OXYGEN-ENHANCED COMBUSTION APPLIED TO GAS POWER CYCLES

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Abstract. The majority of combustion processes use air as oxidant, roughly taken as $21\% O_2$ and $79\% N_2$, by volume. However, if the concentration of nitrogen in the oxidizer is reduced, it's possible to obtain several benefits, including: higher thermal efficiencies, higher heat transfer efficiency, reduction fuel consumption, reduced retrofit cost and reduction in the emission of some polluants. Based on this, this study aims to investigate the influence of oxygen enhanced combustion process (OEC) in the performance and emissions of a gas turbine cycle. Simulations shows that, for the combustion chamber temperature of gas turbine between 1950K and 2250K, the enhancing of the oxidant stream reduced specific fuel consumption on about 1,5% and increase 9,8% the net power. Furthermore, it was also obtained a reduction of 2% in specific emission of CO_2 . However, it was necessary a supply of about 0.13kmol/s of pure O_2 to sustain the process.

Keywords: Oxygen-enhanced combustion, gas power cycle, thermodynamic modeling, chemical equilibrium

1. INTRODUCTION

Many industry areas use large amounts of thermal energy, usually obtained by burning oil, gas or coal. This energy is obtained, in most cases, by combustion of these fuels with air as an oxidant. However, air is mostly made up of nitrogen gas which carries a significant part of the energy of the reaction, lowering the fuel availability.

Thus, the oxygen-enhanced combustion technology (OEC) emerges with a goal of reducing the effects of high concentrations of N_2 in the air. For a given air-fuel ratio, the amount of O_2 can be kept constant with the technique of injecting pure oxygen, thus reducing the participation of N_2 in the oxidant.

Despite the various advantages that can be obtained, the process OEC is still little used. The main applications in industry are in the areas of manufacturing ceramic, metals production and waste incineration. However, there are few studies concerning the use of technology in areas such as energy generation and in internal combustion engines.

The objective of this paper is to analyze how a theoretical heavy duty single-shaft gas turbine cycle responds to airenrichment, during an adiabatic combustion process, by using software EES (http://www.fchart.com) to perform the simulation. The principal analyzed variables are fuel consumption, temperature combustion, net power and emissions for each concentration of O_2 in the oxidant. For all levels of enrichment analyzed, the equivalence ratio and total air flow rate are kept constant. The calculation of emissions is performed with the aid of chemical equilibrium equations.

2. MODEL DESCRIPTION

2.1. Problem studied

The gas turbine cycle studied is shown in Fig. (1) below. It is formed by a turbine and a compressor coupled via a shaft, similarly to that found in heavy duty single-shaft gas turbine.



Figure 1: Schematic diagram of gas turbine cycle studied

In the above scheme, part of the air discharged by the compressor is deviated directly to the turbine inlet. Thus, only a portion of the oxidizing participates of combustion reaction. This is done with the objective to represent the three main regions of a typical combustion chamber (primary, intermediary and dilution zones). The oxygen enhancement is achieved by injecting pure O_2 at point 4 in Fig.(1), so that it is possible obtain in Point 5, an oxygen concentration greater than 21%.

2.2. Main considerations

The equations and the behavior of the thermodynamic cycle of Fig.(1) are based on simplifying assumptions that are valid for all simulations. The main ones are:

- The power cycle operates at steady state;
- The ideal-gas mixtures principles apply for the air and the combustion products;
- The fuel (natural gas) is taken as 100% methane;
- The atmospheric air consists of 79% O_2 and 21% N_2 (in volume);
- All the equipments operate without heat and pressure losses;
- The stream of oxygen injected is composed of pure O₂;
- The combustion reaction occurs until all products are in chemical equilibrium;

2.3. Governing equations

Established the hypotheses, the equations that model the behavior of each device of the thermodynamic cycle studied are detailed in terms of mass and energy balances and the second law of thermodynamics.

The compressor is modeled by continuity and energy balances. The main equation is the definition of isentropic efficiency, η_c , that provides the power consumed by the compressor, $\dot{W}_{c,r}$, according to the isentropic power, $\dot{W}_{c,s}$, given by Eq. (1):

$$\eta_c = \frac{\dot{W}_{c,s}}{\dot{W}_{c,r}} = \frac{(\bar{h}_{2,s} - \bar{h}_1)}{(\bar{h}_2 - \bar{h}_1)} \tag{1}$$

for:

$$\bar{s}_1 = \bar{s}_{2,s} \tag{2}$$

Thus, the energy balance is given by the following equation:

$$\dot{n}_1(\bar{h}_1 - \bar{h}_2) - \dot{W}_{c,r} = 0 \tag{3}$$

where \dot{n}_1 is the air flow, being \bar{h}_1 and \bar{h}_2 the molar specific enthalpy in input and output stream of the compressor, respectively.

The mass balance gives the following equality:

$$\dot{n}_2 = \dot{n}_1 \tag{4}$$

In the splitter, the total air flow coming from the compressor is partially deviated in two different paths. Thus, it's possible obtain of mass balance the Eq.(6) bellow:

$$\dot{n}_3 = y\dot{n}_2 \tag{5}$$

being *y* the fraction of total air flow rate diverted towards the combustion chamber. Furthermore, it's possible to obtain the following equality enthalpies of energy balance applied to the device:

$$\overline{h}_3 = \overline{h}_2 \tag{6}$$

The volume control where the fuel (stream 10) reacts with the oxidizer (stream 5) to form the flue gas (stream 6) corresponds to combustor. The overall reaction of burning fuel is schematically described by Eq. (7) below:

following equations:

$$\dot{n}_{CH_4,10}CH_4 + \dot{n}_{O_2,5}O_2 + \dot{n}_{N_2,2}N_2 \rightarrow \dot{n}_{CO_2,6}CO_2 + \dot{n}_{H_2O,6}H_2O + \dot{n}_{N_2,6}N_2 + \dot{n}_{O_2,6}O_2 + traces$$
(7)

The traces are formed by elements that occur in small concentrations, much lower than those of CO_2 , H_2O , N_2 and O_2 in combustion products. These traces are formed by molecules of CO, NO, NO_2 , H_2 , OH, O, N and H.

$CO_2 \leftrightarrow 2CO + O_2$	(8)
$O_2 + N_2 \leftrightarrow 2NO$	(9)
$2NO + O_2 \leftrightarrow 2NO_2$	(10)
$2H_2O \leftrightarrow H_2 + O_2$	(11)
$2H_2O \leftrightarrow H_2 + 2OH$	(12)
$O_2 \leftrightarrow 2O$	(13)
$N_2 \leftrightarrow 2N$	(14)
	(15)

$$H_2 \leftrightarrow 2H$$
 (15)

Based on the chemical reactions described, the species balances in the combustion chamber are given by the following equations:

$$\dot{n}_{CH_4,10} = \dot{n}_{CO_2,6} + \dot{n}_{CO,6} \tag{16}$$

$$4\dot{n}_{CH_4,10} = 2\dot{n}_{H_20,6} + 2\dot{n}_{H_2,6} + \dot{n}_{OH,6} + \dot{n}_{H,6} \tag{17}$$

$$2\dot{n}_{O_2,5} = 2\dot{n}_{CO_2,6} + \dot{n}_{H_2O,6} + 2\dot{n}_{O_2,6} + \dot{n}_{NO,6} + 2\dot{n}_{NO_2,6} + \dot{n}_{OH,6} + \dot{n}_{O,6}$$
(18)

$$2\dot{n}_{N_{2},5} = 2\dot{n}_{N_{2},6} + \dot{n}_{NO,6} + \dot{n}_{NO_{2},6} + \dot{n}_{N,6} \tag{19}$$

representing, respectively, the atoms balance of carbon, hydrogen, oxygen and nitrogen. This system of equations is completed with the chemical equilibrium equations based on the reactions described in Eq. (5) to Eq. (15). These equations can be represented in a general way by Eq. (20) below:

$$K_{j} = \frac{y_{c}^{x_{c}} y_{d}^{x_{d}}}{y_{a}^{x_{a}} y_{b}^{x_{b}}} \left(\frac{p}{p_{o}}\right)^{x_{c} + x_{d} - x_{a} - x_{b}}$$
(20)

where x_i corresponds to the stoichiometric coefficients of elementary reactions of dissociation and y_i the molar fractions of the flue gas related. In above equation, K_j is the equilibrium constant related to reaction formation of trace *i*.

The energy balance applied to the combustion chamber provides the following equality:

$$H_R = H_P \tag{21}$$

where H_R is the reactants total enthalpy (point 5 and 10) and H_P the products total enthalpy (point 6). The gas mixer corresponds to device between the points 6, 7 and 8 of the cycle. The mixer is used to maintain a prescribed of the turbine inlet flue gases, fixed in 1100 °C (1373.15K). The equations this device are represented by the

$$\dot{n}_6 + \dot{n}_7 - \dot{n}_8 = 0 \tag{22}$$

$$\dot{n}_{6}\bar{h}_{6} + \dot{n}_{7}\bar{h}_{7} - \dot{n}_{8}\bar{h}_{8} = 0 \tag{23}$$

where:

$$\dot{n}_7 = (1 - y)\dot{n}_2$$
 (24)

Analogous to the compressor, the turbine it is modeled by the following equations:

$$\eta_t = \frac{\dot{W}_{t,r}}{\dot{W}_{t,s}} = \frac{(\bar{h}_8 - \bar{h}_9)}{(\bar{h}_8 - \bar{h}_{9,s})}$$
(25)

$$\dot{n}_8(\bar{h}_8 - \bar{h}_9) - \dot{W}_{t,r} = 0 \tag{26}$$

$$\dot{n}_8 = \dot{n}_9 \tag{27}$$

$$\bar{s}_8 = \bar{s}_{9,s} \tag{28}$$

being that $\dot{W}_{t,r}$ represents the actual turbine power and $\dot{W}_{t,s}$ the power obtained through an isentropic expansion. These two variables are associated through the isentropic efficiency η_t of turbine.

Based on the equations presented in previous sections, the net power output, W_{net} , obtained in the cycle is calculated by the Eq. (29), as follow:

$$\dot{W}_{net} = \dot{W}_{t,r} - \dot{W}_{c,r} \tag{29}$$

Being also possible to define the expression for the specific fuel consumption, *sfc*, and thermal efficiency, ε_{cycle} , of cycle studied.

$$sfc = \frac{\dot{m}_{fuel}}{\dot{W}_{net}}$$
(30)

$$\varepsilon_{cycle} = \frac{1}{sfcPCI} \tag{31}$$

where PCI it's the lower heating value of fuel and \dot{m}_{fuel} corresponds is the mass fuel flow rate.

2.4. Parameters and variables

The parameters of the simulation, segregated by equipment, are listed in Tab. 1. The net power output for all the simulations is 45 MW. The fuel has a lower heating value (*PCI*) 50016 kJ/kg. The equivalence ratio is equal to 0.55, which is approximately the optimum value recommended for gas turbines (Lefebvre, 1998). With this value, is obtained by a flame temperature of 1950K to 21% O_2 in point 5.

An opinion
$Q_{S} = 0W; x_{0,3} = 0.21; x_{N,3} = 0.79$
$v_{0,2}^{2,3}$ $v_{1,2}^{2,3}$ $v_{1,2}^{2,3}$
$x_{O_2,7} = 0.21; \ x_{N_2,7} = 0.79$
Combustion Chamber
$Q_{CC} = 0$ W; $\phi = 0.55$
$x_{CH_4,10} = 0; p_{10} = 101.325 \text{ kPa}$
Turbine
$p_9 = 101.325 \text{ kPa}; Q_{T,R} = 0 \text{W}$
$Q_{S} = 0W; \ x_{O_{2},3} = 0.21; \ x_{N_{2},3} = 0.79$ $x_{O_{2},7} = 0.21; \ x_{N_{2},7} = 0.79$ Combustion Chamber $Q_{CC} = 0W; \ \phi = 0.55$ $x_{CH_{4},10} = 0; \ p_{10} = 101.325 \text{ kPa}$ Turbine $p_{9} = 101.325 \text{ kPa}; \ Q_{T,R} = 0W$

Table 1. Simulation parameters

The variables as presented in Tab. 2, also segregated by equipment. The main ones are the mole fractions and temperature of the combustion products. It's allowed that the temperature T_6 varies between 1950K and 2250K, temperature range typically found in combustion chambers of gas turbines (Boyce, 2002).

Air Compressor	Air Splitter
$T_2; T_{2s}; \dot{n}_1; \dot{W}_{c,r}; p_2; \eta_C$	$T_3; p_3; \dot{n}_3; \dot{n}_7$
Oxygen Injector	Combustion Chamber
$T_5; \ \dot{n}_5; \ p_5; \ x_{O_2,5}; \ x_{N_2,5}$	$x_{CO_{2},6}$; $x_{H_{2}O,6}$; $x_{N_{2},6}$; $x_{O_{2},6}$; $x_{CO,6}$; $x_{NO,6}$;
	$x_{NO_2,6}$; $x_{H_2,6}$; $x_{OH,6}$; $x_{O,6}$; $x_{N,6}$; $x_{H,6}$
	$T_6; \dot{n}_6; \dot{n}_{10}; p_6$
Gas Mixer	Turbine
$x_{CO_2,8}$; $x_{H_2O,8}$; $x_{N_2,8}$; $x_{O_2,8}$; $x_{CO,8}$; $x_{NO,8}$;	$T_{9}; T_{9s}; \dot{n}_{8}; \dot{W}_{t,r}; \eta_{T}$
$x_{NO_2,8}; x_{H_2,8}; x_{OH,8} x_{O,8}; x_{N,8}; x_{H,8}$	
$\dot{n}_8; p_8; y$	

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3. MAIN RESULTS AND DISUSSIONS

This section presents the main results of cycle simulation of Fig (1) operating in regime of enhanced combustion (OEC), obtained by the solution the set of equations presented previously in software EES (Engineering Equation Solver, developed by Fchart). The values for the variables are usually presented as a function of oxygen fraction molar in the oxidizer stream of the combustion chamber (in point 5). The range of values of $x_{02,5}$ are such that the temperature T_6 varies in the range proposed (between 1950K and 2250K), as shown in Fig. (2) bellow:



Figure 2. Adiabatic flame temperature, T_6 , obtained for an adiabatic combustion as a function of the oxygen concentration in point 5 of cycle

Thus, based on what was previously presented, the range of temperatures at which turbines can operate is found in oxygen concentrations between 0.21 and 0.29. The Fig. (3) shows the pure O_2 consumption (stream 4) and the variation of net power for this range of $x_{02,5}$:



Figure 3. Pure oxygen consumption, \dot{n}_4 , and net power output, \dot{W}_{liq} , vs. oxygen concentration in point 5 for T_6 between 1950K and 2250K.

As a result of the increase of the net power, the specific fuel consumption, *sfc*, and thermal efficiency, ε , of the cycle exhibit the behavior shown in Fig.(4):



Figure 4. Specific fuel consumption, *sfc*, and thermal efficiency, ε , as a function of the oxygen concentration in point 5 of cycle for T_6 between 1950K and 2250K.

As the equivalence ratio, Φ , remains constant, the increase in oxygen concentration causes a reduction in nitrogen flow in stream 5. This behavior is shown in Fig.(5) below:



Figure 5. Nitrogen molar flow rate of oxidizer and exhaust gases vs. oxygen concentration in point 5 for T_6 between 1950K and 2250K.

The figure above shows a reduction in the total molar flow of combustion products due to the decrease in concentration (and consequently the flow molar) of nitrogen in the oxidizer (stream 5). Despite this, there is an increase in the emission of some pollutants, mainly due to higher temperature in Point 6. These results are presented below:



Figure 6. Main major species formed in combustion vs. $x_{02,5}$ for T_6 between 1950K and 2250K.



Figure 7. Main minor species formed in combustion vs. $x_{02,5}$ for T_6 between 1950K and 2250K.

Since there is a variation in net power cycle, the most relevant pollutants (NO, CO and CO2) can be given in terms of specific mass flow, as shown in the figure below:



Figure 7. Specific emission of CO, CO₂ and NO as a function of the oxygen concentration in point 5 of cycle for T_6 between 1950K and 2250K.

4. CONCLUSIONS

This work was presented and developed a model that could represent thermodynamically the operation of a typical heavy duty single-shaft gas turbine and the effects of oxygen-enhanced combustion (OEC process) in the equipment operation. For this, special attention was given to some components, mainly the combustion chamber, so that the model could represent approximately the behavior of some of the variables of an actual equipment.

Taking how main constraint to operating temperature of the combustion chamber (between 1950K and 2250K), results showed that it's possible to enrich the oxidizer molar concentration of oxygen up to 29%. An increase of 9.5% in net power output and 1.6% in thermal cycle efficiency was obtained with the application process for this concentrations range. As consequence of these results, there was a 1.5% reduction in specific fuel consumption. However, with respect the emissions, there was an absolute increase in formation of main pollutants (CO, CO₂ and NO_x). In specific terms (net mass flow per net power output), CO₂ emissions decreased by up to 2.1%.

As a next step for this research a study of the energy required for oxygen production should be evaluated, since its need a supply of up to 0.1254 kmol/s (4,013 kg/s) of pure oxygen to sustain the process.

5. ACKNOWLEDGEMENTS

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