EFFECTS OF FLUID STREAM IMPURITIES ON PERFORMANCE OF A SUPERCRITICAL CO_2 POWER CONVERSION SYSTEM

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Abstract

A team of professors and students at Carleton University have been working on a designing an S-CO_2 PCS in collaboration with Natural Resources Canada. An important consideration when designing such a cycle is the level of purity of the S-CO_2 working fluid, including the effects of impurities on the critical temperature and pressure. This paper will present an investigation of the influence of impurities on several aspects of cycle performance. For example, it has been found that using low grade commercial CO_2 can produce a cycle thermal efficiency loss in of approximately 5%. The examination was performed using simple analytical techniques and by using HYSYS plant simulation software.

1. Background

The use of supercritical CO_2 (S-CO_2) as the working fluid for next generation power conversion systems (PCS) has many advantages compared to the traditional steam Rakine Cycle PCSs that are in wide spread use today. Most prominent being the large reduction in component size relative to the traditional steam and helium PCSs due to S-CO_2 fluid properties, while retaining high cycle thermal efficiencies. This can cut capital costs and construction times significantly. The goal is to take advantage of the high compressibility of the fluid on or near the critical point. In other words when the fluid is near the critical point, little compression work is needed to increase the fluid stream pressure. However, the fluid properties in this region vary in a highly non-linear fashion, making design of such a cycle a challenging endeavor.

Since 2000, professors and students at Carleton University have been working in collaboration with professionals from Natural Resources Canada on projects under the heading of Zero-Emissions Gas Turbines. Work began on designing a test 100 MW power plant in 2005. The plant specifications were for an externally fired (in-direct) power conversion system (PCS) in which the working fluid would be CO_2 in the supercritical regime. Initial examinations would find that the maximum advantage in terms of cycle thermal efficiency for a CO_2 powered gas turbine arrangement would be for systems with turbine inlet temperatures in the range of 550°C - 950°C. This places next generation (or GEN IV) nuclear power plants, as the most realistic source for such high temperature production.

The cycle design adopted by the team at Carleton University is a simple close loop Brayton cycle with recuperation (Figure 1). The key components of the cycle are: the compressor, the recuperator, the main heat exchanger, the turbine and the precooler. It operates using a supercritical CO_2 working fluid and specified to produce 100 MW of electrical power. In its current form it is designed as an indirect PCS so that it can be applicable to a wider variety of heat sources.

2. Introduction

Much of the design work and modeling of the cycle has relied upon the assumption that the working fluid is 100% pure CO_2, and using the associated fluid properties that can be obtained using this assumption. In most modeling cases this assumption would be perfectly valid. However, the current cycle has regions in which the fluid will pass close to the critical point (i.e. compressor inlet) this leaves room for further investigation of fluid impurity effects. Fluid properties in the critical region vary in a highly non-linear fashion; this results in significant performance variations as well.

This paper examines the possible effects on cycle performance of impurities. The investigation began by contacting an industrial supplier to obtain information on the levels of carbon dioxide (CO_2) purity that could be commercially obtained. Using the information obtained a simple model was setup in HYSYS software to analyze the effects of the impurities.

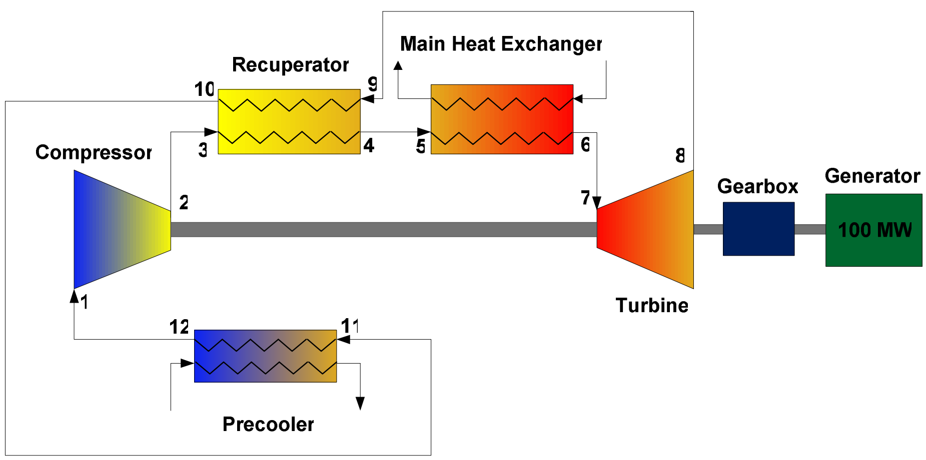

Figure 1 Cycle developed by the Carleton Raven Gas Turbine Team.

3. Best and worst case CO_2

The first step in the analysis was to identify the sources of any working fluid contaminants and the associated concentrations. For this investigation only two sources of contaminants were considered. The first source of contamination that was considered was impurities in the CO_2 purchased from a commercial distributor. The second was possible contamination due to cracked pipes or improperly sealed connections allowing air and other contaminants to enter the fluid stream. However, it was later deemed that the latter case was improbable as the system pressure would be higher than that of the ambient plant atmosphere, and as such any leaks that occurred would be towards the atmosphere and not vice versa.

Information was requested from an industrial supplier of CO_2 gas (Praxair) on the types and concentrations of impurities that are typically found in their CO_2 products. This information was used to formulate a "best" and a "worst" case scenario for analysis.

3.1 Best case

Based on information received from Praxair the best case scenario was determined. Table 1 shows the assumed best case scenario composition.

Compound	Mass fraction (kg/1kg of mixture)
CO_2	0.99998
N_2	$1x10^{-5}$
O_2	$6x10^{-6}$
CH_4	$2x10^{-6}$
H_20	$1x10^{-6}$
CO	$5x10^{-7}$
H_2	$5x10^{-7}$

Table 1 Best case working fluid composition.

3.2 Worst case

For the worst case scenario only the percentage of CO_2 was available. Since it is relatively inexpensive industrial suppliers rarely test this type of gas for the content of impurities. A simple scaling up of the best case components, while keeping the same ratios of concentration was performed (Table 2).

Compound	Mass fraction (kg/1kg of mixture)
CO_2	0.995
N_2	$2.5x10^{-3}$
O_2	$1.5x10^{-3}$
CH_4	$5.0x10^{-4}$
H_20	$2.5x10^{-4}$
CO	$1.25x10^{-4}$
H_2	$1.25x10^{-4}$

Table 2 Worst case working fluid composition.[1]

[1] For the best case you have 20mg of impurities compared to 0.99998kg of CO_2 (1kg – 20mg = 0.99998kg). From this conclusion, the worst case scenario is approximated as 1kg – 0.995kg which leaves 5g of impurities. To get the scaling factor 5g was divided by 20mg to obtain 250.

3.3 Conversion to Mole Fractions

For input into HYSYS it is easiest to have the compositions defined as mole fractions and so a conversion was performed. Using the mass fractions in Tables 1 and 2 the moles of each component was determined with equation 1.

$$n_i = \frac{m_i}{MM_i} \tag{1}$$

Where n_i is the moles of the element, m_i is the mass, and MM_i is the molar mass obtained from [1]. The mole fraction was then calculated using equation 2.

$$y_i = \frac{n_i}{n_{tot}} \tag{2}$$

Where y_i is the mole fraction of the element and n_{tot} is the sum of the moles of each of the components. This method gave the mole fractions that were input into HYSYS to define the mixture stream and they can be found in Tables 3 and 4.

Compound	Mole Fraction
CO_2	≈ 1
N_2	1.6×10^{-5}
O_2	8.2×10^{-6}
CH_4	5.5×10^{-6}
H_20	2.4×10^{-6}
CO	7.8×10^{-7}
H_2	1.0×10^{-5}

Table 3 Best case working fluid mole fractions.

Compound	Mole Fraction
CO_2	0.989
N_2	3.9×10^{-3}
O_2	2.0×10^{-3}
CH_4	1.4×10^{-3}
H_20	6.1×10^{-4}
CO	1.9×10^{-4}
H_2	2.6×10^{-3}

Table 4 Worst case working fluid mole fractions.

4. Investigation of cycle performance in HYSYS

The following section will describe the inputs used in the HYSYS model as well as the results obtained for the best case and worst case scenarios.

4.1 HYSYS model used

In order to perform this investigation a simplified model of the cycle was developed using HYSYS software. Figure 2 shows the overall layout of the cycle in HYSYS based on the current iteration of the Raven Gas Turbine. The cycle remains a closed loop indirect Brayton cycle. The major components of the cycle include: the compressor, the turbine, the pre-cooler, the main heat exchanger and the recuperator. To be able to perform the necessary calculations the model must be in a fully defined state. This means that the minimum number of inputs to solve for all state points must be defined. The inputs used to define the model used in this analysis can be found in Table 5 and are based upon the design best design data available at the time of this investigation.

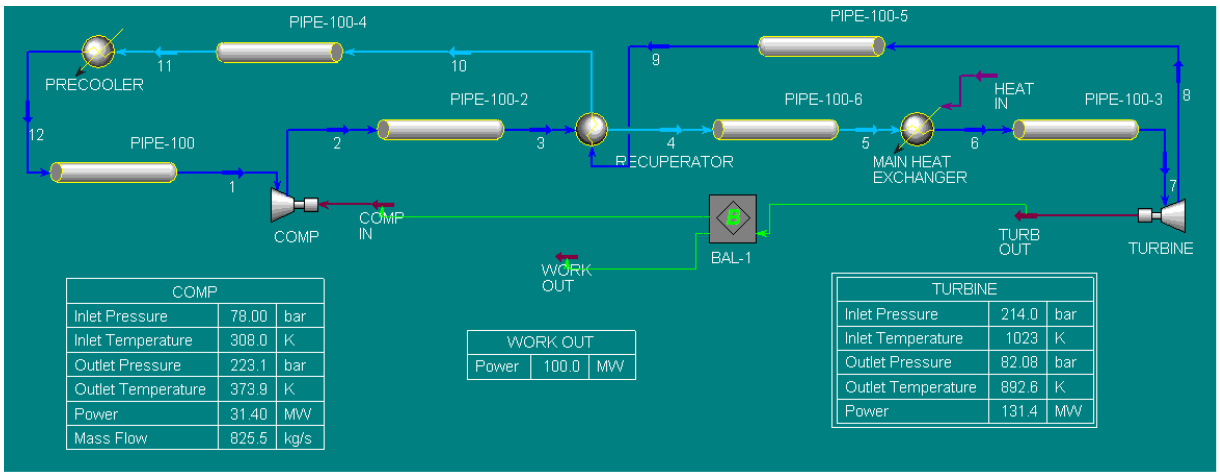

Figure 2 HYSYS model used for the investigation.

Compressor		Turbine	
Inlet pressure	78 bar	Inlet temperature	1023 K
Inlet temperature	308 K	Isentropic efficiency	0.89
Pressure ratio	2.86	Precooler	
Isentropic efficiency	0.89	Pressure loss	2% of inlet pressure
Recuperator		Piping Losses	
Heat sink pressure loss	2% of inlet pressure	Compressor to recuperator	0.00281 bar
Cold sink pressure loss	2% of inlet pressure	Recuperator to main heat exchanger	0 bar
Effectiveness	0.8	Main heat exchanger turbine	0.235 bar
Main Heat Exchanger		Turbine to recuperator	0.6 bar
Pressure loss	2% of inlet pressure	Recuperator to precooler	0.055 bar
		Precooler to compressor	0.2 bar

Table 5 List of inputs into HYSYS model.

In addition it should be noted that the Peng-Robinson equation of state (EOS) was used to model the fluid properties. The selection of this EOS was influenced by the functionality of the EOS with certain utilities within the software necessary for the analysis.

4.2 Reference case

To benchmark the results of the best and worst case CO_2 scenarios they were compared to a reference case. For this investigation the reference case was a model in which the fluid stream was composed solely of CO_2, in other words 100% pure CO_2. The following results were obtained for the benchmark case.

T_c= 304 K
p_c= 7.37 MPa
Specific Power = 121.2 kJ/kg
Cycle Thermal Efficiency = 40.3%

Where T_c is the critical temperature and p_c is the critical pressure.

4.3 Results of "worst case" analysis

Using mole fractions of the worst case CO_2 composition as described earlier in this paper, the following results were obtained from HYSYS.

T_c= 303.0 K
p_c= 7.35 MPa
Specific Power = 119.5 kJ/kg
Cycle Thermal Efficiency = 35.6%

The relatively small amount of impurities (0.5% total) has caused a one degree shift in the critical point which reduced the cycle thermal efficiency from 40.3% to 35.6%. This could be due the fact that the compressor, which operates at an inlet temperature of 308 K, is now one degree further away from the critical point and uses more power to compress the fluid.

4.3 Results of "best case" analysis

When the best case scenario was run in the HYSYS model the new critical properties were obtained. The results were:

T_c= 304 K
p_c= 7.37 MPa
Specific Power = 121.2 kJ/kg
Cycle Thermal Efficiency = 40.3%

These results were identical to the 100% CO_2 reference case. This was expected due to the extremely low concentration of impurities in the fluid stream.

5. Analytical check of results

The results of the HYSYS investigations were reasonable however, there was no way of verifying the math procedures that HYSYS uses directly; the method by which the software calculates the mixture's critical properties was not available. Therefore a simple verification using an independent analytical method was performed to confirm the results. Using the worst case scenario a check was performed using Kay's Rule [1]. This rule defines the critical temperature and pressure of a mixture as:

$$T_c = \sum_{i=1}^{j} (y_i \cdot T_{ci}) \tag{3}$$

$$p_c = \sum_{i=1}^{j} (y_i \cdot p_{ci}) \tag{4}$$

Where T_c is the critical temperature, p_c is the critical pressure and y_i is the mole fraction of a component in the fluid. In essence, Kay's Rule is simply the weighted average of the critical properties of a fluid stream's components. T_c and p_c of the mixture were obtained using the mole fractions calculated and the critical properties of each individual component from as listed in [1]. The results of this check were:

<u>Worst case:</u>
T_c= 302.8 K
p_c= 7.37 MPa

<u>Best case:</u>
T_c= 304.1 K
p_c= 7.39 MPa

The worst case results using Kay's Rule represented a decrease in the listed properties of CO_2 from [1] (T_c= 304.1 K, p_c= 7.39 MPa) and supports the conclusions reached by the HYSYS investigation. Some discrepancy can be attributed to the different pure fluid critical point definitions. Where [1] defines the critical point of CO_2 as T_c= 304.1 K, p_c= 7.39 MPa and HYSYS defines it as T_c= 304 K, p_c= 7.37 MPa. A comparison between the HYSYS and analytical results can be seen in figure 3.

6. Conclusions and recommendations

A study was performed on the effect of impurities on Carleton S-CO_2 cycle performance. This study showed that even at 99.5% pure CO_2, this was enough to shift the critical point of the fluid away from the operating point by approximately 1 K and 0.02 MPa. This lead to a 4.7% drop in cycle thermal efficiency which is significant. As it has been determined that impurities have a large impact on cycle performance, it is recommended that this area be investigated further, such as, which impurities will affect the system the most. Also, the affects of cost and quantity of CO_2 required and initial charging of the cycle after

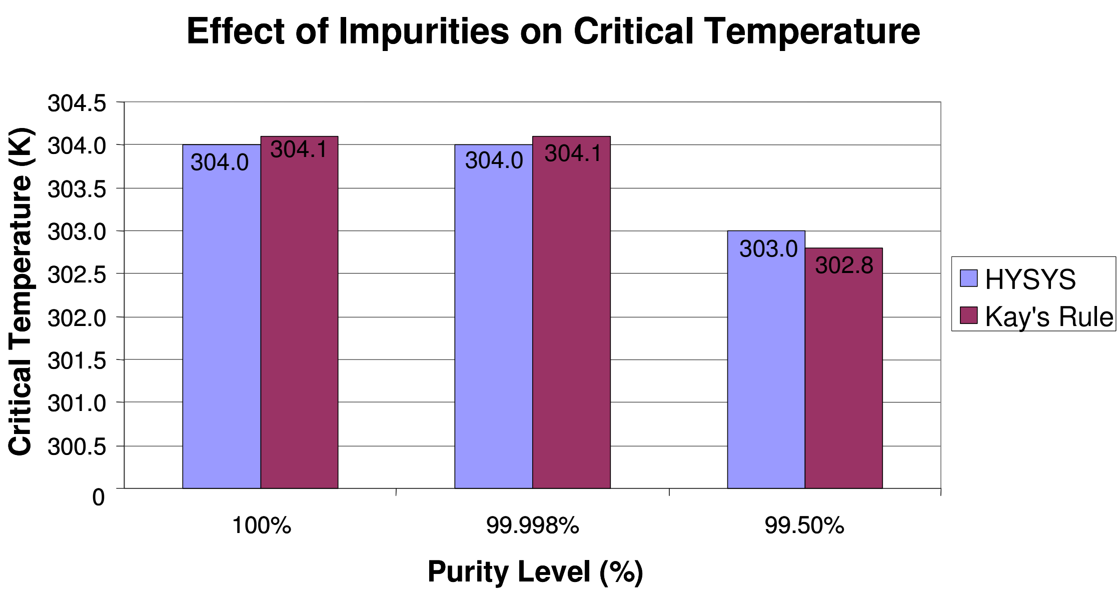

Figure 3 Comparison of results

commissioning and maintenance outages can have a profound effect on performance and should be examined further.

7. References

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