Numerical Simulation of the Combustion Chamber for a New Reference Combustion Calorimeter

Simulación Numérica de la cámara de combustión para un nuevo calorímetro de referencia

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DOI: 10.35429/JRD.2019.16.5.12.20 Received October 26, 2019; Accepted November 24, 2019

Abstract

The Centro Nacional de Metrología is developing a reference calorimeter to measure the superior calorific value of natural gas in collaboration with the Instituto Tecnológico de Celaya. We present the study of the combustion chamber for two formulations a steady state (already published) against the transient state. The study of the combustion chamber is performed employing computational fluid dynamics (CFD) through FLUENT®. For this work, specific parameters were set to define and simulate the combustion process involving the exchange of energy, momentum and mass transfer. In this work, we present simulations performed in steady and transient state, for which was used the Eddy Dissipation Model (EDM). Is shown the simulation of two geometries for the combustion chamber; one cylindrical body a hemispherical lid and the other elliptical, which was proposed to increase the area to heat transfer to the surrounding medium, water in our case. The criterion for selection is the chamber that achieves the lowest temperature for waste combustion gases at the exit. Achieved by the cylindrical chamber with a hemispherical lid in the first 4 seconds with a difference of 0.4 °C lower than the elliptical chamber.

Superior calorific value, Reference calorimeter, Computational Fluid Dynamics

Resumen

El Centro Nacional de Metrología está desarrollando un calorímetro de referencia para medir el poder calorífico superior del gas natural en colaboración con el Instituto Tecnológico de Celaya. Se presenta el estudio de la cámara de combustión para dos formulaciones, una en estado estacionario (ya publicada) contra otra en estado transitorio. El estudio de la cámara de combustión se realiza empleando Dinámica computacional de fluidos (CFD) a través de FLUENT®. Para éste trabajo, se utilizaron parámetros específicos para definir y simular el proceso de combustión que involucra el intercambio de energía, transferencia de masa y momento. En éste trabajo se utilizó el modelo Eddy Dissipation Model (EDM) para las simulaciones realizadas. Se muestra la simulación de dos geometrías para la cámara de combustión; una de cuerpo cilíndrico con tapa hemisférica y la otra elíptica, la cual se propuso para incrementar el área de transferencia de calor a los alrededores. El criterio para la selección, es la cámara que logre la temperatura más baja de los gases residuos de la combustión a la salida. El cual lo obtuvo la cámara cilíndrica en los primeros 4 segundos con una diferencia de 0.4°C, más bajo que la cámara elíptica.

Poder calorífico superior, Calorímetro de referencia, Dinámica Computacional de Fluidos

Citation: GONZÁLEZ-DURÁN, J. Eli E., ZAMORA-ANTUÑANO, Marco, LIRA-CORTES, Leonel and MÉNDEZ-LOZANO, Nestor. Numerical Simulation of the Combustion Chamber for a New Reference Combustion Calorimeter. Journal of Research and Development. 2019 5-16: 12-20

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Introduction

Today natural gas is the third model most widely used fuel in the world. Measuring the amount of heat that would be released by the complete combustion in air of a specified quantity of gas (on a molar, mass or volume basis), in such a way that the pressure *p*, at which the reaction takes place remains constant and all the products of combustion are returned to the same specified temperature, *T*, as that of the reactants, all of these products being in the gaseous state, except for water formed by combustion, which is condensed to the liquid state (ISO 15971:2010, 2008), or superior calorific value (SCV) is essential for billing purposes. Therefore, to perform this task, there are different methods (P. Ulbig, 2002), among them are those that operate under direct combustion calorimetry as the apparatus Cutlass hammer (P. Ulbig, 2002), on the other hand, there are instruments commercial falling in indirect methods and which are the most used. Such devices can calculate the SCV of natural gas by chromatography, supported with ISO 6976 standard (ISO 6976, 1996), the ISO 6976 contain the SCV´s of several pure gases. However, these values for pure gases are based on measurements made in the 1930s and 1970s, and uncertainty involved in the ISO for methane is specified to amount to 0.12 % (two times the standard deviation) (P. Schley, et al., 2010).

Methane is the main constituent of natural gas, measure the value of its SCV is essential because it is used in calorimetry of gases as reference material for calibration to measure SCV by chromatography.

Today several institutions around the world such as (P. Schley, et al., 2010), (Haloua, Filtz, & et.al, 2009) and (A. Dale, et al., 2009), have developed their own devices which operate under the same principle as the calorimeter by (F.D. Rossini, 1931) called Class 0 mass-basis calorimetry by ISO 15971 and its main feature is the accuracy of measuring the SCV of pure gases that can be achieved whit this type of equipment, i.e. uncertainties from about 0.05 % (95% confidence level) (P. Schley, et al., 2010). With the aim to try to get this kind of uncertainty and avoid to use reference materials, a project was initiated jointly by the laboratory calorimetry of CENAM and the ITC to develop a reference calorimeter to measure the heating value of natural gas, based on the principle of (F.D. Rossini, 1931) for combustion calorimetry.

We show in Fig. 1 the main components that comprise these kinds of calorimeters are:

1) The “burner,” which provides and mixes the oxidizer and fuel which generates the flame. The “combustion chamber” and “heat exchanger,” which maximize the heat transfer from the burned gases to the surrounding, generally water.

2) The “calorimeter vessel,” which can contain any fluid, water in this work. Its function is to receive and measure the energy generated by the flame and the burned gases, as well as to maintain a uniform temperature in the fluid contained. The burner, combustion chamber, and heat exchanger are immersing in the calorimeter vessel.

3) The “jacket,” which is a further vessel enclosing the calorimeter vessel and having a temperature either uniform and constant or at least known as regards space and time (Dickinson, 1914).

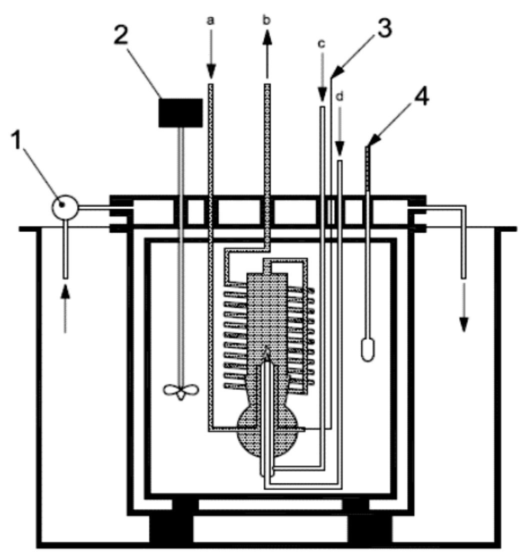

Figure 1 Schematic diagram of class 0 calorimeter. (1) water pump; (2) stirrer motor; (3) spark ignition electrode; (4) thermometer; (a) secondary oxygen; (b) combustion products, (c) primary oxygen plus argon; (d) fuel gas; (CV) calorimeter vessel; (J) jacket; (CH) combustion chamber; (B) burner; (H) heat exchanger.
Source: (ISO 15971:2010, 2008)

The principle under which the calorimeter operates is called Isoperibolic. It consists of a rise of temperature from the calorimeter vessel, containing a stirred liquid, which is watching while the jacket temperature is keeping constant (Dickinson, 1914).

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In Annex C from (ISO 15971:2010, 2008) is presented in more detail operation of called reference calorimeters which objective is to measure the quantity of energy involved in the complete combustion of a specific amount of a hydrocarbon fuel gas (P. Schley, et al., 2010). For a Rossini-type calorimeter, this is achieved by allowing the energy liberated in the reaction to be transferred to a well-stirred bath where is measuring its temperature rise. Do complete isolation of the jacket of a calorimeter is not possible in practice, so then a calorimeter is usually surrounded by a thermostatically controlled jacket, and allowance is made for the various sources and sinks of energy. In calorimetry, this is usually called an isoperibolic principle (P. Schley, et al., 2010).

The combustion chamber is one of the most critical components of the calorimeter because it aims to maximize the heat transfer to the surroundings, water for this work. Hence the Centro Nacional de Metrología (CENAM) and Instituto Tecnológico de Celaya (ITC). In an attempt to increase the heat exchanged through the walls of the combustion chamber, was propose an elliptical chamber and was compared against cylindrical published in the literature by (P. Schley, et al., 2010), (Haloua, Filtz, & et.al, 2009) and (A. Dale, et al., 2009). To test the hypothesis was performed a transient state simulation of temperature distribution into the combustion chamber and the temperature of outside gases to compare the performance of both combustion chambers.

Numerical model

The conservation equations were used for reactive flows in the steady and transient state, for the development of this work was used FLUENT® by ANSYS®. Therefore, the code solves the equation of conservation for chemical species, where the fraction of local mass of each species is predicted through the solution of the equation of convection-diffusion for the species. The conservation equation takes the following general form:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{J}_1 + R_i + S_i. \qquad (1)$$

Where R_i is the net rate of production of species i by chemical reaction and S_i is the rate of creation by addition from the dispersed phase.

In Eq. 1 $\vec{J}_1$ is the diffusion flux of species that arises from the gradients of concentration and temperature, Y_i is the mass fraction of species *i*. The code uses Fick's law to model mass diffusion due to concentration gradients, under which the diffusion flux can be written as:

$$\vec{J}_1 = -(\rho D_{i,m} + \frac{\mu_\tau}{Sc_\tau})\nabla Y_i - D_{T,i}\frac{\nabla T}{T}. \qquad (2)$$

In the Eq. (2), $D_{i,m}$ is the coefficient of diffusion for the species i into the mixture, and $D_{T,i}$ is the thermal diffusion coefficient. Sc_τ is the Schmidt turbulent number (where $\mu_\tau / \rho D_\tau$ is the turbulent viscosity and D_τ is the turbulent diffusivity). Due to the model used for combustion, the net speed of production of species in the Eq. 1 is assumed to be controlled by the turbulence with a two-step reaction mechanism:

$$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O$$
$$CO + 0.5O_2 \rightarrow CO_2$$

Due to the used non-premixed combustion model, the code resolves the total enthalpy of the energy equation:

$$\frac{\partial}{\partial t}(\rho H) + \nabla \cdot (\rho \vec{v} H) = \nabla \cdot (\frac{k_t}{c_p}\nabla H) + S_h. \qquad (3)$$

The terms of conduction and diffusion of species combine to give the first term of the right hand of the Eq. 3, where *H* is the total enthalpy, ρ is density and *v* is the velocity while the contribution of the viscous dissipation S_h appears in the non-conservative form, where k_t is the thermal conductivity and c_p is the heat capacity. And therefore the total enthalpy is defined as:

$$H = \sum_j Y_j H_j. \qquad (4)$$

Where Y_i is the mass fraction of species *j* and

$$H_j = \int_{T_{ref,j}}^{T} cp_j dT + h_j^0(T_{ref,j}). \qquad (5)$$

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Where the enthalpy of formation is $h_j^0\left(T_{ref,j}\right)$ of species j at reference temperature $T_{ref,j}$.

The fluid flow is described using the equation of conservation of momentum as described below:

$$\frac{\partial}{\partial t}(\rho\vec{v})+\nabla\cdot(\rho\vec{v})=-\nabla p+\nabla\cdot(\boldsymbol{\tau})+\rho\vec{g}+\vec{F}. \qquad (6)$$

Where p is the static pressure, $\boldsymbol{\tau}$ is the tensor of efforts, $\rho\vec{g}$ and $\vec{F}$ are the gravitational body force and the external body forces respectively (ANSYS FLUENT 14.0, 2011). Simulations were made using Fluent®. Nonlinear equations along with boundary conditions were solved using an iterative numerical method using the finite volume method (Versteeg & Malalasekera, 1995).

Methodology

After reviewing and analyzing the combustion chambers used by (P. Schley, et al., 2010), (Haloua, Filtz, & et.al, 2009) and (A. Dale, et al., 2009); it is seen to be the cylindrical body with hemispherical lid. Therefore, was proposed one elliptical combustion chamber, under the hypothesis that by increasing the area, the temperature of the waste gases of combustion is reduced. The restriction to evaluate the chambers was to have the same height and diameter, so was achieved increase by 10 cm^2 the elliptical combustion chamber against another one.

To select the best chamber was established that the waste gases of combustion should have the lowest temperature and that to transfer as much energy to its surrounding environment, in our case water. Fig. 2 and Fig. 3 shows the combustion chamber from literature with heat exchanger and the elliptical chamber.

Figure 2 Combustion chamber published in the literature.
Source: Own Elaboration

Figure 3 Combustion chamber from this work.
Source: Own Elaboration

For this work we realized all the simulations in FLUENT® (ANSYS FLUENT 14.0, 2011), an iterative numerical approximation solved the nonlinear governing equations together with the boundary conditions by finite volume method (Versteeg & Malalasekera, 1995). In the solution of the transport equations and turbulence model, in this work, we used the algorithm PISO (Pressure-Implicit with Splitting of Operators) for coupling the pressure and speed.

Grid generation is done using (ANSYS ICEM CFD 14.0, 2011). For the meshes, an unstructured mesh with tetrahedral elements was used, due to the complex geometry, Fig. 4 and Fig. 5 shows the result of this discretization. In this work, two fluid domains and one solid domain were established. The first fluid domain represents the zone which provides fuel and oxidant, mixes both and generates flame and burned gases. Coupled to it, we have one solid domain, which represents the burner and the heat exchanger made of glass whose thermophysical properties, such as density, thermal conductivity, and heat capacity were obtained from (Incropera & DeWitt, 1999). The second fluid domain represents the water contained inside the calorimeter vessel, which receives all the heat due to combustion and burned gases.

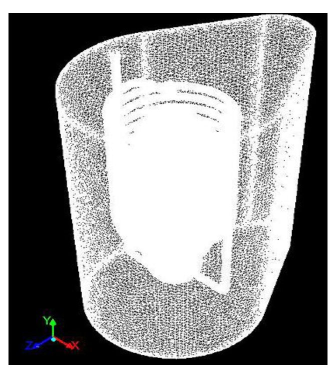

Figure 4 Picture shows discretization of calorimeter with burner, heat exchanger and combustion chamber. From as (P. Schley, et al., 2010), (Haloua, Filtz, & et.al, 2009) and (A. Dale, et al., 2009) with 1 133 433 nodes

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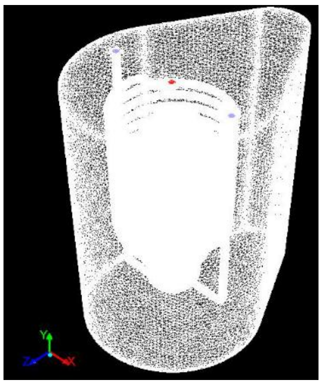

Figure 5 Picture shows discretization of calorimeter with burner, heat exchanger and combustion chamber from this work. with 1 403 244 nodes
Source: Source: Own Elaboration

In this work, we carried out simulations in transient and steady state at 3D for proposed combustion chambers, the elliptical and cylindrical with hemispherical lid. The flow fuel is 76 cm^3min^{-1} for methane, and the oxidant is oxygen, and its flow is three times the fuel flow.

The molar fractions established were of 0.96 for methane and 0.9 for oxygen with an input temperature of 23.5 °C for both flows, furthermore, the initial temperature for all the system of 23.5 °C.

For simulations carried out in this work, the combustion chamber, the burner and heat exchanger are inside of the calorimeter vessel, represented by a water volume of geometry similar to those published in the literature by (Rauch, et al., 2008) and (Haloua, Filtz, & et.al, 2009). The walls of the vessel calorimeter were established at 25 °C to simulate the isoperibolic environment (see Fig. 6).

We established the boundary conditions and initial condition above mentioned for the following cases: constant and variable density water and the last par transient case, shown in the results of this work.

Results analysis

Our aim in this work was determining the best kind of geometry to the reference calorimeter to develop. We used computational fluid dynamics to evaluate the performance of the chamber proposed (elliptical) and compare against published in the literature, to improve the chambers published by other authors. Our hypothesis was if we increase the area of heat exchanged we will improve the performance.

To achieve the above exposed, we designed virtual models by computer-aided design, which were discretized to be evaluated in FLUENT, data input, boundary and initial conditions were the same. We carry out the analysis in the transient state. The restriction established was diameter and height equal. We use the lowest temperature obtained of exhaust gases like a parameter to choose the best chamber.

Taking account, the results obtained in the transient state, we figure out that the cylindrical chamber with hemispherical lid has better performance that elliptical one. The area that we have to increase to improve heat exchange is where exhausted gases are accumulated in the chamber.

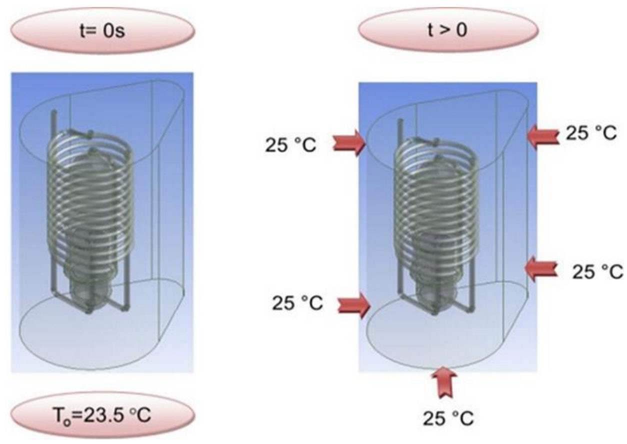

Figure 6 Analyzed diagram by numerical simulation with initial and boundary conditions.
Source: Own Elaboration

Results

For the case at steady state, we made two additional formulations; one keeping the constant density of water whose detailed work is presented in (Gonzalez, Estrada, & Lira, 2015) and the second was established a ratio with density-temperature for the water in the calorimeter vessel.

For the first case Table 1, shows that average temperature of the gases at the exit is lower in the elliptical chamber by 0.49 °C, as the average water temperature which is calculated based on the volume of water contained in the calorimeter vessel. The maximum temperature represents the temperature reached by the water in the calorimeter vessel by heat transfer from the burner. In the top of the burner are presented the higher temperatures.

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	Elliptical chamber	Cylindrical chamber
Average temperature of the exit gases	27.71 °C	28.20 °C
Average temperature water	26.45 °C	26.80 °C
Maximum water temperature	68.43 °C	80.23 °C
Minimum water temperature	24.93 °C	24.95 °C

Table 1 Evaluation results of the combustion chamber with the constant density of water
Source: Own Elaboration

For this case, water with the constant density, the behavior of heat transfer through water is like a thermal conductivity case instead of a convective case, hereby from Table 1, we can see that the cylindrical chamber transferred more heat to water surrounding, because the maximum temperature in the water is higher than the another chamber.

The minimum water temperature is 25 °C as the boundary condition established. It is because we not used a stirrer in all simulations.

In the second case, to take account variable density of water, we take information of density and temperature from (Incropera & DeWitt, 1999), we generate a polynomial relation that we input to the code through functions, and these results are showing in Table 2. Here it is seen a difference of 0.27 °C, for the residual gases from the combustion chamber concerning each other; almost half regarding the analysis of -the constant density-. Generally, temperatures obtained to the burner exit and in the water are lower, concerning for to the results of constant density. Due in this case we consider the effect of buoyancy forces, we got lower temperatures than the last case, mentioned above.

	Elliptical chamber	Cylindrical chamber
Average temperature of the exit gases	28.48 °C	28.75 °C
Average temperature water	26.41 °C	25.29 °C
Maximum water temperature	37.24 °C	45.40 °C
Minimum water temperature	25.00 °C	20.00 °C

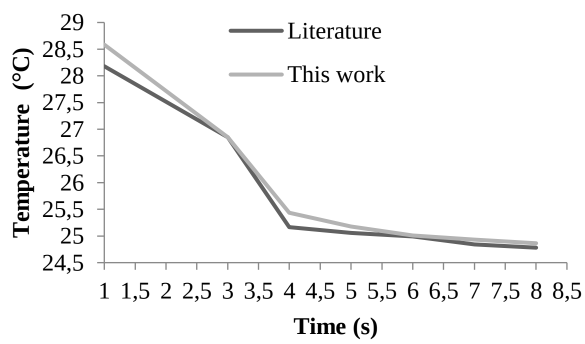
Table 1 Evaluation results of the combustion chamber with the constant density of water
Source: Own Elaboration

The difference among both formulations shown in Table 1 and Table 2 is due to the variable density because, for this case with the polynomial functions introduced, we are closer of the convective model than another case where density is constant.

Maximum water temperatures for the case with variable density were lower than constant density, due which the case of constant density, the code simulate like a phenomenon of pure conduction, with variable density we are modeling the behavior of water with a heat transfer mode by convection.

To the transient state, one aim of this work was to monitor the temperature of residual gases of combustion under transient formulation.

Therefore Graphic 7 shows the values of the mean temperature in the first 8 seconds, where under the legend "this work" shows the evolution over time of the behavior of the chamber proposed for this work and "literature" from (P. Schley, et al., 2010), (Haloua, Filtz, & et.al, 2009) and (A. Dale, et al., 2009), to identify the chamber with the cylindrical body and hemispherical lid.



Graphic 7 Graph of the temperature last the first 8 seconds from the residual gases of the combustion to the exit of the heat exchanger. For the elliptical chamber the legend "this work" is used and for the cylindrical chamber with hemispherical cover the legend "literature".
Source: Own Elaboration

For the first 4 seconds is important analyze how temperature to the exit is high, probably could be have a negative effect to the moment to calculate the SCV. We could reduce this temperature by the stirrer, increasing its rotary velocity. From Graphic 7 we can analyze performance from both chambers, with the slope.

The cylindrical chamber has a quick rate of temperature decrescent. It is mean that heat exchanged to water is more significant than the elliptical chamber. We only show 8 seconds because it is where the changes in temperature are abrupt.

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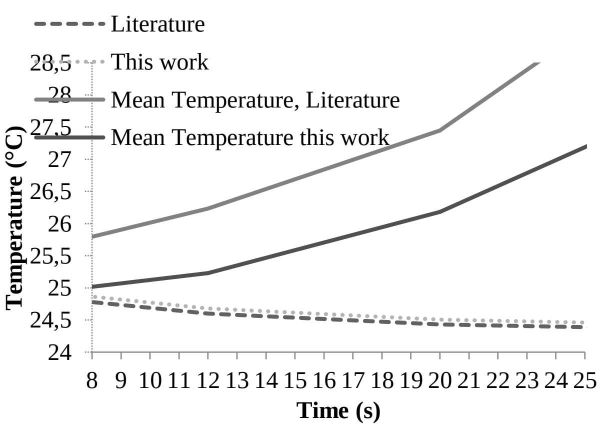
Graphic 8 shows evolution temperature from second 8 to the second 25. For this time interval analyzed, the maximum difference is 0.08 °C at the second 12 and continues going down a rate of 0.003 °C / s. Additionally Fig. 6 shows the comparison from mean temperature from the water bath for this work against literature as (P. Schley, et al., 2010), (Haloua, Filtz, & et.al, 2009) and (A. Dale, et al., 2009) and we can see the difference in temperature 8 second, this due to the performance of the combustion chamber cylindrical.

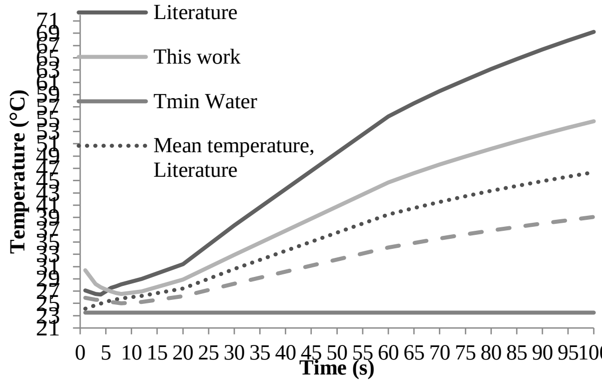
From Graphic 8 we can see that combustion chamber from literature as (P. Schley, et al., 2010), (Haloua, Filtz, & et.al, 2009) and (A. Dale, et al., 2009) is more efficient than proposed in this work, this taking account the slopes among both chambers because the mean temperature from literature as (P. Schley, et al., 2010), (Haloua, Filtz, & et.al, 2009) and (A. Dale, et al., 2009) is growing up more and quicker than elliptical. So performance is better than the elliptical chamber.

As we can see in Graphic 8 the temperature of residual gases from combustion is practically constant, approximately 24.3 °C. This temperature is higher than 23.5 °C, and under the definition of superior calorific value from (ISO 15971:2010, 2008), the exhaust gases should return to initial temperature. However, we can reach the temperature using a stirrer, which is not taking account for simulations in this work.



Graphic 8 Graph of the temperature of the residual gases of the combustion to the exit of the heat exchanger from 8 to 25 seconds. For the elliptical chamber the legend "this work" is used and for the cylindrical chamber with hemispherical cover the legend "literature"
Source: Own Elaboration

From Graphic 8 can see how the mean temperature inside of water bath from the cylindrical body is higher than elliptical because heat exchanged by the combustion chamber is better than the elliptical. Thus temperature in exit gases is lower than exit gases from elliptical chamber.



Graphic 9 Graph of the evolution of the maximum temperature inside the calorimeter vessel, mean temperature and minimum temperature for 100 seconds of simulation
Source: Own Elaboration

Graphic 9 shows that the maximum temperature inside the calorimeter vessel is higher in the chamber published in the literature because of cylindrical chamber exchanges more energy to the water surrounding it, unlike the elliptical chamber. The value of the minimum temperature of the water in the calorimeter vessel under legend T_{min} is also displayed.

As we can see minimum temperatures are constant for the 100 seconds shown, this meant that in that time not all the water inside has a homogenous temperature.

Then is necessary develops and locate a stirrer that can assure a uniform temperature inside of the vessel calorimeter.

Figure 10 and Figure 11 are pictures that show the temperature gradients for elliptical chamber in the second 100, through a cut plane.

We can see in both pictures a white zone which indicate temperature higher than 30°C, so we can see the contour of burner, combustion chamber, and helicoidal heat exchanger with several turns. By the side of the circles of heat exchanger we can see two tubes vertical, these represent the inlet and outlet of methane and oxygen.

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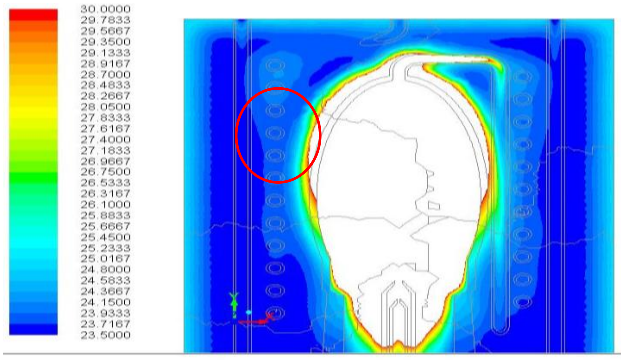

Figure 10 Temperature distribution (in °C) for elliptical chamber at 100 seconds of simulation in a transient state
Source: Own Elaboration

In Figure 10 can be seen that in the last turn, from heat exchanger for elliptical chamber has a higher temperature than the same heat exchanger used for the cylindrical chamber (red circle), as shown in Figure 11. which is observing that the distribution of temperature gradients is different for both chambers and that may be due to the accumulation zone of residual gases of the combustion. We can also observe as the elliptical chamber has higher temperature zones at the top the calorimeter vessel, which implies that the temperature of the residual gases is slightly larger than that of the chamber generated by the cylindrical body. As the Fig. 5 and Fig. 6 shown. Where is possible analyse than the lowest temperature last 100 seconds of simulation is for combustion chamber with the cylindrical body.

In Figure 11 we can see that gradients temperature are more uniform than the elliptical chamber. It is possible since temperature around tubes of the inlet of oxygen and methane conserve the lowest temperature, this for the cylindrical chamber. However, according to Figure 10, we can see like tubes of inlets for methane and oxygen are perturbed by a temperature at least 1°C more than the cylindrical chamber.

Figure 11 Temperature distribution (in °C) for cylindrical chamber at 100 seconds of simulation in a transient state.
Source: Own Elaboration

From Figure 11 we can see the temperature distribution, and it shows a critical zone between the burner and heat exchanger. This zone is locating at the end of de chamber, the little tube that turns to the side and takes the combustions gases to the heat exchanger, this part is close to the tube that exit from the vessel. If they are very close to each other the temperature of gases at exit can be higher than required by definition of Superior Calorific Value. We figure out through simulations an optimum distant among these parts.

Conclusions

In this work was shown two numerical simulations in a transient state of two combustion chambers for possible employment in the reference calorimeter to measure SCV of natural gas. The goal of the work was to test the hypothesis that increasing the heat transfer area by an elliptical chamber proposed by this work the temperature of the residual gases would be lower than used by the authors (P. Schley, et al., 2010), (Haloua, Filtz, & et.al, 2009) and (A. Dale, et al., 2009) of the cylindrical body and hemispherical lid. With the aim to select the most appropriate combustion chamber for the reference calorimeter developing by CENAM.

The lowest temperature of the residual gases of combustion was obtained by cylindrical chamber with hemispherical lid with a maximum difference of 0.40°C in the first second, and a temperature in the rest of the simulation which was descending at rate of 0.003 °C /s for which the second 100 the difference is 0.005°C. Therefore, in the transient state, the performance of the chamber cylindrical with hemispherical lid is better than elliptical chamber proposed by this work. The above can be possible because the residual gases of the combustion accumulate in the top of the combustion chamber and therefore this area is larger in the hemispherical lid than in the elliptical chamber. Then to improve heat exchanged from residual gases of combustion, we need to increase the area at the top of the combustion chamber, due it is here where they are accumulated.

The graph in Graphic 9 show the maximum value of temperature for the elliptical chamber, and it is lower than the cylindrical chamber. It is possible because by increasing the area, its mass increases, therefore at that time the mass of the chamber absorbs heat before to be transferred to the surrounding water.

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Due to the established criteria and the fact that is less complicated and have more repeatability to build a chamber with a cylindrical body and hemispherical lid, this geometry was selected for the chamber to be used in the calorimeter under development by the CENAM and ITC.

Acknowledgments

The authors are grateful to all who have contributed to this work.

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