Effect of turbulence model on flameless combustion simulation of a regenerative furnace

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Abstract: The high energy consumes have generated the need of developing higher efficiency devices, in this sense flameless combustion is a great alternative. The design of flameless combustion systems by means of Computational Flow Dynamics simulation is an alternative value to reduce costs, however it required an adequate model selection. In the present study a capability evaluation of standard and realizable versions of k-e turbulence model was carried out. Experimental measurements of temperature and chemical species were performed in combustion chamber of a regenerative furnace in order to compare this with numerical data and in this way determinate the performance and the incidence of the selected models. The realizable version shows better results regarding at changes of flow direction and recirculation patterns inside the furnace.

1. Introduction
The increase in global energy demand has been inherently translated into a greater amount of polluting gases since fossil fuels have been the main resource to satisfy the requirements [1]. In this sense, the implementation of alternatives such as flameless combustion, a process in which the energy released during the reaction of the fuel develops under highly diluted conditions, due to a high rate of recirculation of combustion products, generating a reaction zone distributed and thus eliminating the visible flame front, it becomes very promising since it allows to obtain more uniform temperature profile and reduce the losses due to incomplete combustion and therefore the emissions of CO and hydrocarbons [2], which improves the efficiency of the system.

Computational flow dynamics (CFD) was used for the design and evaluation of the devices that operate under this regime is increasingly recurrent, since it allows to optimize the designs and to avoid expenses in previous prototypes to the definite version. However, to obtain reliable results, the suitable selection of the models for each one of the phenomena associated is crucial, in particular in the process of design where there is no previous experimental data to realize comparisons. In this sense, models associated with flow conditions or the turbulence models play a vital role in the simulation processes to obtain results close to reality within the flameless combustion regime [3], due to the strong dependence on the regime of recirculation levels. Several authors have conducted studies focused on the effect of the most commonly used models on the predictions the flameless combustion regime. The different version of the k-e model has been evaluated in various combustion devices and compared with other models in order to establish the prediction capacity with different conclusions. The standard version of
the model has showed better results in a different configuration, even compared with the other models like the Reynolds stress model (RSM) and modified version of the same, when temperature, chemical species and velocity profiles inside of the thermal system have been compared with the obtained by CFD simulation. However, in some cases the same uncertainties in the measurements of the velocities do not allow to clarify that this is the best model. However, not always the standard version have the best performance, the realizable version of the κ-ε model is considered the most suitable due to its capacity in the modeling of round jets according to other studies, this capability is important in flameless combustion systems where jets have this shape [4-6].

In the previously mentioned studies, the systems do not take into account the heat regeneration and only put its attention on one output for the combustion gases, which limits to a certain extent extrapolating the performance of the models considered more suitable for these studies to other geometries. In this way, the present study is conducted and within this two of the models that have presented the best results in the flameless combustion regime are evaluated by simulating a regenerative furnace with two outputs, comparing the results with experimental measurements of temperatures and chemical species

2. Experimental setup
The experimental tests were developed in a combustion flameless furnace of square cross section, equipped with a regenerative burner. Details of the associated experimental assembly can be found in the references [7], also, in the present research a brief description will be made highlighting the most relevant aspects, specifically the operating conditions. The furnace used has four tubes inside the combustion chamber through which air flows as a thermal load. In the final part of the oven located on the roof is the smokestack. The burner also has 4 nozzles located peripherally around the fuel discharge for the air discharge and gas suction to the regenerators. Natural gas (CH₄) was used as a fuel at a power of 25kW, with an excess of air of 20% (Vol.) and a load air flow of 107.89 m³/h.

To carry out the comparison with the simulations conducted and to assess the effect of the turbulence model, measurements of chemical species (O₂, CO, CO and CH₄) and temperature inside the combustion chamber were made. For this, the specific probe of each parameter was entered through the back of the oven through holes designed for data collection. In the case of temperature, a probe with two concentric shields and an annular gas section was used to reduce the effects of radiation on the measurement [8].

3. Simulation methodology

3.1. Computational domain
The computational domain was built conserving the geometrical characteristics of the furnace, using a non-structured meshing of 405632 hexahedral cells. (See Figure 1).

Figure 1. Combustion chamber meshing.
The simulations were carried out through the Ansys - Fluent 15.0 program, solving the Navier - Stokes equations with the Favre average due to the reactive nature of the phenomenon, inside the combustion chamber of the furnace. Due to the symmetrical configuration of the furnace and in order to reduce the computational cost, only half of the combustion chamber was considered, using a condition of symmetry along a plane in the axial direction of the furnace. The meshing was built particularly dense in the areas where the reactants are expected to interact most, as well as between the discharges and it was gradually increasing, as the high gradients are reduced.

3.2. Turbulence models
The \( \kappa-\varepsilon \) model in its standard and realizable versions, present suitable results for systems of flameless combustion, this is why they were selected to be evaluated in the present work. Both versions of the model are based in the approximation of Boussinesq, which establishes a relation of proportion between the Reynolds stress and the gradients of the mean velocity, defining a fictitious designated turbulent viscosity \( (\mu_t) \) [9]. The calculation of \( \mu_t \) in both cases is done by solving two additional transport equations, one for the turbulent kinetic energy \( (\kappa) \) and another for the dissipation rate \( (\varepsilon) \) [10], through the Equation (1)

\[
\mu_t = \rho C_\mu \frac{\kappa^3}{\varepsilon}
\]

Where \( \rho \) is the density and \( C_\mu \) is a constant of the model whose value is of 0.09. The expressions of transport for \( \kappa \) and \( \varepsilon \) are given by the Equation (2) and Equation (3).

\[
\frac{\partial(\rho \kappa)}{\partial t} + \nabla \cdot (\rho \kappa \mathbf{U}) = \nabla \cdot \left[ \frac{\mu_t}{\sigma_k} \nabla \kappa \right] + 2\mu_t S_{ij} S_{ij} + G_\kappa
\]

\[
\frac{\partial(\rho \varepsilon)}{\partial t} + \nabla \cdot (\rho \varepsilon \mathbf{U}) = \nabla \cdot \left[ \frac{\mu_t}{\sigma_\varepsilon} \nabla \varepsilon \right] + C_{1\varepsilon} \frac{\varepsilon}{\kappa} 2\mu_t S_{ij} S_{ij} + G_\varepsilon - C_2\rho \frac{\varepsilon}{\kappa+\sqrt{\varepsilon}}
\]

Where \( \sigma \) is the number of Prandtl turbulent in each case, \( \mathbf{U} \) is the velocity, \( S_{ij} \) is the average rate of of the fluid, \( C_1 \) and \( C_2 \) are constant of the model whereas the term \( G \) groups additional source terms.

The realizable version of the model, takes into account the fact that the normal efforts inside the flow have to be positive quantities and limits mathematically the obtaining of negative values, by adjusting the constant \( C_\mu \), in this version the mentioned parameter is a variable associated precisely with the rotation and deformation rates of the flow. Additionally, this version modifies the equation of transport for \( \varepsilon \), changing the term from the right of the Equation (3) by the expression defined through the Equation (4).

\[
\nabla \cdot \left[ \frac{\mu_t}{\sigma \varepsilon} \nabla \varepsilon \right] + \rho C_1 \varepsilon \sqrt{2S_{ij}S_{ij}} + G_\varepsilon - C_2\rho \frac{\varepsilon}{\kappa+\sqrt{\varepsilon}}
\]

The changes are given in the second and last term of the right side of the equation, modifying the production and destruction, this allows a better representation of the energy spectrum transfer.

3.3. Complementary models and convergence
For the radiation phenomenon and the mode of interaction between chemical reactions and turbulence, the discrete ordinate models and the eddy dissipation concept (EDC) were selected, respectively. The selection of them was made from the results obtained according to several studies recorded in the literature [11]. The modified Westbrook and Dryer reaction mechanism was used [12]. The criteria established by Tu et al. were used as convergence criteria [13].
4. Results

The profile of temperatures along the combustion chamber in the central line shown in Figure 2(a), shows the obtaining of the regime by not presenting peaks in this variable, this was also verified visually by means of the monitoring windows with that the furnace counts.

![Temperature profiles](image)

**Figure 2.** Measurements and temperature predictions inside the furnace. (a) Center line, (b) Left line.

Aimed at quantifying the uniformity of the temperatures profile, it was calculated the factor of thermal uniformity (RTU) defined by Rafidi and Blasiak [14], between closer to zero this parameter greater uniformity is in the temperature profile. For this calculation it was used the data of temperature along the 3 lines measured in the half plane of the furnace, obtaining a value of 0.186, which is characteristic of the flameless combustion, very underneath of the one reported in conventional systems by Rafidi and Blasiak, confirming thus the obtaining of the regimen. From Figure ¡Error! No se encuentra el origen de la referencia. it is possible to appreciate that both models predict adequately the values of temperature from a distance of 0.45 m in the axial direction, the average deviation for the realizable model is of 3.9% whereas in the case of the standard is 6%.

For these positions it can be seen that the standard model slightly underestimates the experimental values, while the realizable version better predicts the temperatures in that area. In the first part of the furnace (before 0.45m) neither of models adequately predicts the behavior of the temperature. However, the gap may be associated with the preheating effect of the fuel generated by the temperature increase in the previous components of the burner, which are not included in the CFD simulation.

Regarding the temperatures measured in the left line of the furnace, as shown in Figure 2(b), where the effect mentioned above does not take place, it is observed that the simulation adequately reproduces the temperatures also in the primary zone of the combustion chamber, confirming the hypothesis raised regarding the lag in the central line. In the case of the left line, the predictions of both models are very similar. The maximum deviations for the standard version and realizable in the whole line are of 5.6 and 6.6%, while the average deviations are of 3.4% and 4.2% respectively. These values indicate suitable predictions in both cases, but evidence that the realizable version presents a better behavior in the zones where has curves flows or give drastic changes in the direction of the same, whereas the standard version achieves a main precision in the initial zones where in principle the flow is more axial given the vicinity to the downloads of the reagents.

To analyze the reproduction capacity in a more adequate way, the chemical species inside the furnace were also analyzed, in Figure 3(a) the experimental measurements and the predictions of both models for CO\textsubscript{2} are shown. In this case, a similar behavior is found in terms of the predictive capacity, reproducing the general behavior in an appropriate way by both models. This indicates that globally both models capture the flow patterns inside the furnace, since CO\textsubscript{2} can be taken as a reference of the internal recirculation level of combustion gases and in both cases the levels presented by the simulations are consistent, with differences lower than 9.4% in the final zone.
However, in the middle zone of the furnace, the gap increases, reaching maximum values of 14% for the realizable version and 13.3% for the standard version. Is in this said middle zone where it is expected that the mixing of the reactants takes place and where the largest recirculation zone appears, therefore where the prediction can be more difficult. Although it may sound contradictory the fact that it reproduces the flow patterns adequately but the greatest differences in CO$_2$ are present in these zones, this lag is not necessarily associated with dynamic fluid behavior, but with the reaction kinetic process, this is checking to see the profiles of CO and CH$_4$, shown in Figure 3(b) and Figure 4(a) respectively.

The CO profile shows in a clear way that the simulations overestimate the present quantity of this species in comparison with the experimental data, in addition these differences becomes larger for the realizable version compared to the standard version. This important difference shows that the reaction rate in the conversion of CH$_4$ to CO$_2$ calculated by the models is lower than the real one, generating higher CO concentrations in that middle zone, this behavior is related to the way to determine the reaction process of the EDC model. In this sense, it should be taken into account that the development of models for the reaction process under the flameless combustion regime is still a hard studying area, given the marked differences of this with respect to conventional combustion.

The CH$_4$ profile shown in Figure 4(a) confirms this behavior. According to the predictions, the concentration of this species in the central zone of the furnace is much greater than experimentally measured, confirming the effect of a reaction rate described by the simulation lower than the real for both versions evaluated. Although the above mentioned associates the difference of the simulations with respect to the experimental data in the center of the combustion chamber with the reaction model, it is evident that the turbulence model has an important incidence in the calculations associated to the kinetics chemical and although as previously mentioned, both models achieve an adequate prediction of fluid dynamic behavior, there are marked differences regarding their influence on the modeling of the reaction process.

Both for the case of CO and CH$_4$, the imprecision in the data is greater when the simulation was done with the realizable version of the model, presenting higher values compared to the standard version. In this way, the standard version allows apparently to obtain more adequate results regarding the reaction process. In order to corroborate this behavior, it is necessary to complete the analysis of chemical species, for which the profile of O$_2$ inside the combustion chamber is shown in Figure 4(b). In this case, both models have difficulty predicting the behavior of this species; however the realizable version presents results much closer to the experimental data than those obtained with the standard version. The standard version shows a higher concentration of O$_2$, which indicates that its apparent better behavior with respect to chemical species (CO and CH$_4$) is not to contribute to a better performance of the reaction model, if not because of difficulties in predicting specific flow patterns.
Namely, if the standard version does indeed allow a better performance of the kinetic model, the concentration of O_2 in the central zone of the furnace should be lower since part of this is consumed more quickly and therefore the conversion of CH_4 to CO_2 occurs from the same way at a higher rate compared to the exposed by the realizable version, allowing lower concentrations of CH_4 and CO to be generated. However, the concentration of O_2 is much higher than those experimentally measured. From this last behavior it can be inferred that the higher reaction rate that is generated when the standard version is used is due to the difficulty of the model to predict changes in direction and recirculation processes inside the combustion chamber. Which result in a lower level of dilution of the mixture and therefore an increase in the rate at which the fuel conversion takes place. When comparing the predictions of the realizable model with the experimental data, a greater agreement is found in order of magnitude, especially in the central part of the furnace, location of the reaction zone and recirculation zones. Confirming that this version presents a better behavior in the reproduction of the fluid dynamics patterns, given that it is evident that the lower concentration of O_2 is not due to a higher consumption according to the behavior shown in the predictions of CH_4, CO and CO_2, but because of the level of dilution that is reached due to the recirculation of combustion gases. In the Figure 5(a) it is shown the concentration of CO_2, O_2 and CH_4 in the flue gases. Both simulations report small concentrations of CH_4 that could be associated with the effects of the kinetic model generating that part of the fuel is not consummated, nevertheless, because there are values underneath of 0.06% it could be associated with the numerical uncertainty.

This is further corroborated if CO_2 is analyzed where the measurements and predictions show differences less than 0.4. In the case of O_2, the differences are also small, although a little greater than the case of CO_2. The CO shown in Figure 5(b) is associated with the above, as it is possible to be seen the simulations report a greater amount of this species in the combustion gases of the chimney indicating that part of this cannot be converted into CO_2, thus the highest concentration of O_2 mentioned previously. This behavior is also directly related to reaction rates underestimated by the EDC model, since the actual experimental values are well below of the predictions (<25 ppm).
5. Conclusions
In the present study, the evaluation of two versions of the $\kappa$-$\varepsilon$ model for turbulence, standard and realizable, was carried out within a regenerative furnace operating under the flameless combustion regime, by comparing temperature and chemical species data. The results showed that the standard version of the model presents difficulties to capture effects of change of direction in the flows, as well as recirculation processes, which generates that the dilution rates inside the furnace are lower, causing higher reaction rates and apparent better predictability. On the other hand, the realizable version captures in a better way the process of recirculation and changes of direction in the flows, which allows to better predict the levels of dilution in the combustion chamber. Finally, it can be established that the chemical interaction - turbulence EDC model underestimates the reaction rates inside the furnace operating under the flameless combustion regime due to the high levels of dilution, which makes the simulation overestimate the concentration of intermediate species as the CO.

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References
[1] Kibria A, Akhundjanov S B and Oladi R 2019 Fossil fuel share in the energy mix and economic growth Int. Rev. Econ. Financ. 59 253–264
[2] Cavaliere A, Joannon M de and Ragucci R 2008 Highly Preheated Lean Combustion D-R Derek (ed) Lean Combustion Technology and Control (Amsterdam: Academic Press) Chapter 3 pp 55–94
[3] Moussa O and Driss Z 2017 Numerical investigation of the turbulence models effect on the combustion characteristics in a non-premixed turbulent flame methane-air Am. J. Energy Res. 5 85–93
[4] Rebola A, Coelho P J and Costa M 2013 Assessment of the performance of several turbulence and combustion models in the numerical simulation of a flameless combustor Combust. Sci. Technol. 185 600–626
[5] Fortunato V, Galletti C, Tognotti L and Parente A 2015 Influence of modelling and scenario uncertainties on the numerical simulation of a semi-industrial flameless furnace Appl. Therm. Eng. 76 324–334
[6] Arghode V K and Gupta A K 2011 Hydrogen addition effects on methane-air colorless distributed combustion flames Int. J. Hydrogen Energy 36 6292–6302
[7] Echavarria J D and Arrieta A A 2017 Estudio del régimen de combustión sin llama ante la variación de la carga térmica Ingenieria y Ciencia 13 185–208
[8] Brohez S, Delvosalle C and Marlair G 2004 A two-thermocouples probe for radiation corrections of measured temperatures in compartment fires Fire Saf. J. 39 399–411
[9] Turns S R 2000 An introduction to combustion: concepts and applications (Singapore: McGraw-Hill)
[10] Ansys Inc 2013 ANSYS Fluent Theory Guide (Canonsburg: ANSYS Inc)
[11] Tu Y, Liu H, Chen S, Liu Z, Zhao H and Zheng C 2015 Numerical study of combustion characteristics for pulverized coal under oxy-MILD operation Fuel Process. Technol. 135 80-90
[12] Wang L, Liu Z, Chen S and Zheng C 2012 Comparison of different global combustion mechanisms under hot and diluted oxidation conditions Combust. Sci. Technol. 184 259–276
[13] Tu Y, Liu H, Chen S, Liu Z, Zhao H and Zheng C 2015 Effects of furnace chamber shape on the MILD combustion of natural gas Appl. Therm. Eng. 76 64–75
[14] Rafidi N and Blasiak W 2006 Heat transfer characteristics of HiTAC heating furnace using regenerative burners Appl. Therm. Eng. 26 2027–2034