CO_2 -Argon-steam oxy-fuel (CARSOXY) combustion for CCS inert gas atmospheres in gas turbines

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Sharp demand for electricity consumption is a serious problem that has led to excessive emissions of CO_2 with its inherent climate change consequences. Oxy-fuel combustion for Carbon Capture and Storage (CCS), a technique which uses pure Oxygen with recirculation of CO_2 gas in the combustion process, may provide one path for the solution of the aforementioned issues by decreasing the emissions from power station plants using gas turbine cycles.

This paper investigates how advanced blends from a combination of concepts such as Oxyfuel combustion, Advanced Humidified (AH) injection and CCS can be used without significantly changing efficiency and power outputs. In this study, 0-D chemical kinetic software (GASEQ) is utilized to generate 120 blends of Argon, H_2O and CO_2. Furthermore, an empirical approach combined with the design of experimental models are implemented. Finally, software (CHEMKIN - PRO) using GRI-3.0 reaction mechanism is utilized. The obtained results from these investigation process indicate elimination of NOx, with enough CO_2 and H_2O in the flue gases to be sequestrated for further treatment or recirculation. Most promising blends have thermodynamic properties similar to those of air Methane, thus ensuring that current systems can go through as less refitting as possible.

Keywords: Inert gases, gas turbine cycle, carbon capture and storage.

1. Introduction

Growing awareness of greenhouse gas (GHG) emissions' increase has driven the development of new approaches that mitigate carbon dioxide CO_2 emissions(Hong et al. 2009). Specifically, Carbon Capture and Storage (CCS) has the potential to mitigate the climate change issue by applying different techniques (Hallett & Haszeldine 2014; World IEA 2012). In brief, CCS is used for capturing carbon dioxide from an abundant source and depositing it into a storage site, such as underground, to keep the atmosphere clean (Figueroa et al. 2008; Sharman 2014). One of the most promising approaches of CCS is Oxyfuel (OF) combustion, which may be required for future power generation plants to mitigate CO_2 emissions (Wall et al. 2013; Anderson et al. 2008). In the OF combustion process, fuel is burned in a pure domain of Oxygen and a portion of the CO_2 products is recycled while the residual CO_2 can be treated (Li et al. 2016).

However, using CO_2 as a working fluid in a gas turbine power plant has a direct impact on thermodynamic properties, such as specific heat ratio and heat capacity. Thus, it reduces the overall efficiency. To address these drawbacks, using a direct injection of up to 10% of water-air mixtures into a combustion chamber can enhance power output up to 15% (Kayhan & Ust 2013; Cheng & Nelson 2002; Bouam et al. 2008). The technique allows that overall efficiency rises and emissions of NOx, which also have an effect on the GHG, decrease (Katharina et al. 2010). The Advanced Humidified Air Turbine (AHAT) cycle represents a new generation of the Humidified cycles, which uses a water atomization cooling (WAC) system, humidifier and water recovery system to enhance the thermal efficiency of the power plant with low NOx emissions compared to a combined cycle (Takeda et al. 2014; Rao 2012; Gotoh 2011).

However, using water restrains inlet temperature, which leads to the issue of flame blowoff and system shutdown. Thus, water injection, which has a theoretical value up to 30% in mass (Goke, 2012), is limited by the combustion process in highly turbulent flames. Thus, Argon could be utilised due to its relatively high concentration in the atmosphere with CO_2-H2O-oxyfuel combustion to raise thermodynamic parameters and increase water content, thus increasing power output whilst allowing CCS. The mixture of these gases can produce a blend which makes possible to overcome the issues in gas turbine cycles such as efficiency, power output and stabilisation of both inlet temperature and flame.

Within the scope of this work, a huge number of blends of Carbon dioxide, Water, Argon and Oxygen have been numerically tested. The goal of these tests is to find the best mixture which has similar thermodynamic properties to that of the current methane-air cycles. Moreover, the selected mixture needs to produce water and CO_2 in exhaust gas that makes possible to utilise CCS technology to reduce the GHG effect while the remaining portion of these products can be used for OF through the AHAT cycle

2. SETUP

The best blend investigation process began by utilising 0- D chemical kinetic model Gaseq to generate 120 blends of Argon, water and CO_2 with pure Oxygen and Methane as fuel. In all of these blends, thermodynamic properties such as outlet temperature, specific heat ratio and heat capacity were calculated. Moreover, mole fractions of both CO_2 and H_2O were determined at 10 bar and 900K conditions, which can be considered industrial operation conditions. For simplicity, each of the blends will be presented with their number and the acronym "(X-Y-Z)", in which "X" stands for the molar percentage of Argon in the blend, "Y" for H_2O and "Z" for CO_2, whilst the remaining of the blend is oxygen and methane at the particular equivalence ratio.
Using this software, different stoichiometric values between 0.667 and 1 within the adiabatic process were considered for each blend. The basis of this software is the complex balance approach at a certain pressure. This method was defined by Sanford Gordon and Bonnie J. McBridge for NASA (Morely 2010). Products have been calculated according to Gibbs free energy equation for n species as indicated in Eq(1).

$$\frac{G}{RT} = \sum_{i=1}^{nSp} \left(\frac{x_i \, G_i^o}{RT} + x_i \ln \frac{x_i}{\sum x_i} + x_i \ln p \right) \quad (1)$$

G_i^o : is the molar free energy at the atmospheric pressure of species i [J/mol]
$\sum x_i$: is the total number of moles in the mixture, *G*: Gibbs free energy [J], *nSp*: Species n
p: Pressure [Pa], *T*: Temperature [K], *R*: Universal Gas Constant [J/mol K]
Results obtained from the 0-D simulation model were fed into an empirical approach comparing to conventional fuel-air mixtures which were used as reference. The maximum and minimum values for each property were selected for these blends in order to divide these values into equal intervals, each of which was given (+,-) signs according to their direction from the reference. In this method, four intervals were taken for each property. A Design of Experiments (DOE) was devised and applied to this study in order to quantify the cause and effect relationship between factors (Anon 2012), which were represented by Argon, water and CO2 and the yields that were determined by the Gaseq program according to the design of the experimental model. This approach also indicates a response by these outputs towards any interaction between the inputs, while saving the cost and efforts of an experiment. In terms of the tool used to apply the D.O. E. approach, Minitab 17 statistical analysis software released in 2014 was selected. This version of the program was utilised in this paper with a two-level full factorial design, as well as random variability while minimizing the number of runs (Minitab Inc. 2014).
Finally, CHEMKIN – PRO was used by applying GRI–Mech 3.0, which provides reliability by considering different critical species for the 1-D combustion chamber model. The reactor configuration consists of two clusters. A perfectly Stirred Reactor (PSR), represents the first cluster in which three distinct zones are used; a mixing zone where fuel is partly premixed, a flame region directly connected to the former and the central recirculation zone (CRZ) where the products are recirculated. The second cluster utilizes a Plug Flow Reactor (PFR) for post-flame operation along a 0.1m duct (Reaction Design 2011). This hybrid PSR- PFR network was used to simulate the flame speed of a gas turbine combustor, Figure 1.

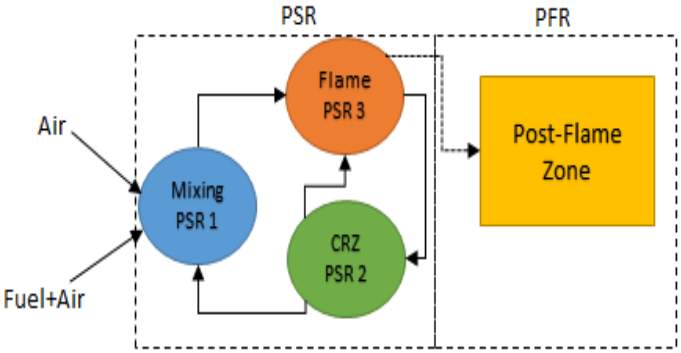


Figure 1. PSR-PFR Schematic.

3. RESULTS AND DISCUSSION

3.1 0-D Chemical Reaction Analysis

Gaseq was applied to determine the thermodynamic properties for each blend, using conversional methane fuel values as a reference for each property. Figures 2, 3, 4, and 5 show outlet temperature, specific heat ratio (ɣ), heat capacity (Cp), and CO_2 product for some selected blends against a range of equivalence ratios. The outlet temperature, Figure 2, indicates that blends 79 (24-19-19) and 109 (24-8-29) have the highest values while the others are just a few degrees lower than those obtained with current air cycles. In one case only, blend 58 (25-

23-19) has approximately the same temperatures as those of pure Methane. Moreover, results show improvement in specific heat ratio in some cases and the increase of heat capacity, Figures 3 and 4, thus enhancing output power. Figures 5 represents complete combustion products. Mole fraction of CO_2 rises around 40% compared to about 10% with air. These concentrations might enable mitigation of a portion of CO_2 products by condensing some of the water, thus capturing both molecules by producing carbon acid. The residual of inert gas and CO2 would have to be recirculated in the cycle.

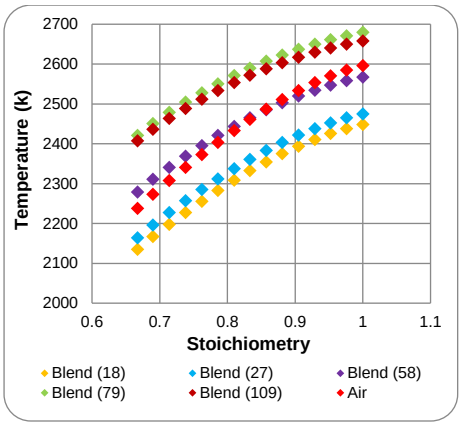


Figure 2. Product Temperatures

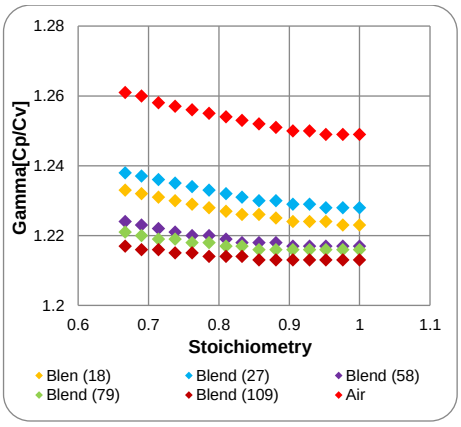


Figure 3. Product Specific Heat Ratio

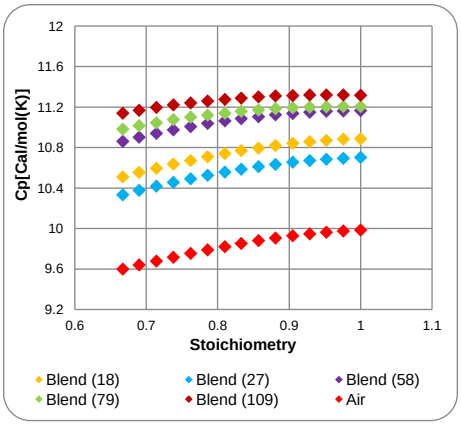


Figure 4. Product Heat capacity

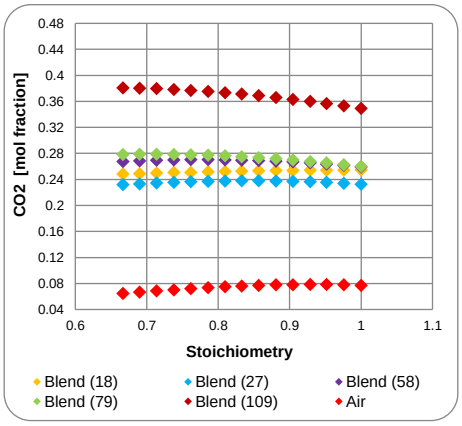


Figure 5. CO_2 Product

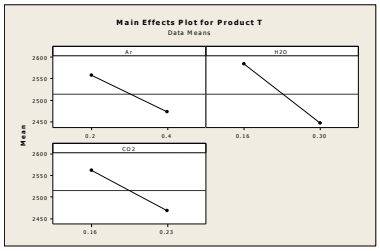
A matrix was created using data obtained from Gaseq, Table 1. The signs (- and +) indicate that the thermodynamic property is higher or lower than the reference one while single, double and even triple numbers for these signs indicate how far or close that blend's properties are to the reference value of Air as the working fluid, Table 1. The presented 16 blends represent the best blends out of 120 cases.

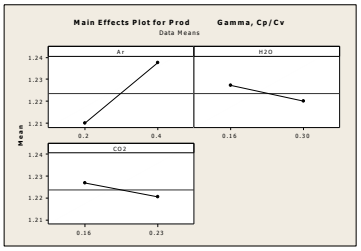
Table 1. The best blends have been selected using empirical method

Case	Ar [Mole fraction]	H2O [Mole fraction]	CO2 [Mole fraction]	T(K)	Cp. [Cal/mole. K]	Gamma [Cp/Cv]	H2O [Mole fraction]	CO2 [Mole fraction]
Air				2596.4	9.983	1.249	0.177607	0.076828
4	0.24434	0.27149	0.1991	- -	++	- -	+++	++
5	0.262443	0.271493	0.180995	-	++	--	+++	++
6	0.2271493	0.2271493	0.171946	-	++	- -	+++	++
18	0.287	0.25112	0.17937	-	+	- -	+++	++
20	0.23963	0.24885	0.2212	-	++	- -	+++	++
26	0.34335	0.23176	0.15451	-	+	-	+++	+
27	0.30769	0.24434	0.1629	-	+	-	+++	++
32	0.2467	0.22907	0.2467	- -	++	- -	+++	++
33	0.29224	0.23744	0.18265	-	+	- -	+++	++
34	0.26484	0.23744	0.21005	-	++	- -	+++	++
49	0.26906	0.2242	0.2242	- -	++	- -	+++	++
58	0.25131	0.23037	0.18848	0	++	- -	+++	++
59	0.2654	0.20853	0.22749	-	++	- -	+++	++
69	0.25571	0.18265	0.27397	- -	++	- -	++	++
79	0.23952	0.19162	0.19162	+	++	- -	+++	++
109	0.24242	0.08485	0.29091	0	++	- -	++	+++

3.2 DOE Analysis

The essential finding in DOE process is how these factors affect the thermodynamic properties positively and negatively. As Figure 6 shows, the temperature responds inversely to all factors: Ar, H_2O and CO_2. Figure 7 illustrates the response in Gamma, which is enhanced by Argon while there is a negative impact on its value by water and CO_2. For specific heat ratio both water and CO_2 have a positive impact on its amount. On the other hand, an increase in inert gas has reflected negatively on its value as illustrated in Figure 8.





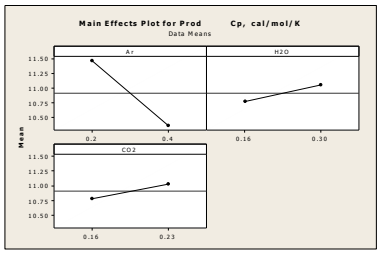


Figure 6. Main effects. Temp. **Figure 7. Main effects. Gamma** **Figure 8. Main effects. Cp.**

3.3 Combustion Characteristics

Flame speeds were calculated for the 8 most promising blends, Table 2. Out these blends, 3 blends, i.e. 58 (25-23-19), 79 (24-19-19) and 109 (24-8-29), were selected for further studies because they had flame speeds close to that of pure methane-air. A forth blend, i.e. 27 (30-24-16), was also included for comparison purposes, although its flame speed falls to half of that of methane-air.

Data obtained from the 1-D simulation model in the PSR-PFR reactor cluster show the temperature of the blend 58 (25-23-19) approximately matching the one of pure methane, Figure 9. Furthermore, Figures 10, 11 and 12 show that this blend produces elevated CO_2 in the flue gases, ~1.5 times CO than pure methane and high H_2O concentration for recovery purposes.

Table 2. Flame speed at 1 and 10 Bar for selected blends.

Pressure condition (bar)	Flame Speed (cm/sec.)								
	Pure Methane	Blend (Table 1)							
		27	58	79	109	33	26	18	6
1	43.1	21.8	31.2	45.3	38.4	21.7	20.3	20.1	20.4
10	15.1	7.97	12.7	21.2	17.8	7.23	6.4	6.5	6.76

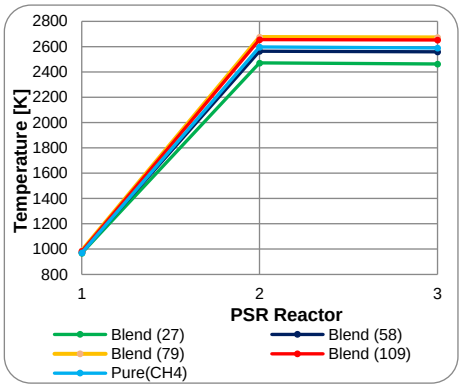


Figure 9. Temperature at PSR

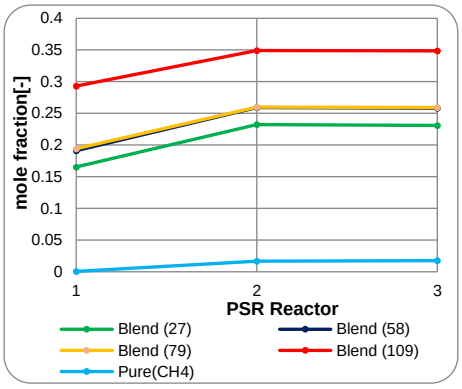


Figure 10. Mole fraction of CO_2 at PSR

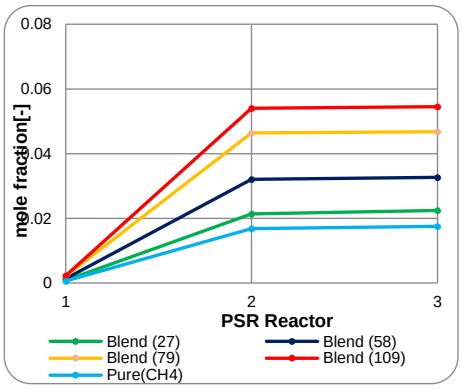


Figure 11. Mole fraction of CO at PSR

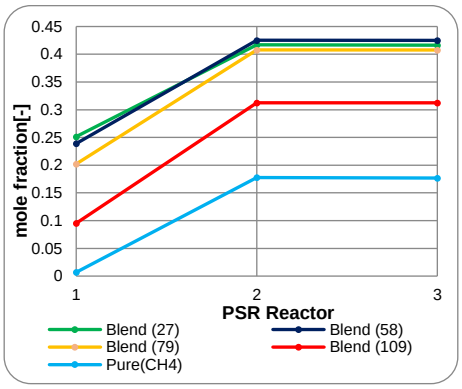


Figure 12. Mole fraction of H_2O at PSR

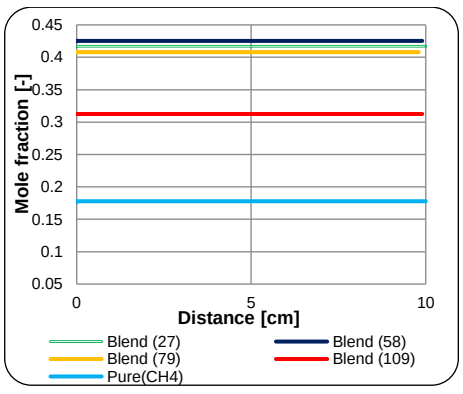


Figure 13. Mole fraction of H2O at PFR

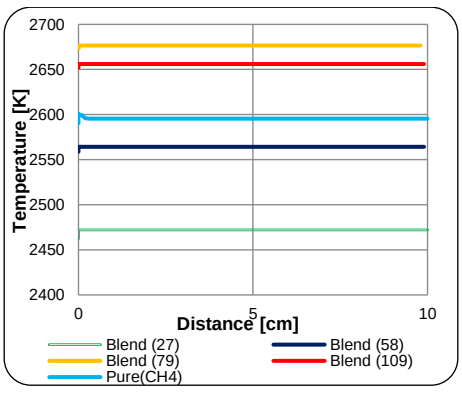


Figure 14. Temperature at (PFR)

Further downstream the reaction zone, mole fraction of water and carbon dioxide remain high, showing a drop in ~50K for the temperature of the flue gases for blend 58 (25-23-19), Figures 13 and 14. The results also show how a high inert blend with vast water content such as 27 (30-24-16) can still have acceptable parameters

through its combustion, Figures 13 and 14. However, the considerable reduction of flame speed, i.e. higher propensity to blowoff, demonstrated that although good properties can be obtained from some blends, definition of the best inert/water/carbon dioxide concentration requires a deep understanding of not only their thermodynamic properties when burned, but also knowledge of their flame and combustion characteristics. Thus, further research is required to demonstrate that the best blend, 58 (25-23-19), can be used under real gas turbine operating conditions.

4. CONCLUSIONS

This study was carried out to utilise oxyfuel, CCS and AHAT techniques in a gas turbine combustor by finding the best blend out of a number of mixtures consisting of CO_2, water and Argon with pure oxygen and methane. Simulations integrated with empirical approach data show that blend 58 (25% Ar-23% H_2O-19% CO_2) has approximately similar outlet temperature to that obtained for current air cycle. Additionally, the flame speed of this blend is just lower than for conventional fuel in an air domain at the same pressure conditions. This blend also has the highest mole fraction of water product with high mole fraction of CO_2, gases that might enable to be captured and stored away from the atmosphere with zero percentage of NOx. The residual part of CO_2 could be recirculated through the cycle. Thus, future work is recommended to demonstrate that this blend can be used for real operating gas turbine conditions, showing through an analytical study the power outputs and efficiency of the final cycle.

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