoir only when the pocket pressure has reached the reservoir pressure. In a scroll expander, the port at the center of the scroll is the inlet port. The use of a reed valve for the timing of the port is not possible. An external control is necessary to adjust the built-in volume ratio to the operating conditions.

The built-in volume ratio in screw compressors can be adjusted by a slide vane controlling the axial discharge port (variable Vi, Shaw 1988). It may be possible to use a similar mechanism for the slide valve in a scroll compressor. The technology for the actuation of the valve is already developed. Nippon Soken and Denso (1997) developed a control valve for a CO₂ cycle with isenthalpic expansion valve, which adjusts the high-side pressure to the optimum value depending on the operating conditions. This valve does not require an external control.

While the low volumetric efficiency of the reciprocating piston compressor is due to the large clearance volume in this device, the low volumetric efficiency of the scroll compressor is due to leakage and indicates real losses. Comparing the results of the scroll
compressor and expander indicates that the compressor performance may be improved by using a design with longer wraps to reduce driving pressure differences across the leaks. However, this option was not found in the optimization of the compressor. The optimization algorithm moved the design more in the direction of short wraps and high wall thickness. This means leakage in the compressor can best be reduced by increasing the flow resistance in the leaks (rather than reducing the driving force as in the expander). Therefore, it may be advantageous to deviate from the involute design to more advanced geometries, for example the two-turn scroll presented by Lindsay and Radermacher (2000).

The effect of friction has not been included in these simulations. The losses due to friction depend on the mechanisms as well as the specific design within each mechanism. More detailed simulation is necessary in order predict the performance of a compressor or expander including the effect of friction.

The first experimental results of the performance of a semi-hermetic reciprocating piston CO₂ compressor indicate that the isentropic efficiency is approximately 15% lower than the indicated efficiency (Neksa et al.1999). To obtain an approximation for the isentropic efficiency of other compressor types and expanders, it is assumed that all devices dissipate a constant amount of energy through friction and other losses. Using the published data for the semi-hermetic CO₂ compressor as a baseline, the work dissipated in the devices is determined such that the isentropic efficiencies of the reciprocating type devices with a leakage gap size of 10µm is 15% below the respective indicated efficiencies at the relevant operating conditions. The isentropic efficiencies for the compressor and expander, respectively, can then be written as:

\[
\eta_{is} = \frac{W_{is}^{Comp}}{W_{is}^{Comp} + x_{Comp} \cdot W_{is}^{Comp}} \quad \text{Compressor}
\]

\[
\eta_{is} = \frac{W_{is}^{Exp} - x_{Exp} \cdot W_{is}^{Exp}}{W_{ind}^{Exp}} \quad \text{Expander}
\]

Equation 37

where \(x_{Comp}\) and \(x_{Exp}\) are fractions of the isentropic work of the compressor and expander, respectively, which are adjusted to achieve the desired results. Table 10 and
Table 11 lists the values of the isentropic efficiencies for the different compressor and expander types at the range of leakage gap sizes considered.

Table 8: Compressor isentropic efficiency vs. leakage gap size

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<th></th>
<th>5 µm</th>
<th>10 µm</th>
<th>15 µm</th>
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<tbody>
<tr>
<td>Recip piston</td>
<td>0.77</td>
<td>0.76</td>
<td>0.72</td>
</tr>
<tr>
<td>Rotary piston</td>
<td>0.79</td>
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<tr>
<td>Scroll</td>
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<td>0.56</td>
<td>0.36</td>
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Table 9: Expander isentropic efficiency vs. leakage gap size

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<th>15 µm</th>
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</thead>
<tbody>
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<td>0.75</td>
<td>0.72</td>
<td>0.66</td>
</tr>
<tr>
<td>Rotary piston</td>
<td>0.79</td>
<td>0.69</td>
<td>0.63</td>
</tr>
<tr>
<td>Scroll</td>
<td>0.78</td>
<td>0.60</td>
<td>0.32</td>
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</table>
7 INTEGRATION CONCEPTS

To minimize energy conversion losses the expander work should be directly utilized as mechanical work input to the compressor. The integration of the expander work in the cycle reduces the need for energy storage because the energy supply from the expander always coincides with the energy demand from the compressor. In order to reduce coupling and gear losses, the compressor and expander should be connected through a common shaft (Figure 33).

Figure 33: System with integrated compressor–expander

The concept of direct mechanical coupling is generally possible with all the displacement mechanisms analyzed in this report. Heyl (2000) has demonstrated this concept for a reciprocating piston compressor–expander and Smith et al. (1995) for an integrated screw device (Expressor) (CITY 2002).

With the expander coupled directly to the compressor shaft, the control of the high-side pressure requires special attention. Different from sub-critical cycles, the transcritical cycle with CO₂ as refrigerant has an optimum high-side pressure at which the COP reaches a maximum at given ambient conditions. In a CO₂ cycle with an isenthalpic expansion valve, the optimum high-side pressure is adjusted by the expansion valve setting. In a cycle with an expander, the high-side pressure can be optimized by adjusting the mass flow rate through the expander (assuming constant compressor speed and displacement volume). The expander mass flow rate can be varied by the expander speed or displacement volume. In a cycle with an integrated compressor–expander, the expander speed cannot be adjusted independently of the compressor speed. This means in a system with integrated compressor–expander (Figure 33), the expander mass flow rate can only be modified with a variable expander displacement volume. Another option is to introduce an additional expansion valve into the cycle, which can be operated independently from the compressor and expander.

Figure 34 shows block diagrams of possible circuitries, which can control the high-side pressure independently from the compressor shaft speed.
Figure 34: Circuitry options for high-side pressure control in expander systems

Option (a) in is a system with independent compressor and expander speeds. In options (b) and (c), the high-side pressure may be adjusted by increasing the total flow resistance across the expansion section by introducing an additional, adjustable pressure drop. Option (c) adjusts the flow resistance across the expansion section by introducing an adjustable bypass to the expander. In options (e) and (f), the compression is divided into two sections. The expander speed is determined by the operating conditions. The low-stage compressor (e) or the high-stage compressor (f) is independent of the expander speed. Option (f) is patented by Sanden and has been investigated experimentally by Heyl and Quack (2000). The expander used therein had an isentropic efficiency of 51% and the system COP was improved by 30% compared to the two-stage system without expander. Due to problems with valve operation, the expander was operated with a full-pressure stroke, and only the flow work of the process was utilized. Option (f) offers the possibility of placing the expander and the low-stage compressor close to the evaporator inlet, so that the heat transfer to the refrigerant in the liquid line is minimized, resulting in higher capacity. With the first compression stage close to the evaporator outlet, the heat transfer to the refrigerant can be reduced, minimizing the suction heating to the high-stage compressor and reducing the discharge temperature. A lower discharge temperature reduces the compressor work and the heat load that must be rejected in the gas cooler.
7.1 Performance Analysis

The circuitries (a) to (f) in Figure 34 have been analyzed assuming the following simplifications:

- Constant volumetric and isentropic efficiency of compressor and expander
- Constant UA value for heat exchangers
- Saturated vapor at evaporator outlet
- Energy balance, mass balance, and heat transfer determine high-side and low-side pressure

For each circuitry or option, the appropriate control parameter was varied in order to investigate its feasibility to control the high-side pressure.

Figure 35 shows results of the simulation of option (a), expander speed independent from compressor speed. The P-h diagram (B) shows three cycles with different expander speeds. This option allows adjusting the high-side pressure. The COP undergoes a maximum as the expander speed varies (C).

Figure 35: High-side pressure control with independent expander speed

Figure 36 shows the results for option (b), adjustable expansion valve upstream of expander. The P-h diagram (B) shows the cycle without expansion valve (solid) and with expansion valve (dashed). The flow restriction of the expansion valve has almost no effect on the high-side pressure. The plot (C) shows the performance of the system and the performance of the system with independent compressor and expander. The system for option (b) is designed such that the high-side pressure is approximately 1000 kPa below the optimum pressure with the expansion valve fully open. As the expansion valve opening is reduced, the high-side pressure is expected to increase. However, the graphs show that the pressure changes insignificantly. The COP does not reach a maximum, but decreases constantly as the flow restriction is increased. This means that option (b) cannot be used to control the system.
Figure 36: High-side pressure control with expansion valve before expander.

Figure 37 shows the results for option (c). The findings are similar to the ones for option (b). The expansion valve opening has no distinguishable effect on the high-side pressure (plot B) and the COP cannot be optimized (plot C). Thus, circuitry (c) is not a viable option for controlling the system.

Figure 38 shows the results for circuitry (d). The by-pass to the expander allows only reducing the high-side pressure. The system is designed such that high-side pressure is approximately 3000 kPa above the optimum pressure when the by-pass is closed. As the expansion valve is opened, the high-side pressure decreases (plot B) and the COP undergoes a maximum (plot C). However, the maximum found with this circuitry is significantly below the performance found with compressor and expander operated independently. Thus, this circuitry cannot be considered an appropriate option for the system control.

The by-pass to the expander can be interpreted as controlled internal leakage in the device. Revisiting the results of the simulation implies that there is an “optimum” leak...
flow rate (greater than zero) for the expander if the compressor and expander speeds are coupled and the system operates off the optimum expander speed. The expansion valves before and after the expander can be interpreted as adjustable valve losses at the expander inlet and outlet. Accordingly, the results make sense, since the performance is expected to drop as the valve losses increase.

The results of the analysis show that the expander speed is the only acceptable control variable in the expander systems considered. **Figure 39** shows the performance of the system with independent expander speed versus high-side pressure and versus the expander speed for a range of gas cooler air temperatures.

![Figure 39: (a) COP vs. high-side pressure and (b) vs. expander speed](image)

For all air temperatures considered, the maximum COP occurs at the same expander speed. Since the compressor speed was kept constant, this result implies that the optimum ratio of compressor speed to expander speed is constant over the range of operating conditions considered (gas cooler air inlet temperature 35°C to 55°C, evaporator air inlet temperature 27°C at 50 relative humidity). Hence, the displacement volumes of the devices can be designed such that the ratio of speeds is equal to unity and the compressor and expander can be operated with the same speed.

**Figure 40** shows the system performance for various values of the compressor speed for a range of gas cooler air temperatures. The graphs show that the system can be operated close to the maximum COP for all operating conditions considered with a constant ratio of compressor speed to expander speed, if the ratio is chosen appropriately. The lines for constant ratio of compressor RPM to expander RPM indicate the same ratio in all graphs. The COP is within 3% of the maximum COP at the respective operating point. This means that it may be possible to design the system such that no additional control for the high-side pressure is necessary even if the speed of the integrated device is varied.
Figure 40: COP vs. expander speed of directly coupled system for range of compressor RPM and gas cooler air temperatures.
8 SUMMARY AND CONCLUSIONS

Performance Potential of CO₂ Systems with Expander

An ideal expander can improve the energy efficiency of a transcritical CO₂ system under typical residential A/C operating conditions of ambient temperatures between 28°C and 50°C by 41% to 81%, respectively. Simulation results are shown in Figure 41. With an expander of 80% efficiency, the system performance can be improved by 31% to 56% and with an expander of 60% efficiency by 22% to 38%, at ambient temperatures between 28°C and 50°C, respectively. Compared to a conventional R22 system, the energy efficiency of a CO₂ system with an ideal expander is higher at all ambient temperatures considered. With an 80% efficient expander, the CO₂ system performs better than a conventional R22 system at ambient temperatures below 36°C. At 28°C, the CO₂ system performs 22% better and at 50°C, it performs 11% worse. A CO₂ system with an expander of 60% efficiency operates 13% more energy efficiently than the R22 system at ambient temperatures of 28°C and 21% less energy efficiently at ambient temperatures of 50°C. At approximately 31°C, both systems operate with the same energy efficiency.

Figure 41: Performance of CO₂ expander system and conventional R22 system

Under most operating conditions, the performance of a CO₂ expander system does not benefit from a suction line heat exchanger. Although the SLHX increases the specific cooling capacity, it also reduces the expander work output and increases the compressor work input. If more than 30% of the expander work output can be recovered, the SLHX does not benefit the system performance. However, when designing a system, other factors than the energy efficiency may influence the decision regarding the integration of an SLHX.
Analysis of Expander and Compressor Performance

The performance of expanders and compressors depends on irreversible processes during the expansion/compression process. The dominating irreversibilities in positive displacement machines are:
- Internal leakage
- Valve losses
- Over/under compression/expansion
- Internal heat transfer

Internal heat transfer has a negligible effect on the performance of a compressor in a residential size CO₂ air-conditioning system. In an expander for this type of application, internal heat transfer can affect the performance significantly due to the increased heat transfer coefficient during evaporation. At adiabatic operating conditions, i.e. when the net heat transfer between fluid and expander wall is equal to zero, internal heat transfer affects the expander performance by less than 3%. An integrated compressor–expander device operates adiabatically when the net heat transfer between compressor and expander is equal to zero. The heat transfer is dominated by the expander. Therefore, the adiabatic operating point of the integrated device is close to the adiabatic operating point of the expander alone. Hence, the effect of internal heat transfer on the performance of an integrated device is in the order of a few percent and is thus neglected in the simulations.

The performance of three positive displacement mechanisms as expander and compressor in a CO₂ system has been analyzed considering the losses mentioned above:
- Reciprocating piston
- Rotary piston
- Scroll

Tables 8 and 9 list the expected performance of the mechanisms with optimized geometry at ASHRAE A operating conditions depending on the leakage gap size. For all simulations, the valve timing was assumed ideal for all devices.

Table 10: Compressor indicated, isentropic, volumetric efficiency vs. leakage gap size

<table>
<thead>
<tr>
<th>Leakage gap size</th>
<th>Recip. piston</th>
<th>Rotary piston</th>
<th>Scroll</th>
</tr>
</thead>
<tbody>
<tr>
<td>5 µm</td>
<td>η_ind 0.93</td>
<td>η_is 0.77</td>
<td>η_vol 0.88</td>
</tr>
<tr>
<td></td>
<td>η_ind 0.91</td>
<td>η_is 0.76</td>
<td>η_vol 0.84</td>
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<tr>
<td></td>
<td>η_ind 0.85</td>
<td>η_is 0.72</td>
<td>η_vol 0.79</td>
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<tr>
<td>10 µm</td>
<td>η_ind 0.96</td>
<td>η_is 0.79</td>
<td>η_vol 0.96</td>
</tr>
<tr>
<td></td>
<td>η_ind 0.90</td>
<td>η_is 0.75</td>
<td>η_vol 0.92</td>
</tr>
<tr>
<td></td>
<td>η_ind 0.85</td>
<td>η_is 0.72</td>
<td>η_vol 0.87</td>
</tr>
<tr>
<td>15 µm</td>
<td>η_ind 0.87</td>
<td>η_is 0.73</td>
<td>η_vol 0.88</td>
</tr>
<tr>
<td></td>
<td>η_ind 0.64</td>
<td>η_is 0.56</td>
<td>η_vol 0.65</td>
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<tr>
<td></td>
<td>η_ind 0.39</td>
<td>η_is 0.36</td>
<td>η_vol 0.38</td>
</tr>
</tbody>
</table>

3 For the isentropic efficiency assumptions, see Section 6.5, p. 40
The reciprocating piston and rotary piston mechanisms perform similarly at all leakage clearances. The performance of the scroll mechanism is the most dependent on the leakage gap size. At machining tolerances above 5 µm, the scroll mechanism performs significantly worse than the other mechanisms. The performance of the scroll mechanism is dominated by the leakage across the tips of the scroll wraps. If this leakage path is eliminated, the indicated efficiency of a scroll expander, for instance, is above 90% for a flank clearance of 15 µm.

Figure 42 shows the indicated compressor and expander efficiency over the range of pressure ratios at typical A/C operating conditions.

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Table 11: Expander indicated and isentropic efficiency vs. leakage gap size

<table>
<thead>
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<th></th>
<th>5 µm</th>
<th>10 µm</th>
<th>15 µm</th>
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<td></td>
<td>( \eta_{\text{ind}} )</td>
<td>( \eta_{\text{is}} )</td>
<td>( \eta_{\text{ind}} )</td>
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<tr>
<td>Recip. piston</td>
<td>0.90</td>
<td>0.75</td>
<td>0.87</td>
</tr>
<tr>
<td>Rotary piston</td>
<td>0.94</td>
<td>0.79</td>
<td>0.84</td>
</tr>
<tr>
<td>Scroll</td>
<td>0.93</td>
<td>0.78</td>
<td>0.75</td>
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</table>

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4 For the isentropic efficiency assumptions, see Section 6.5, p. 40
The piston compressors perform similarly over the range of pressure ratios. The performance of the rotary piston compressor falls behind that of the reciprocating piston compressor at higher pressure ratios. The scroll mechanism performs poorer as compressor than the other mechanisms. As in the expander application, the mechanism is dominated by leakage across the tip of the scroll wraps. If this leakage path can be reduced, the scroll could perform similarly to the other mechanisms. Experience with scroll compressors for conventional refrigerants indicates that efficient sealing mechanisms are available.

The valve operation for the two piston type expanders requires special attention. Since it is not possible to use reed valves in an expander application, externally controlled valves must be used for these mechanisms. Previous experiments with reciprocating piston expanders revealed that the valve control might be a major challenge. If the volume ratio is optimized for one operating condition and not adjusted for others, the losses due to over/under expansion are in the range of 10% of indicated efficiency at typical A/C operating conditions.

The effect of friction was not considered in the simulation. The losses due to friction depend on the type of device and the individual design of the machine. Detailed research on the individual design level is necessary to reliably predict the performance potential of a specific machine.

**Integration Concepts**

In order to efficiently utilize the work produced by the expander, the compressor and expander should be integrated on a common shaft. With this design, the adjustment of the high-side pressure to the operating conditions requires special attention. Since the expander speed is coupled to the compressor speed, the high-side pressure cannot be adjusted by the expander RPM. The system cannot be controlled by an additional expansion valve in series or in parallel to the expander. However, the system can be operated at or close to the optimum performance over the range of typical A/C operating conditions (ambient temperature between 30°C and 50°C, evaporating temperature 7°C) at constant ratio of compressor speed to expander speed if compressor and expander displacement volumes are designed appropriately. Simulation shows that this control concept is also applicable for integrated devices with variable speed.

**Expected Performance of Residential CO₂ Air-Conditioning System with Expander**

Assuming an effective leakage gap size of 10 μm, the indicated efficiency of a reciprocating piston compressor is in the order of 91% and the indicated efficiency of a reciprocating piston expander is in the order of 87% at ambient temperatures of 28°C to 50°C. Additional losses due to bearing friction, suction heating, and entrance and exit effects to the compressor/expander shell reduce the expander efficiency by approximately 15% below the indicated efficiency. With this estimation, the isentropic efficiency of the compressor is approximately 76% and the isentropic efficiency of the expander is approximately 72%. The resulting COP of an expander system is 6.6 at 28°C ambient
temperature and 2.4 at 50°C ambient temperature. At 28°C, the CO₂ expander system performs 20% more energy-efficiently than a conventional R22 system. At 50°C, the CO₂ system performs 14% less energy-efficiently than the R22 system. At approximately 34°C, both systems perform with the same energy efficiency.
APPENDIX A

Modeling Assumptions for the Comparison of CO₂ and R22

Both systems are simulated with constant cooling capacity, independent of the operating conditions. For both systems, the evaporator pressure is assumed to be an independent variable, fixed for all operating conditions. The evaporating temperature is assumed to be 0 – 2K higher in the CO₂ systems than in the R22 system, reflecting the potential of superior heat transfer properties of CO₂. The evaporating temperature in the R22 system is 9°C and in the CO₂ system 9°C - 11°C. The refrigerant leaves the evaporator as saturated vapor for all cases in both systems. Unless otherwise stated, the evaporator secondary fluid is air with 27°C inlet temperature and 50% relative humidity. The compression is assumed adiabatic with constant isentropic efficiency. The isentropic efficiency for the R22 compressor is 0.7 and for the CO₂ compressor slightly higher at 0.75. The higher efficiency of the CO₂ compressor is due to a smaller pressure ratio across the compressor (Preissner 2001, Sakamoto and Giese 2000). The condensation temperature in the subcritical cycle is assumed to be 12K above the air inlet temperature and the refrigerant leaves the condenser with a sub-cooling of 8.6K. The gas cooler outlet temperature in the CO₂ system is set to 2.5K above the air inlet temperature. The high-side pressure is optimized for each operating condition. The refrigerant pressure drop in the gas cooler/condenser is constant in both systems at 100 kPa. The pressure drop in the evaporator of the subcritical R22 system is 25 kPa and in the CO₂ system 50 kPa.
APPENDIX B

Geometry data for scroll device

% Device identification, type, length unit  
XXX  
accll  
0.00100  
% Number of pockets  
2  
% Table of crank angle, chamber volume, area, moment area  
64.00000 19.00000 63.00000  
% Table of dimensions  

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