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Simulation and Performance Correlation for Transcritical CO₂ Heat Pump Cycle

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ABSTRACT

For more than a decade, carbon dioxide (R744) has been revived as a natural environmentally friendly refrigerant. Compared to HFC refrigerants with a global warming potential (GWP) in the order of 1300-1900, R744 has a GWP of 1. As it is relevant for R744 heat pumps, a transcritical cycle has an extra degree of freedom with the gas cooler pressure and outlet temperature being thermodynamically independent of each other. Utilizing MATLAB integrated with the NIST REFPROP thermodynamic database, a single stage transcritical R744 heat pump cycle is modeled and simulated. The isentropic and volumetric efficiency correlations of a commercial semi-hermetic reciprocating compressor are generated as a function of pressure ratio, based on simulated data obtained from the manufacturer’s software. Developed with the cycle model, an optimized control correlation is presented that relates the gas cooler pressure to the gas cooler outlet temperature. The correlations are compared to correlations available in the literature. The range of the gas cooler pressure varies from 75 to 140 bar, the gas cooler outlet temperature from 32 °C to 53 °C, and the evaporation temperature from -30 °C to 15 °C. The developed correlations are for maximizing the coefficient of performance (COP) of the cycle during operation in the range of the above operating conditions.

1. INTRODUCTION

Under Kyoto protocol regulations (adopted in 1997 and entered into force in 2005), the phasing out of HFC refrigerants is underway due to their global warming potential (GWP). The US EPA listed R134a as unacceptable for newly manufactured light-duty vehicles beginning in Model Year 2021 (Chakrabarti et al., 2017). Since CO₂ has GWP of only 1, it is considered a strong alternative solution. The revival of CO₂ as a natural refrigerant has been supported by Lorentzen (1994). Several contributions to the CO₂ transcritical cycle analysis and understanding have been carried out by Robinson and Groll (1998), Kim et al. (2004), Neksà (2004), Li and Groll (2005), and Müller and Joseph (2009). In particular, CO₂ distinguishes itself from common refrigerants by its relative low critical temperature and high critical pressure of 31.1 °C and 73.8 bar respectively. Hence, for a CO₂ heat pump cycle, that can be used for cooling and heating applications, the heat rejection process at the high-pressure side will take place above the critical point for high ambient/sink temperatures. In this supercritical region there is no clear distinction between gas/vapor and liquid. Thus, there is no phase change in the supercritical area. Therefore, the heat exchanger that would ordinarily condense the refrigerant leaving the compressor is instead referred to as a gas cooler (GC). While in the subcritical 2-phase region, pressure and temperature are coupled by the saturation curve; in the supercritical region, pressure and temperature are independent of each other. Therefore, for a given ambient temperature that can be related to the GC outlet temperature, the GC pressure (high-side pressure) can be controlled independently. Controlling the high-side pressure affects the cycle COP (Lorentzen and Pettersen, 1993). Previous studies (Liao et al., 2000) and (Müller and Joseph, 2009) have shown that the high-side pressure optimized for highest COP is affected by the GC outlet temperature, evaporation temperature, amount of superheat at the compressor suction, and compressor isentropic efficiency.

Some researchers focused on developing control correlations for the GC pressure to maximize the COP either through simulations or experiments. These correlations have been developed as a function of the GC outlet temperature such as those of Kauf (1999), Chen and Gu (2005), Kim et al. (2009), and Qi et al. (2013); and in a few cases as a function of both the GC outlet temperature and evaporation temperature such as Sarkar et al. (2004) and Liao et al. (2000),
where the latter one additionally includes a term for the compressor isentropic efficiency. The evaporation temperature has less effect on the COP compared to the GC outlet temperature, while the compressor performance depends on the compressor isentropic efficiency. Each of these correlations is valid for a specific range of operating parameters.

Furthermore, some real time algorithms such as Zhang and Zhang (2011), Cecchinato et al. (2012), Kim et al. (2014), and Hu et al. (2015) have been recently developed to maximize the COP online while obtaining some data measurements. This requires continuous measurement of input parameters such as compressor suction and discharge temperatures, GC pressure, and outlet temperature. In some of these methods, the convergence time of the COP to its optimum value is relatively long. The improvement of these approaches is still an ongoing work especially for transient operation. Not all these developed methods have been verified experimentally. Still, the developed offline control correlations are a good guide for a system to maximize the COP, even if they may have some deviations due to the regression analysis.

In the work discussed here, the isentropic and volumetric efficiency correlations for a semi-hermetic reciprocating compressor are developed from simulated data points. The developed efficiency correlations are compared to several available in the literature. Based on the developed compressor correlations, the CO2 transcritical cycle performance is modeled in a MATLAB environment and analyzed to investigate the effect of the GC outlet temperature, the evaporation temperature, and the superheat on the COP. An optimized control correlation is generated and compared to the common ones in the literature, which relates the optimized GC pressure to the GC outlet temperature. The correlation can be used to maximize the COP in the specified range of operating conditions.

2. THERMODYNAMIC MODELING

The cycle considered in this analysis is for the basic transcritical CO2 system, which is shown in Figure 1. The assumptions considered for the cycle simulation and analysis are as follows: the cycle is assumed to operate at steady state, the compression process is adiabatic but non-isentropic, the heat transfer with the ambient of components other than the heat the exchangers is neglected, the evaporation and the gas cooling processes are isobaric, the pressure drop in heat exchangers and CO2 tube lines are neglected, and CO2 is considered as a pure fluid neglecting the effect of the lubricant on the properties.

![Figure 1: Basic Transcritical CO2 heat pump cycle, with Ts and ph diagram](image)

3.1 Compressor modeling

The compressor selected for this study is a commercially available, 3-phase, 230 V, and 60 Hz, with 1.34 kW rated input power. Additional specifications are shown in Table 1, and its operating envelope is shown in Figure 2. The compressor supports evaporation temperatures ranging from -30 °C to 15 °C. To simulate the cycle behavior, compressor efficiency correlations are needed to calculate the compressor discharge enthalpy and the mass flow rate. The compressor isentropic and volumetric efficiency correlations are expressed as (Boewe et al., 1999)
\[
\eta_{is} = \frac{\dot{m}_r (h_{2s} - h_1)}{W_{comp}} \\
\eta_v = \frac{\dot{m}_r v_t}{N V_d}
\]

(1)  
(2)

**Table 1: Compressor specifications**

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore</td>
<td>22 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>17 mm</td>
</tr>
<tr>
<td>Swept volume (V_d)</td>
<td>12.9/10^6 m³</td>
</tr>
<tr>
<td>Displacement</td>
<td>1.35 m³/h @ 60 Hz</td>
</tr>
<tr>
<td>Speed</td>
<td>1740 rpm @ 60 Hz</td>
</tr>
<tr>
<td>Max low side pressure</td>
<td>100 bar</td>
</tr>
<tr>
<td>Max high side pressure</td>
<td>150 bar</td>
</tr>
</tbody>
</table>

![Figure 2: Compressor Envelope]

Since there were no available efficiency correlations from the manufacturer, the manufacturer’s software was used to simulate the compressor behavior at different operating conditions. The compressor discharge pressure \(p_2\) was swept from 75 bar to 140 bar at constant GC outlet temperature of 35 °C and a total superheating of 1K. The superheat can take place either inside the evaporator, which adds to the cooling capacity, and/or it can be generated outside the evaporator, which is usually due to the pressure drop in the connecting lines between the evaporator outlet and the compressor suction and/or external heat transfer to the line. Eqns. (1) and (2) are used to calculate the isentropic and volumetric efficiency for each data point. A MATLAB code was written to determine the efficiency correlations using regression analysis. For each iteration, the code takes the mass flow rate \(\dot{m}_r\), and the compressor consumed power \(W_{comp}\) as input from the manufacturer’s software and calculates the efficiency. The NIST REFPROP database (Lemmon et al., 2013) is used within the MATLAB code to retrieve the thermodynamic properties of CO₂.

The compressor envelope is shown in Figure 2 which shows the compressor’s maximum high side pressure for the evaporation temperature range from -30 °C to 15 °C. This line can be expressed with Eqn. (3). For instance, at a \(T_1\) of -30 °C and -8 °C, the equation gives that the maximum high side pressure as 82 bar and 140 bar respectively. This equation is used in the MATLAB code to ensure that the high side pressure in each sweep iteration is within the compressor envelope.

\[
p_2 < 2.63 T_1 + 160.9
\]

(3)

Most of the compressor’s efficiency correlations found in the literature were developed at a selected evaporation temperature. For the work discussed here, the efficiency correlations are developed at evaporation temperatures of -8 °C, 0 °C, and 15 °C. Compared to relying on a set of correlations developed at a single evaporation temperature, this was found to provide more accurate results when the correlations are used at different evaporation temperatures in the cycle analysis. A third-order polynomial fit that takes the form of Eqns. (4) and (5) has been adapted for the resulting efficiencies as a function of the compressor pressure ratio \(r_p = p_2/p_1\). Table 2 presents the polynomial coefficients for the different evaporation temperatures. Using the developed correlations, the maximum deviation of the calculated mass flow rate and the compressor power from the manufacturer’s software values used in generating the correlations was ±0.34 %. Figure 3 shows the developed compressor volumetric and isentropic efficiency correlations represented by Eqns. (4) and (5) along with Table 2, compared to CO₂ compressor correlations used in the literature. The correlations of Sarkar et al. (2009), Casson et al. (2003), Ortiz et al. (2003), and Liao et al. (2000) are estimated or based on experimental data fitting for a semi-hermetic compressor, while no information was provided for the Robinson and Groll (1998) correlations. It can be noted that the isentropic efficiency varies considerably between different compressors, hence selecting the appropriate correlations for simulating the cycle behavior is important.
\[ \eta_v = a_0 + a_1 r_p + a_2 r_p^2 + a_3 r_p^3 \]  
(4)

\[ \eta_{is} = b_0 + b_1 r_p + b_2 r_p^2 + b_3 r_p^3 \]  
(5)

**Table 2.** Developed volumetric and isentropic efficiency correlations at different evaporation temperatures

<table>
<thead>
<tr>
<th></th>
<th>( \eta_v )</th>
<th></th>
<th>( \eta_{is} )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( a_0 )</td>
<td>( a_1 )</td>
<td>( a_2 )</td>
</tr>
<tr>
<td>-8 °C</td>
<td>1.0904</td>
<td>-0.1929</td>
<td>0.0189</td>
</tr>
<tr>
<td>0 °C</td>
<td>1.0829</td>
<td>-0.1965</td>
<td>0.0202</td>
</tr>
<tr>
<td>15 °C</td>
<td>1.0380</td>
<td>-0.2044</td>
<td>0.0249</td>
</tr>
</tbody>
</table>

![Figure 3](image.png)

**Figure 3:** Compressor developed (a) Volumetric efficiency correlations, and (b) Isentropic efficiency correlations; compared to correlations from the literature

### 3.2 Cycle modeling

By referring to Figure 1, and considering the compression process is adiabatic but not isentropic, the enthalpy at the compressor discharge can be written as

\[ h_2 = h_1 + \frac{h_{2s} - h_1}{\eta_{is}} \]  
(6)

The expansion process is considered isenthalpic, hence

\[ h_3 = h_4 \]  
(7)

The power consumed by the compressor is calculated as

\[ W = \dot{m} (h_2 - h_1) \]  
(8)
The cooling capacity is the enthalpy difference across the evaporator times the mass flow rate

\[ Q_c = \dot{m} (h_1 - h_4) \quad (9) \]

Thus, the cooling coefficient of performance is written as

\[ COP = \frac{h_1 - h_3}{h_2 - h_4} \quad (10) \]

### 3. RESULTS AND DISCUSSION

A parametric study is carried out to show the effect of several parameters on the cooling COP. The range of the GC pressure is varied from 75 to 140 bar, the GC outlet pressure from 32 °C to 53 °C, the evaporation temperature from -30 °C to 15 °C, and the superheat from 0.5 K to 1.5 K.

#### 3.1 Analysis

Figure 4a shows the influence of varying GC pressure on the COP at different GC outlet temperatures at a 15 °C evaporation temperature and 1K superheat. Clearly, there is an optimum GC pressure for each GC outlet temperature where the COP is maximum. This is shown by the green curve polynomial fit connecting those optimum points. Apparently, and as indicated by Yang et al. (2015) the accurate determination of the optimum GC pressure is much more sensitive close to the critical point than at higher pressures. At higher GC pressures, the COP curves are flatter; hence, the maximum COP becomes almost insensitive to the estimate of optimal high pressure.

The effect of changing the GC pressure on the COP at different evaporation temperatures at 35 °C GC outlet temperature is shown in Figure 4b. The evaporation temperature of -30 °C was excluded from this simulation because of the limited allowed high-side pressure of 82 bar at this evaporation temperature. The green curve connects the optimum pressure points. From the graph, at the two extreme evaporation temperatures, -25 °C and 15 °C, the optimum GC pressure is 90.5 bar and 86.2 bar respectively. In fact, if 86.2 bar pressure is applied as a GC pressure for the whole evaporation temperature range, the resulting COP is no more than 1.5% (at either -15 °C or -25 °C) away from the optimum COP. Hence, the effect of the evaporation temperature on the optimum GC pressure is negligible compared to the more considerable effect that the GC outlet temperature has on the optimum GC pressure.

The effect of changing the GC outlet temperature on the COP at different GC pressures at 15 °C evaporation temperature is shown in Figure 5a. It can be noted that the optimum GC pressure increases with the increase of the...
GC outlet temperature. It is also clear for the shown range that the COP is maximum at the lowest GC outlet temperature. Hence, for the best COP the cooling process in the GC should be the best possible.

Figure 5b shows that COP increases with the increase of the evaporation temperature as in conventional (subcritical) heat pump cycles. This graph is generated for GC outlet temperature of 35 °C where the 86.2 bar GC pressure line represents the maximum COP line neglecting the effect that the changing evaporation temperature has on the optimum GC pressure. Considering the GC pressure curves for 75, 86.2, and 100 bar, it can be noted that the under-estimation of the optimum GC pressure generates higher reduction in COP compared to the over-estimation of the optimum GC pressure. For instance, at 10 °C evaporation temperature, the COP is 2.85 at 86.2 bar, while the COP at 75 and 100 bar is 0.82 and 2.65 respectively.

The impact of the amount of the superheating taking place inside the evaporator, which adds to the cooling capacity at various GC pressures is plotted in Figure 6 for GC outlet temperatures of 35 °C and 45 °C, both at 15 °C evaporation temperature. At 35 °C, the superheating has negligible effect at all GC pressure except at 75 bar. At 45 °C, the superheating has a considerable effect on the COP for 75 and 100 bar GC pressures. It can be concluded that at most GC pressures, the superheating has hardly an influence on the COP, especially if the GC pressure is much greater than the critical pressure. However, if the GC pressure is close to the critical pressure, COP can significantly increase with an increasing amount of superheating, and even more so if additionally the GC outlet temperature is high.

![Figure 5](image1.png) **Figure 5**: (a) The impact of varying the GC outlet temperature on the COP at different GC pressures and at 15 °C evaporation temperature (b) The effect of changing the evaporation temperature on the COP at different GC pressures and at 35 °C GC outlet temperature

![Figure 6](image2.png) **Figure 6**: (a) The influence of the superheating on the COP at 15 °C evaporation temperature; and (a) 35 °C GC outlet temperature and (b) 45 °C GC outlet temperature
3.2 Optimization Correlation
Based on the analysis, the GC outlet temperature is the most influential parameter on the optimum GC pressure. A second-order polynomial is developed based on the simulated points shown in Figure 7, which is calculated at a 15 °C evaporation temperature and 1K total superheat. Using regression analysis, the polynomial fit has coefficient of determination (R²) of 1.

\[
p_{GCopt} = 8.197 + 1.717 \cdot T_{GCo} + 0.01448 \cdot T_{GCo}^2
\]  

(11)

This correlation is developed for the range of operating conditions of 32 °C < T_{GCo} < 53 °C and 75 bar < p_{GCopt} < 140 bar. Figure 7 shows the developed correlation in comparison with the common ones in the literature displayed with their respective valid range.

![Figure 7: Developed correlation for optimized GC pressure shown in thick green curve compared to correlations available in the literature](image)

4. CONCLUSION

In this paper, the CO₂ transcritical cycle is modeled and analyzed. For the sourced compressor, the isentropic and volumetric efficiency correlations are developed from simulated data points at three different evaporation temperatures. The efficiency correlations are compared to correlations from the literature. The isentropic efficiency varies considerably between different compressors, hence selecting the appropriate correlations for simulating the cycle behavior is important. The effect of the GC outlet pressure and temperature, the evaporation temperature, and the useful superheat taking place inside the evaporator on the COP are investigated and discussed. The GC outlet temperature is the most influential parameter on the optimum GC pressure. The evaporation temperature has a negligible effect on the optimum GC pressure. An optimized control correlation is developed, and compared to common ones in the literature. The correlation relates the optimized GC pressure to the GC outlet temperature which can be used to maximize the transcritical cycle COP for relevant range of operating conditions.

**NOMENCLATURE**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>COP</td>
<td>coefficient of performance</td>
<td>(-)</td>
</tr>
<tr>
<td>GC</td>
<td>gas cooler</td>
<td>(-)</td>
</tr>
<tr>
<td>GWP</td>
<td>global warming potential</td>
<td>(-)</td>
</tr>
<tr>
<td>h</td>
<td>specific enthalpy</td>
<td>(J/kg)</td>
</tr>
</tbody>
</table>
\( \dot{m} \)  
mass flow rate  
(kg/s)

\( N \)  
compressor speed  
(rev/sec)

\( p \)  
pressure  
(bar)

\( \dot{Q} \)  
capacity  
(W)

\( r_p \)  
compressor pressure ratio  
(-)

\( T \)  
temperature  
(°C or K)

\( V_d \)  
compressor swept volume  
(m³)

\( W \)  
work per unit time (power)  
(W)

**Greek symbols**

\( \eta \)  
efficiency  
(-)

\( \rho \)  
density  
(kg/m³)

\( \nu \)  
specific volume  
(m³/kg)

**Subscripts**

1,2, etc.  
state points

comp  
compressor

c  
cooling

o  
outlet

opt  
optimum

v  
volumetric

is  
isentropic

r  
refrigerant

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**REFERENCES**


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