GLYCEROL, AN ALTERNATIVE ENERGY SOURCE: COMBUSTION AND DESIGN OF A Y-JET ATOMIZER

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Abstract. *The depletion of fossil fuels and environmental problems involving the burning of these fuels is a major environmental concern worldwide. As a consequence, there is a search for processes and energy sources that do not degrade the environment, are energy efficient and meet the demand of energy required. At the peak of biodiesel production, a relevant issue is the amount of waste produced. In this case, glycerol is the main byproduct.*
With an increased amount of glycerol on the market, concerns arise both in the economic and environmental spheres, including issues such as the drop in the price of glycerol as it is stocked by manufacturers and, secondly glycerol cannot be freely disposed of in the environment. This article will discuss a study of the combustion of four different types of glycerol: the most economically viable type, crude glycerol; methylated glycerol; demethylated glycerol; pure glycerol and glycerol mixture with pure ethanol. Both a theoretical thermochemical analysis (adiabatic flame temperature and enthalpy of formation) and gas emissions analysis of the combustion of these types of glycerol will be presented. A Y-Jet Atomizer to burn pure glycerol and ethanol blends, by calculating the average droplet diameter and main dimensions of the atomizer will also be carried out.
Keywords: *Glycerol, combustion, atomization, emissions,*

1. INTRODUCION

Biodiesel is produced from transesterification of triglycerides (oils, fats or lipids) with an alcohol reagent, for example, methanol or ethanol. Glycerol is the main byproduct of biodiesel production, which generates about 10% (w / w). The excess glycerol produced can become an environmental problem, since it cannot be disposed of in the environment. Currently glycerol is used in beverage and food, pharmaceutical, chemical, cosmetic, petrochemical, and textile industrial sectors, etc. These industries are not absorbing all production. An alternative way of using large amounts of glycerol is to burn it. An example of this would be for combustion chambers of small size. However, the combustion process of glycerol is not easy and presents some technological difficulties. On the other hand, there are several benefits such as reducing the use of fossil fuels, storage, and emissions of greenhouse gases. Biodiesel production has increased considerably, so an excess of glycerol on the market and looking for a solution for this by-product is of great importance both economically and environmentally.

The current price of crude glycerin is so low (0.04 to 0.11 $ / kg, $ 0.02-0.05 / lb.) that many producers prefer to store biodiesel glycerol while waiting for better market prices.

In this article, a study of combustion and thermochemical properties of the main several glycerol types: raw glycerol, methylated, and demethylated glycerol and mixtures with ethanol at different percentages were performed. As glycerol is becoming an alternative energy source, being a biofuel, it is important to develop technologies for atomization and combustion, for example, a Y-Jet Atomizer. This type of Y-Jet Atomizer is currently used to burn other fuels, such as diesel and alcohol and especially fuels with high rate of viscosity. In this study, a method for scaling the atomizer is done for pure glycerol and mixtures with ethanol.

2. FUEL

There are variations in the composition and physic-chemical state of different types of glycerol, which generally determine the degree of ease for its combustion or use in acceptable conditions, considering the technical point of view, economic and environmental point of view. Commercially there are several types of glycerol, such as raw glycerol, methylated and demethylated glycerol (blond glycerin, as it is known in Brazil) and refined glycerol (USP° Glycerin – *U. S. Pharmacopeia)*, all with different percentages of purity which depend on final application. This article will examine the first three mentioned types as well as mixtures with ethanol, USP° Glycerin combustion was not taken into account seeing that the USP° Glycerin is the most expensive as it is the most refined, invalidating its combustion in the

economic realm. Crude glycerol contains from 40 to 80% glycerol and other components such as salts, water, matter organic non-glycerol (MONG) and other residues from the production of biodiesel. (MATURANA, 2011). Methylated glycerol has from 50 to 70% glycerol, 10-20% methanol, 5-10% salts, <3-10% water, <5-1% MONG. Demethylated glycerol (blond glycerin) 70-88% glycerol, <1% methanol, 5-15% salts, <5-15% water, <1-5% free fatty acids and <1-5% MONG. (BOHON, 2011). USP Glycerin (refined) has 99% purity. (MATURANA 2011; HESS, 2007; THOMPSON, 2006 e HE, 2006). The blends have 25% pure glycerol ($C_3H_8O_3$) and 75% ethanol, 50% pure glycerol and 50% ethanol and finally 25% pure glycerol and 75% ethanol.   .

Table 1 presents wt % values for different types of glycerol for this study. The concentrations of salts such as sodium, potassium and magnesium were added to the ash content, since they do not react in the combustion reaction.

Table 1 - wt % values for different types of glycerol

	Crude Glycerol[1]	Methylated Glycerol[2]	Demethylated Glycerol[3]	°USP Glycerin[2]
% C	50.29	42.05	49.46	39.1
% H	9.66	10.14	9.57	8.7
% N	2.6	<0.05	<0.27	0
% O	37.21	43.32	37.72	52.2
% S	0.24	0.078	<0.2	0
% H$_2$O	--	1.03	2.48	0
% Ash	--	3.06	3.12	0
HHV (MJ/kg)	25.5	21.8	26	16

[1] Maturana,2011, [2] Bohon 2011, [3] Steinmetz,2013.

It is important to mention that during the research there was a high deviation in the oxygen concentration of demethylated glycerol reported by Bohon *et al.* (2011) which did not coincide with the theoretical Higher Heating Value (HHV) calculated from the mass composition of this glycerol; so demethylated glycerol was used in other literature. The case in question referenced here is demethylated glycerol, reported by Steimetz (2013). An important property of the fuel is its calorific value, as this demonstrates the chemical energy of the fuel. The calorific value of glycerol depends on the raw material used in their production. (THOMPSON and HE, 2006). Many researchers have reported different values for the glycerol Lower Heating Value (LHV), among them, Soares *et al.* (2006) reported a LHV of 16.07 MJ / kg, Da Silva and Müller (2010) reported 16.18 MJ / kg; Vaz *et al.* (2010) reported a LHV approximately 19.0 MJ / kg. Moreover, Thamsiriroj and Murphy (2010) reported for the glycerol residue obtained as biodiesel from rapeseed and corn for example, a LHV 19.2 MJ / kg and for the glycerol obtained from waste fats its LHV is 14.82 MJ / kg. The heat of combustion of the virgin oils had an average of 19.56 MJ / kg which is about 10% higher than that obtained from crude glycerol, which was approximately 18 MJ/kg according to Lide (1999). The glycerol's combustion heat is about two times lesser than that of fossil fuels; but it is comparable to most types of biomass, such as wood, straw, bagasse, oil, bark, sawdust and willow. The calorific value is lower due to the high presence of water which is obtained (STEMELMACHOWKI, 2011).

3. COMBUSTION

There are several factors and thermochemical properties relevant to the study of the combustion of a fuel, especially for liquid fuels. Among them are: the calorific value; the amount of excess air; turbulence for atomization; adiabatic flame temperature and enthalpy of formation. For a specific study of the combustion about the glycerols mentioned above, the combustion was realized at 20% excess air to utilize it on a Y-type atomizer, thus favoring the complete combustion of a fuel with high viscosity. Sprays are generally burned with excess air of 5 to 25%. (WILLIAMS, 1990, PÉREZ, 2007). However, the combustion process in crude glycerol is not easy from a technological point of view. According to some researchers METZGER, (2007) and (BOHON) *et al.,* 2011, among the difficulties for the burning of glycerol, the following can be cited:

a) LHV has between 16 and 21 MJ/kg, which makes it unable to maintain a stable flame in a conventional burner, besides being hampered by the presence of water in the mix.

b) High auto-ignition temperature, i.e., around 370ºC as compared to 280ºC for gasoline and 210ºC for kerosene;

c) The burning of glycerol can produce acrolein;

d) High viscosity at room temperature (kinematic viscosity of about 450 cSt for refined glycerol), making it difficult to atomize with standard atomizers;

e) The presence of salt contents causes corrosion problems in the burner's atomizers and in the post-combustion system, being also flame inhibitors, therefore hindering the glycerol combustion.

There are effective methods to tackle or minimize many of these obstacles, such as the emission of acrolein, a carcinogen substance. It has been reported that, when heated above 280ºC, this substance cannot be produced, moreover, under controlled combustion and good atomization this problem could be overcome (MATURANA, 2011). Salts can be removed or reduced by filtration. The other obstacles mentioned above can be overcome with a mixture of glycerol and low-viscosity fuel, whereas the development of technologies suitable for its burning with mixtures would be decisive.

Based on the combustion heat, a direct thermal utilization of crude glycerol is an obvious choice. Studies have reported that the co-firing of crude glycerol with other biomasses would yield favorable results (OBERBERG and JAUSCHENG, 1998). An attractive and simple option for the use of crude glycerol would be as a fuel for boilers in heat and power production (EPP, 2008).

According to DAF (2006) and BOMBOS *et al.* (2011), modern boilers are designed to bear certain thermal stresses in fireboxes; therefore, the direct utilization of glycerol in the existing boilers is unacceptable due to its high combustion heat and low adiabatic flame temperature. Nowadays, the most common uses of crude glycerol as biofuel and alternative energy sources are for incineration (DAF, 2006). Thus, taking into account an average calorific value of 17.5 MJ/kg, and an average cost of 0.08 US$/kg, the thermal energy produced has an average cost of 0.0045 US$/MJ, which is slightly lower than an equivalent amount of heat burning natural gas. The co-combustion of glycerol with other liquid or solid fuels has not been carried out in large scales yet (STELMACHOWSKI, 2011).

Another relevant point of this study regards turbulence as the most difficult factor to be achieved and essential to assure a satisfactory fuel-air mixture, blaze shape and total fuel burning.

In order to achieve satisfactory combustion, the following parameters are necessary:
1) Fuel atomization;
2) Fuel vaporization;
3) Air-fuel mixture.

Consequences of inefficiency in these phases can generate:
- Nebulization: Dripping, coking in the torch, sparking, defective vaporization.
- Vaporization: Dripping, coking, sparkling, poor air mixture.
- Mixture: Incomplete combustion, formation of CO and soot, long oscillating flame, unnecessary air in excess.

In the industrial combustion process it is practically impossible to obtain a complete combustion without having air in excess, due to the lack of a perfect homogenization between the air and the fuel. Stoichiometric combustion would be the ideal process as heat would not be lost for heating the excess air.

Summarizing, in order to achieve complete combustion, with stable and short flame and low excess air, a satisfactory air-fuel ratio is essential. To do so, suitable turbulence must be obtained. In liquid fuels, to enable a good mixture, good vaporization and atomization is fundamental. For these motives, liquid combustion is more complex (ASSUNÇÃO *et.al.*, 1993).

Relevant results obtained through this study on fuel combustion are adiabatic flame temperature (T_{ad}), enthalpy formation (h_f), low heat value (LHV) and air-fuel ratio (AF). For crude glycerol and ethanol the LHV used is that provided in scientific literature. From the mass percentage in the referred literature (Table 1) molar compositions were determined for the combustion reaction, and, with the chemical balance an algorithm in Fortran programming language was developed to achieve T_{ad} e h_f

4. ATOMIZER

For the dimensioning of the Y-Jet Atomizer, a point to be studied is fuel atomization and its leading factors. Atomization involves the formation of pellicles and/or ligaments around the atomizer and the further formation of droplets. This phase is extremely important, and a good atomization is essential for the combustion process. Atomization is strongly influenced by the atomizer's geometry and diameter, fuel properties, atomization fluid and its relative velocity, as well as by the surrounding environmental conditions (temperature, humidity, among others). Basically, atomization consists of increasing the surface area of the fluid. In this process, a liquid jet, film or sheet is disintegrated by the kinetic energy of the liquid itself or by exposure to high velocity air or gas, or even as a result of external mechanical energy applied through rotating devices.

Aerodynamic forces act on the surface of the liquid causing disruptions that disseminate like waves and contribute to the instability of liquid jet, film or sheet. Liquid breakup and ligament formation occur when the magnitude of the disruptive force exceeds the liquid surface tension force. In the disintegration process, where ligaments are fragmented into drops, many of the larger drops produced are unstable and undergo further disintegration into smaller droplets resulting in spray (LACAVA, 2009).

4.1 Y-Jet Atomizer

Y-Jet atomizers are widely used in industrial furnaces, moreover with high-viscous liquids (SONG and LEE, 1994). It may have between six and thirty jets, arranged in a way to produce a hollow cone spray pattern, according to

Mattos Ana Paula, Quintero Juan Gabriel, Velásquez Elkin, Coronado Christian R., Nascimento Marco Antônio R.
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Mullinger and Chigier (1974), Lacava (2000) and Pacifico (2000). Y-Jets are widely used due to their advantages as simple configuration and adaptability, stable pulverization angle when fuel or atomization gas flow varies, good spray quality with low consumption being operational with highly viscous fuels.

In order to build one, further studies on geometric dimensions must be carried out, such as Figure 1 (PÉREZ, 2007), which will be approached in the dimensioning of the atomizer.

- Diameter of the air inlet pipe (d_a),
- Diameter of the glycerol inlet pipe (d_c),
- Diameter of the mixing chamber (d_m),
- Length of the pre-mixture (l),
- Length of the mixture (l_m),
- Length of the air inlet pipe (l_a),
- Length of the fuel inlet pipe (l_c),
- Angle of the fuel inlet channel (θ),
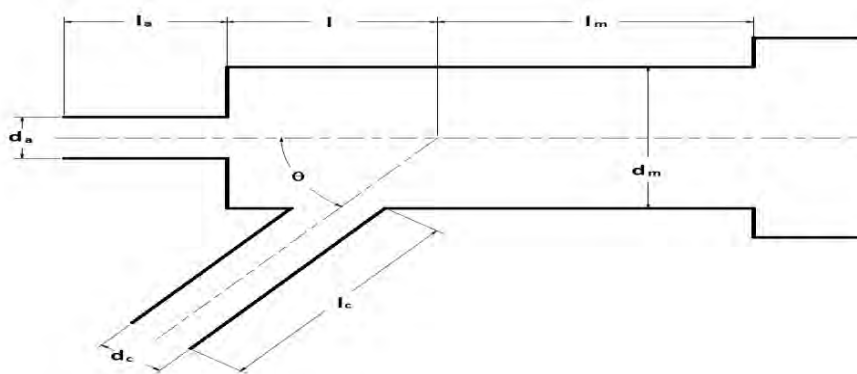- Analysis of the fuel flow conditions.

Figure 1 - Schematic drawing of the atomizer

5. EMISSIONS

One key feature of biomass fuels is its high oxygen content, which results in low production of particulate matter (PM), carbon monoxide (CO), total hydrocarbons (HCT) and the absence of sulfur oxide (SOx) (MATURANA, 2011).

Glycerol is a renewable, biodegradable biologically-based product. Its production process is connected to green refineries having high environmental value, besides contributing to the independence of fossil fuels (RAHMAT *et al.*, 2010). Its use as a burning fuel does not increase the emission of pollutants in the atmosphere. Therefore, the use of glycerol as a fuel in industrial processes has several advantages, mostly in cogeneration.

Emission calculations were performed for carbon dioxide and sulfur dioxide, as both have high pollutant potential, and are one of the main greenhouse effect gases.

Eqs. (1) and (2) were used for the calculation of carbon dioxide and sulfur dioxide emissions, respectively.

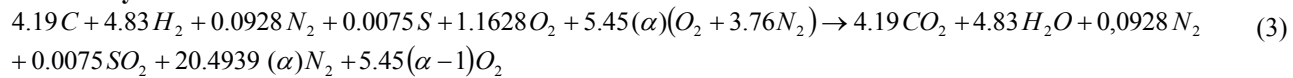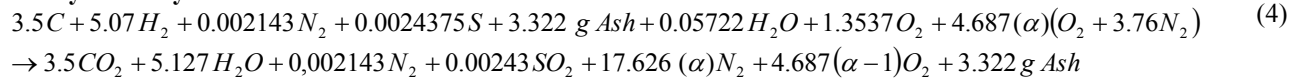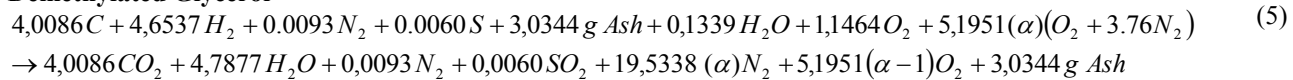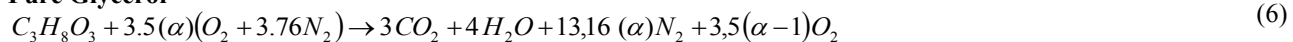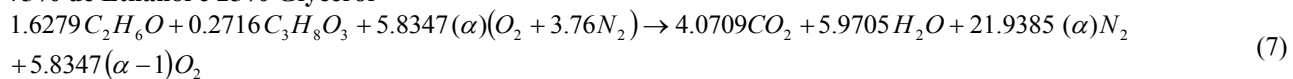$$P_{CO_2} = \frac{n_{CO_2}\, M_{CO_2}}{n_c\, M_c\, PCI} \tag{1}$$

$$P_{SO_2} = \left(\frac{\%\ the\ mass\ of\ sulfur\ in\ fuel.\, MM\ SO_2}{100}\ \frac{}{MM\ S}\right)\left(\frac{1\ kg\ fuel.}{PCI\, fuel.}\right)\left(\frac{10^6\ kJ}{1GJ}\right)\left(\frac{1000\ gr}{1\ kg}\right) \tag{2}$$

6. METHODOLOGY MATHEMATICS - THERMOCHEMISTRY:

6.1 Combustion

To start the combustion calculations, it is first necessary to determine the mass percentages of the types of glycerol (Table 1) to perform the chemical balance, as well as the LHV of the fuel to calculate T_{ad} and h_f.

Eqs. (3-10) demonstrates the combustion reactions to crude glycerol, methylated glycerol, demethylated glycerol, pure glycerol and mixtures and ethanol. The chemical compositions of Table 1 were corrected to close the balance to 100%.

Crude Glycerol

$$4.19\,C + 4.83\,H_2 + 0.0928\,N_2 + 0.0075\,S + 1.1628\,O_2 + 5.45\,(\alpha)(O_2 + 3.76\,N_2) \rightarrow 4.19\,CO_2 + 4.83\,H_2O + 0.0928\,N_2 \quad (3)$$
$$+ 0.0075\,SO_2 + 20.4939\,(\alpha)N_2 + 5.45\,(\alpha - 1)O_2$$

Methylated Glycerol

$$3.5\,C + 5.07\,H_2 + 0.002143\,N_2 + 0.0024375\,S + 3.322\,g\,Ash + 0.05722\,H_2O + 1.3537\,O_2 + 4.687\,(\alpha)(O_2 + 3.76\,N_2) \quad (4)$$
$$\rightarrow 3.5\,CO_2 + 5.127\,H_2O + 0.002143\,N_2 + 0.00243\,SO_2 + 17.626\,(\alpha)N_2 + 4.687\,(\alpha - 1)O_2 + 3.322\,g\,Ash$$

Demethylated Glycerol

$$4.0086\,C + 4.6537\,H_2 + 0.0093\,N_2 + 0.0060\,S + 3.0344\,g\,Ash + 0.1339\,H_2O + 1.1464\,O_2 + 5.1951\,(\alpha)(O_2 + 3.76\,N_2) \quad (5)$$
$$\rightarrow 4.0086\,CO_2 + 4.7877\,H_2O + 0.0093\,N_2 + 0.0060\,SO_2 + 19.5338\,(\alpha)N_2 + 5.1951\,(\alpha - 1)O_2 + 3.0344\,g\,Ash$$

Pure Glycerol

$$C_3H_8O_3 + 3.5\,(\alpha)(O_2 + 3.76\,N_2) \rightarrow 3\,CO_2 + 4\,H_2O + 13.16\,(\alpha)N_2 + 3.5\,(\alpha - 1)O_2 \quad (6)$$

75% de Ethanol e 25% Glycerol

$$1.6279\,C_2H_6O + 0.2716\,C_3H_8O_3 + 5.8347\,(\alpha)(O_2 + 3.76\,N_2) \rightarrow 4.0709\,CO_2 + 5.9705\,H_2O + 21.9385\,(\alpha)N_2 \quad (7)$$
$$+ 5.8347\,(\alpha - 1)O_2$$

50% de Ethanol e 50% Glycerol

$$1.0853\,C_2H_6O + 0.5433\,C_3H_8O_3 + 5.1576\,(\alpha)(O_2 + 3.76\,N_2) \rightarrow 3.8006\,CO_2 + 5.4293\,H_2O + 19.3928\,(\alpha)N_2 \quad (8)$$
$$+ 5.1576\,(\alpha - 1)O_2$$
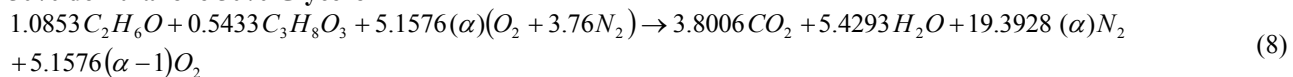
25% de Ethanol e 75% Glycerol

$$0.5426\,C_2H_6O + 0.8150\,C_3H_8O_3 + 4.4805\,(\alpha)(O_2 + 3.76\,N_2) \rightarrow 3.5304\,CO_2 + 4.8881\,H_2O + 16.8466\,(\alpha)N_2 \quad (9)$$
$$+ 4.4805\,(\alpha - 1)O_2$$

Ethanol

$$C_2H_6O + 3\,(\alpha)(O_2 + 3.76\,N_2) \rightarrow 2\,CO_2 + 3\,H_2O + 11.28\,(\alpha)N_2 + 3\,(\alpha - 1)O_2 \quad (10)$$
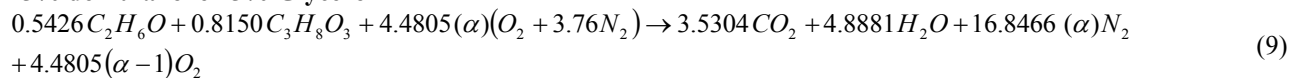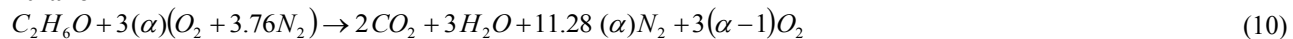
6.2 Higher and Lower Heating Value (HHV, LHV)

Analyses for the higher and lower heating values were used for two empirical Mendeleev formulations Eq. (11) and Eq. (12) respectively, held a comparison with the scientific literature. This calculation was not performed for pure glycerol and mixtures with ethanol. This value utilized was obtained directly from the scientific literature.

$$Q^h = 4.187\,(81C + 300H - 26(O - S)) \quad (11)$$

$$Q^l = 4.187\,(81C + 300H - 26(O - S) - 6(W + 9H)) \quad (12)$$

6.3 Adibatic Flame Temperature (T$_{ad}$)

T_{ad} is the highest temperature that can be obtained for combustion products. This temperature can be reached if there is no loss in the process. (CARVALHO, 2007). In order to calculate this temperature, two methods can be employed: specific heats, Equation (13) or enthalpy tables, Equation (14):

$$\Delta H_c = \int_{T_I}^{T_F} \sum_i n_i\,c_{p,i}\,dT \quad (13)$$

$$\sum_{Products} n_i\,(\bar{h}_f + \Delta\bar{h}) = \sum_{Reagents} n_i\,(\bar{h}_f + \Delta\bar{h}) \quad (14)$$

For this study, T_{ad} was calculated using specific heats methods due to the fact that there are insufficient data available in the scientific literature about the enthalpy of formation "h_f" of different types of glycerol being analyzed in this article. Conversely, there are no enthalpy values for a given temperature $\bar{h}_T$ of some components (SO$_2$, ash).

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To use this method, it is necessary to calculate the specific heat of different gases. The polynomial equation Eq. (15) of the specific heat is: (CENGEL, 2007).

$$c_p = a + bT + cT^2 + dT^3 \tag{15}$$

The coefficients used in Eq (15) are shown in Table 2.

Table 2 – Coefficients to calculate specific heat.

	a	b	c	d
CO_2	22.26	$5.981*10^{-2}$	$-3.501*10^{-5}$	$7.469*10^{-9}$
H_2O	32.24	$0.1923*10^{-2}$	$1.055*10^{-5}$	$-3.595*10^{-9}$
N_2	28.90	$-0.01571*10^{-2}$	$0.8081*10^{-5}$	$-2.873*10^{-9}$
O_2	25.48	$1.520*10^{-2}$	$-0.7155*10^{-5}$	$1.312*10^{-9}$
SO_2	25.78	$5.795*10^{-2}$	$-3.812*10^{-5}$	$8.612*10^{-9}$

The ashes were assumed as graphite, therefore, c_p of the ash is a function of temperature and can be calculated according to Eq (16) (CARVALHO, 2007):

$$c_{p(Ash)} = 2.673 + 0.00217\,T - \frac{116900}{T^2} \tag{16}$$

The T_{ad} is normally higher than 2000 K. Owing to the heat transfer for the materials and processes in the combustion chamber, the adiabatic flame temperature of liquid fuel is approximately 1400 to 1900 K. [PÉREZ, 2007].

6.4 Entalphy of Formation

To calculate the enthalpy of formation, T_{ad} must be known and through the use of the second method to calculate this parameter, or by using the enthalpy tables Eq (14), the enthalpy of formation of each type of glycerol analyzed in this article can be calculated. It is necessary to know the values of the enthalpy of formation $\bar{h}_f$ of the elements involved in combustion for this calculation. These values are found in any book on thermodynamics (CENGEL, 2007).

6.5 Air – Fuel Ratio

It is important to determine the air fuel ratio (AF) for efficient combustion, in order to not cause incomplete combustion, in which soot occurs (unburned C) and CO forms. Furthermore, inappropriate excess of air should be avoided in order to not diminish the flame temperature because of the inert gas N_2. To calculate the air-fuel ratio, see Eq (17).

$$AF = \frac{Mass\ Air}{Mass\ Fuel} \tag{17}$$

6.6 Atomizer:

To calculate the atomizer, it is first necessary to obtain the average fuel droplet diameter (SMD). This diameter for the Y-Jet atomizer can be calculated with the empirical formulation of Eq. (18), proposed by Wigg (CHIGIER and MULLINGER, 1974):

$$D_m = \frac{200.v^{0,5}\dot{m}_c^{0,1}\left(1+{\dot{m}_c}/{\dot{m}_{at}}\right)^{0,5}h^{0,1}\sigma^{0,2}}{\rho_{at}^{0,3}V_a} \tag{18}$$

With this diameter, it is possible to follow the recommendations of Chigier and Mullinger (1974), based on experimental results. In Eq (18) it can be observed that the factors that influence the droplet size of the spray produced

by the Y-Jet atomizer can be geometric, operational and physicochemical properties of the fluids. Mullinger and Chigier (1974) presented some technical recommendations for dimensioning a J-Jet atomizer. Table 3 shows the measurements of this atomizer, expressed as a function of diameter of the air inlet pipe (da):

Table 3 – Recommended values for the Y-Jet Atomizer dimensions

Diameter of the air line pipe (mm)	d_a *(calculated)*
Diameter of the glycerol inlet pipe	$d_c = d_a$
Diameter of the mixing chamber	$d_m = (1.4\text{-}1.8)d_a$
Length of the pre-mixture	$l = (1\text{-}2)\ d_a$
Length of the mixture	$l_m = (4\text{-}5)\ d_a$
Length of the air inlet pipe	$l_a > 2\ d_a$
Length of the fuel inlet pipe	$L_c > 2\ d_c$
Angle of the fuel inlet channel	$\theta = 52°$

The Diameter of the air inlet pipe, d_a, can be calculated using the equation of continuity, Eq. (19) in the pipe (PÉREZ, 2007).

$$\dot{m}_{at} = \frac{\pi \cdot d_a^2 \rho_{at} V_{at}}{4} \tag{19}$$

Where:
The rate of spray is described by equation (20).

$$V_{at} = Ma\sqrt{\gamma.R.T} \tag{20}$$

In addition to the geometric recommendations , Mullinger and Chigier (1974) also elaborated suggestions with respect to fuel flow conditions:
• The ratio between mass flow rate of atomizing AF ratio should be greater than or equal to 0.1 or 0.15;
• The speed of atomizing air is equal to critical velocity flow conditions. The Mach number = 1.
• The pressure drop coefficient through the fuel supply pipe = 0.75.
After all these considerations, the design geometry for the Y-Jet Atomizer was obtained and which was used for combustion of several kinds of glycerol under study.

7. RESULTS AND CONCLUSIONS

7.1 Combustion reaction

Chemical balance was carried out for 100 grams of fuel. At 20% excess air, just consider α = 1.2 and using the coefficients of the stoichiometric reaction.
The next step is to calculate the upper and lower calorific values. Table 4 shows the results of HHV and LHV found in the scientific literature and calculated using the Eqs. (11) and (12).

Table 4 - HHV and LHV comparisons.

	Crude Glycerol	Methylated Glycerol	Demethylated Glycerol	Glycerol	75% Glycerol + 25% Ethanol	50% Glycerol + 50% Ethanol	25% Glycerol + 75% Ethanol	Ethanol
HHV [1] (MJ/Kg)	25.53	21.80	26.00	16.00	--	--	--	--
LHV [1] (MJ/kg)	20.424	17.44	20.80	12.80	--	--	--	28.22
LHV [2] (MJ/kg)	22.980	19.972	22.484	--	16.65	20.51	24.37	--
LHV Deviation	12.51%	14.50%	8.10%	--	--	--	--	--

[1] Values found in the literature. [2]Calculation values.

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Table 5 shows the values found for the adiabatic flame temperature (T_{ad}), enthalpy of formation (h_f) and air-fuel ratio (AF), with 20% excess air for calculated LHV.

Table 5 - Thermochemical properties of fuels.

	Crude Glycerol	Methylated Glycerol	Demethylated Glycerol	Glycerol	75% Glycerol + 25% Ethanol	50% Glycerol + 50% Ethanol	25% Glycerol + 75% Ethanol	Ethanol
T_{ad} (K)[1]	1899.61	1842.05	1984.65	1673,8	--	--	--	
T_{ad} (K)[2]	2081.55	2043.95	2109.36	--	1786.15	1958.50	2056.90	--
h_f (kJ/kmol)[1]	-777005.12	-873918.33	-657108.08	-969994	--	--	--	-212079.50
h_f (kJ/kmol)[2]	-521404.31	-620718.19	-488705.29	--	-938364.5	-1023180.8	-577402.7	--
AF	8.98	7.71	8.55	6.17	7.38	8.49	9.61	6.60

[1] LHV from literature data. [2] Calculated LHV data.

Figures 2 and 3 show the behavior of h_f and T_{ad} in respect to maximum and minimum LHV values found in the literature for different types of glycerol.
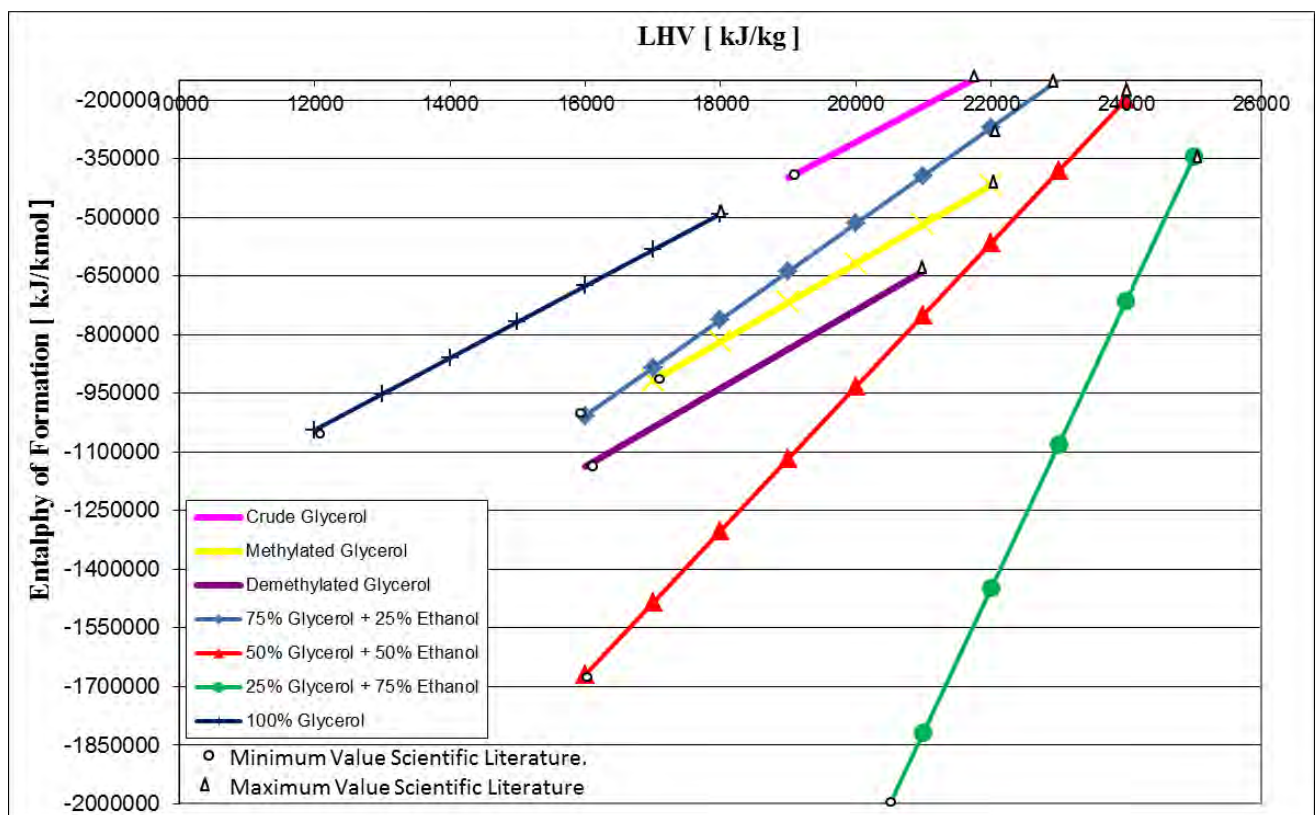

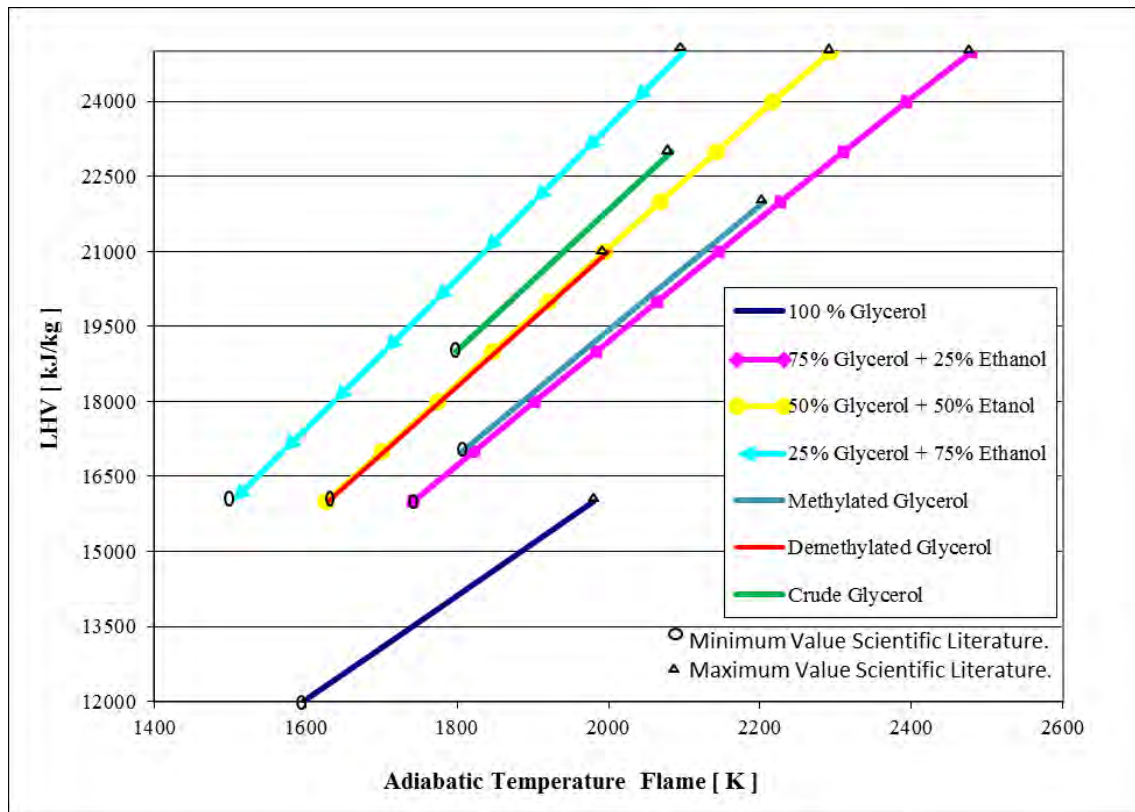Figure 2 - Correlation between the fuel enthalpy of formation and LHV.

Figure 3 - Correlation between fuel adiabatic temperature flame and LHV.

7.2 Atomizer

An atomizer was scaled to burn glycerol with ethanol due to the difficulty of burning glycerol as a result of its viscosity and other barriers already mentioned.

Table 6 shows the properties of each fuel for droplets diameter of fuel (SMD) calculation in Eq. (18). Table 7 shows general data for the design of the atomizer. The properties are used for the temperature of 294 K. Mullinger and Chigier (1974) related recommendations generated Tab. (3) for an atomizer with the geometric parameters of a Y-Jet Atomizer. As an initial condition, the project was established which would generate 100 kW power.

Table 6 – Properties for fuel droplet diameter calculation (SMD**)**.

Properties	Glycerol	Ethanol	75% Glycerol +25% Ethanol	50% Glycerol +50% Ethanol	25% Glycerol +75% Ethanol
Specific Mass (kg/m^3)[1]	1261.51	789.91	943.62	1070.14	1174
Viscosities (µPa s)[1]	1390	1.214	8.74	48.56	256
Kinematics Viscosities (cst)[2]	1101.854	1.536	9.262	45.377	218.057
Surface Tension (dyn/cm)[1]	63.1	22.2	23.5	28.16	38.37

[1]Literature Values (ALKINDI, *et al*, 2008). [2] Calculated data.

Table 7 – Generation data for atomizer.

Data	Values
Mach Number	1
Stagnation Air temperature (T_0)(K)	300
Stagnation Air pressure (P0) (kPa)	500
Air constant	287
γ	1.4

Table 8 shows the calculations results of average droplet diameter for pure glycerol and mixtures with ethanol for the dimensioning of the atomizer shown in Table 9.

Table 8 – Results of the average droplet diameters

Fuel	$D_m (\mu)$
100% Ethanol	17.28
25% Glycerol +75% Ethanol	43.56
50% Glycerol + 50% Ethanol	101.72
75% Glycerol + 25% Ethanol	242.35
100% Glycerol	617.47

It can be noted from Table 8, that the average droplet diameter for atomization of pure glycerol is very high. It can be verified that by mixing glycerol with ethanol, a large reduction in this diameter is achieved. Crude glycerol difference would attain an even greater reduction. Therefore, a preheat methylated or demethylated glycerol for atomization projects atomization would be widely recommended.

Table 9 – Results of the dimensions of the atomizer.

Parameter	Dm (Assumed value)	Value (mm)
Diameter of the air line	0.9	0.9
Diameter of the fuel line	0.9	0.9
Diameter of the mixing chamber	1.675	1.50
Premix length	1.67	1.5
Mixing length	5	4.5
Total length of the chamber	6.67	6.0
Airline Length	2.78	2.5
Fuel line length	5.65	5.0
Angle between the axis of the feed lines	$\Theta = 52°$	$\Theta = 52°$

Figure 4 shows the geometry of the atomizer to the values of Table 9**.**
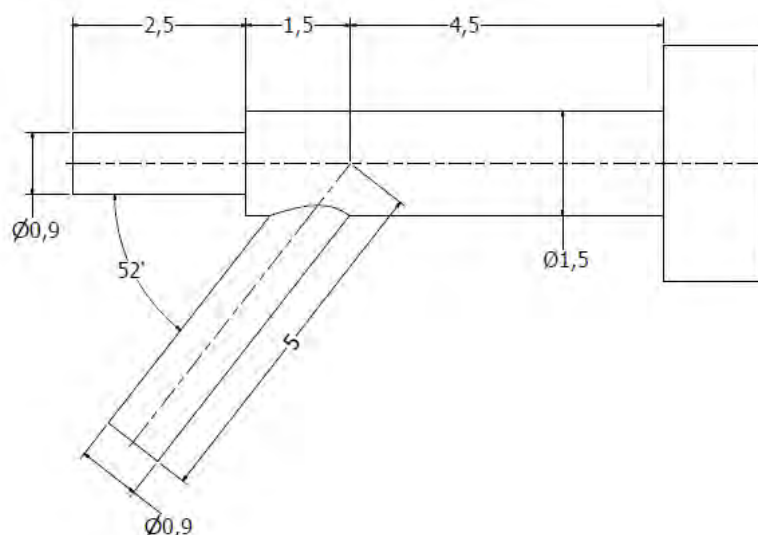

Figure 4 - Design of the atomizer, dimensions in mm.

7.3 Emissions

Table 10 presents carbon dioxide (CO_2) emission analysis for all fuels and sulfur dioxide (SO_2) for fuels containing sulfur in its composition.

Table 10 - Values of formation of CO_2 and SO_2, from combustion of each type of glycerol.

	Crude Glycerol	Methylated Glycerol	Demethylated Glycerol	Glycerol	75% Glycerol + 25% Ethanol	50% Glycerol + 50% Ethanol	25% Glycerol + 75% Ethanol	Ethanol
n CO_2	4.19	3.5	4.0086	3	3.5304	3.8006	4.0709	2
MM Fuel. (kg/kmol)	--	54.11	69.18	92.02	73.65	61.39	52.64	46.07
LHV (kJ/kg)	20454	17440	16480	12800	16556	20512	24368	28225
% Mass S	0.24	0.078	0.05	--	--	--	--	--
P CO_2 (kg/kJ)E^{-4}	--	0.8830	1.0702	1.1206	0.9326	0.8152	0.7350	0.6767
P SO_2 (g/GJ)	234.67	89.44	242.71	--	--	--	--	--

From Table 10, it can be observed that pure glycerol emits more CO_2 because it contains lower LHV despite not containing more CO_2. Crude Glycerol CO_2 emissions were not calculated due to inconsistency in molecular weight. The demethylated glycerol released more SO_2. For pure glycerol and mixtures with ethanol which do not contain sulfur in its composition, there are no SO_2 emissions. Eventually a simulation in CFD will be carried out in order to validate the calculations or recommendations made to design the atomizer.

8. ACKNOWLEDGEMENTS

9. REFERENCES

Alkindi S.A.,Al-Wahaibi M.Y., Muggeridge H.A., 2008. "*Physical Properties (Density, Excess Molar Volume, Viscosity, Surface Tension and Refractive Index) of Ethanol + Glicerol*". Department of Earth Science and Engineering, Imperial College, London SW7 2AZ, United Kingdom,53,2793 – 2796.

Assunção V.J,Yamagata S.,Oliveira S.,1993, Apostila do Curso " *A Combustão e o Meio Ambiente*",

Bohon D.M., Metzger A.B., Linak P.W.,King J.C.,Roberts L.W.,2011. "*Glycerol combustion and emissions*". North   Caroline State University, USA, Proceedings of the Combustion Institute 33 2717-2724.

Bombos D, Mihaescu L, Pisa I, Bolma I, Vasilievici G, Zaharia E.Burning,2011.*" Glycerol emulsion in Liquid Fossil Fuel, Revista de Chimie",* , vol. 62. Nº 5, pp. 562 – 566. Bucharest

 Carvalho, M.Q. McQuay,2007. "*Principles of Applied Combustion*" ,UNESP, SãoPaulo, Brazil, (in Portuguese).

Da Silva AL, Müller IL,2010. "*Operation of solid oxide fuel cells on glycerol fuel: A thermodynamic analysis using the Gibbs free energy minimization approach*"; Journal of Power Sources, v. 195, p. 5637-5644.

Cengel,2007. "*Thermodynamics an Engineering Approach*". Editora McGraw-Hll.

DAF, Department of Agriculture and Food, Government of Western Australia, Glycerin Overview, 2006, <http://www.agric.wa.gov.au/PC_93205.html?s=0>.

EPP T, 2008. *"Combustion of Glycerine for Combined Heat And Power Systems in Biodiesel Processing Facilities"*,   Bachelor Thesis, University of Manitoba, Canada

Hess, 2007. *"Value of crude Glycerin for Ruminant Livestock".* Journal of University of Wyoming.

Lacava, P. T, Oliveira, a. A.; Gurguel, C. A.; Figueira, L. T. 2009 " *Curso de combustão"*, Apostila. II Escola de Combustão , Rede Nacional de Combustão, p 68-103,.

Lide DR (ed.). 1999. *Handbook of Chemistry and Physics*, 84th ed. Boca Raton, Fla.: CRC Press, Inc.

Maturana C,A.Y. ,2011. "E*studo da combustão direta da glicerina bruta e loira como alternativa de aproveitamento energético sustentável*". Thesis (Doutorado) - Escola de Engenharia de São Carlos, Universidade de São   Paulo,São Carlos

Metzger B,2007. "*Glycerol Combustion*". MSc. Thesis, North Carolina State University, Raleigh, NC, USA.

Moran,Shapiro,2002. "*Fundamentals of Engineering Thermodynamics*", Nova York, 4a Edição.

Mattos Ana Paula, Quintero Juan Gabriel, Velásquez Elkin, Coronado Christian R., Nascimento Marco Antônio R.
GLYCEROL AN ALTERNATIVE ENERGY SOURCE: COMBUSTION AND PROJECT OF ATOMIZER Y-JET

Mullinger, P. J.; Chigier, N. A. 1974. "*The design and performance of internal mixing multi jet twin fluid atomizers".* Journal of the Institute of Fuel", v.47, p.251-261.

Rahmat N, Abdullah AZ, Mohamed AR, 2010. Recent progress on innovative and potential technologies for glycerol transformation into fuel additives: A critical review. Renewable and Sustainable Energy Reviews,
vol. 14, pp. 987–1000.

Pacifico, A. L.2000." *Analise Teórico experimental bifásico no interior de Bocais nebulizadores do tipo Y-Jet."* Thesis (Doutorado em Engenharia Mecânica) – Escola Politécnica da Universidade de São Paulo, São   Paulo.

Pérez, E. P.,2007. " *Substituição do diesel usado nos queimadores industriais por álcool combustível*" , Tese (Doutorado) – Universidade Estadual Paulista, Faculdade de Engenharia de Guaratinguetá.

Song,S.H.;Lee, S.Y.1994. "*An examination of spraying performance of Y-Jet Twin – Fluid Atomizers: Effect of mixing port length*". International Conference on Liquid Atomization an sprays s sistems." França, S.E.D,p.616-623.

Steinmetz. S, Herrington. J, Winterrowd. C, Roberts. W, Wendt J, Linak W.,2013. "*Crude glycerol combustion: Particulate, acrolein, and other volatile organic emissions*", Proceedings of the Combustion Institute 34 2749–2757.

Stelmachowski, M,2011. *"Utilization of glycerol, a by-product of the transesterification process of vegetable oils: A Review*". Ecological Chemistry and Engineering's; 18, 1, 9-30.

Soares RR, Simonetti DA, Dumesic JA.2006. "*Glycerol as a source for fuels and chemicals by low-temperature catalytic processing*", Angewandte Chemie, International Edition;45(24):3982-3985.

Thamsiriroj T, Murphy JD. "*Can rape seed biodiesel meet the European Union sustainability criteria for biofuels?"* , Energy Fuels, 2010, v. 24. pp. 1720 -1730.

Thompson, He, 2006. "*Characterization of crude glycerol from biodiesel production from multiplied feedstocks*".

Vaz VHS, Carvalho JBR, Sant'anna MC, Silva MS, 2010. "*Viabilidade de usina de briquete de casca de coco e glicerina em Sergipe"*, II Fórum Brasileiro de Energia, Bento Gonçalves–RS–Brasil, <http://www.institutoventuri.com.br/energia/trabalhos/05.pdf/>.

Williams,2006. "*Combustion of liquid fuel sprays*". London: Butterwoths,289p.

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