24th COBEM - 2017

24th ABCM International Congress of Mechanical Engineering
December 3-8, 2017, Curitiba, PR, Brazil

COBEM-2017-1976
NUMERICAL CFD EVALUATION OF A FLAMELESS BURNER USING DETAILED CHEMICAL KINETICS

Fagner Luís Goulart Dias
Marco Antonio Rosa do Nascimento
Lucilene de Oliveira Rodrigues
Federal Univerty of Itajubá - Mechanical Engineering Institute - Av. BPS, 1303, bairro Pinheirinho, cx postal 50, CEP: 37500-903
fagner@unifei.edu.br; marcoantonio@unifei.edu.br; lucilener@unifei.edu.br.

Abstract. *Flameless combustion regime has been shown to be promising because of the high combustion efficiency coupled with low levels of pollutant emissions, especially nitrogen oxides, NO_x. Over the last few years, numerous studies have investigated the main features of the flameless combustion regime and also seeking to obtain their numerical modeling. Among the numerical models the most widely used in the turbulence modeling is the k-ε realizable (KER), the Eddy Dissipation Concept (EDC) for combustion and the Discrete Ordinates (DO) for radiation modeling, as well as use of detailed reaction mechanisms. Based on experimental data, those models that would be more suitable for numerical prediction of this regime, as well as the needs of adjustments were investigated. Therefore, this work aims to present a numerical investigation using ANSYS Fluent about the burning process, through detailed chemical kinetics using the CHEMKIN package. Initial results with global reaction mechanism showed elevated temperatures, especially close to the burner injector, which reflected negatively on the NO_x content at radial planes plotted. In the case of GRIMech3.0 detailed reactions, the temperatures remained moderate, but with a CO and NO_x levels above the experimental data, beyond the large computational time used. New investigations will be needed to better represent the burning process, especially in the content of the pollutants formed*

Keywords: *numerical modeling, flameless, CFD, MILD combustion*

1. INTRODUCTION

Numerous alternatives to increase the efficiency of the energy conversion process have been developed, especially about the technology used in regenerative furnaces. However, some disadvantages are attributed to this technology, mainly due to the high cost of the modern heat exchangers required, besides the increase in the emission of polluting gases, mainly of oxides of nitrogen or nitrogen oxides, named NO_x (Gomez-Garcia *et al.*, 2002). The NO_x contribute to air pollution mainly through the formation of photochemical smog, which frequently occurs in large cities. Also, NO_x emissions causes acid rain phenomena, eutrophication of ecosystems and partly responsible for the formation of tropospheric ozone, a harmful gas to human health and agricultural production (EDP, 2012; Skalska *et al.*, 2010).

There are several technologies used to reduce the emission of NO_x, such as the Lean Premixed Combustion and the gas recirculation technique (Quaresma, 2010). There is still the staged combustion by fractional injection of fuel and oxidant, creating a combination of rich and poor regions. In this context, from the 1990s, the flameless combustion regime has emerged with high energy efficiency, as well as low pollutant emissions and low combustion noise levels, making it a viable alternative (economically and environmentally) to conventional combustion regimes.

The flameless combustion operation is shown in Fig. 1. It can observed, the emergence of the regime as the dilution content is varied, in this case by increasing the content of N_2 and CO_2. This procedure reproduces a necessary condition for the existence of the phenomenon, through the recirculation of products and inert elements, that distributes the combustion along the burner, eliminating the existence of a defined flame front, and then, a concentrated peak of temperature. In this case, among other reasons, the flame does not remain visible, outside the spectrum visible (Szego, 2010).

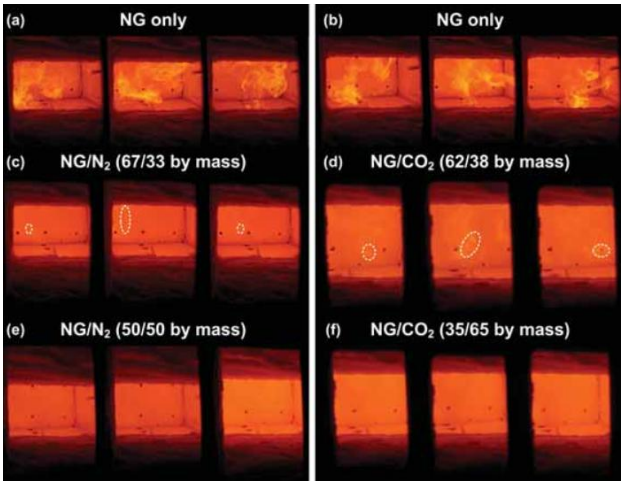
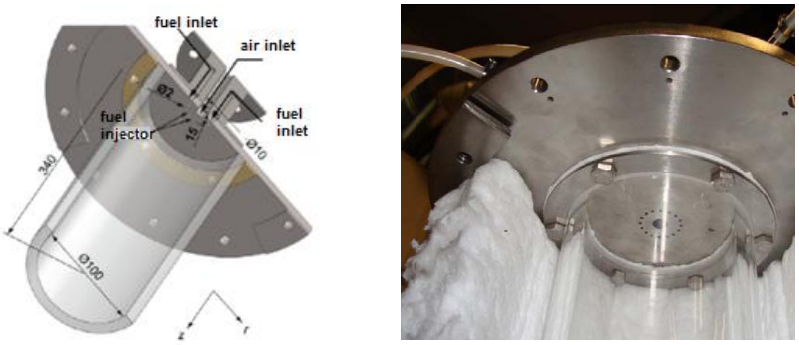


Figure 1. Instantaneous images of the burning of natural gas with progressive dilution by N_2 and CO_2 (Szego, 2010).

According to the interest of the industrial sector by the flameless combustion technology, several researches have been carried out around the world, not only in an experimental method but numerically, generally through Computational Fluid Dynamics, CFD techniques. So, considering the complexity of the combustion regime and the importance of NO_x levels, the CFD analysis through detailed chemistry becomes essential for investigations and better understanding of the phenomena involved. Finally, through the detailed chemical kinetics, more information about the temperature field and the chemical elements of the combustion can be revealed, improving the investigation of this combustion regime and, approaching the real phenomena occurred.

2. NUMERICAL PROCEDURE

The burner geometry used was the object of study of the doctoral thesis of Veríssimo (2011). It is a cylindrical geometry burner with central combustion air flow and 16 fuel injectors, arranged radially at a distance of 15 mm from the center of the burner, like a burner design shown in Fig. 2, containing the major dimensions.



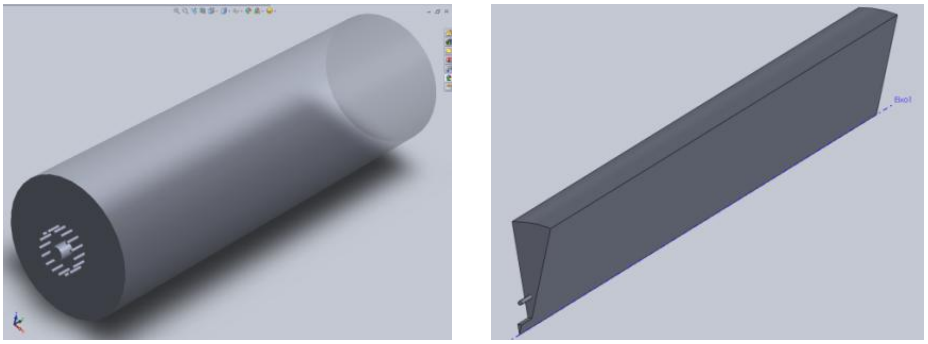
(a) (b)

Figure 2. Schematic domain representation
(a) three-dimensional perspective b) positioning of the injectors and the coating (Veríssimo, 2011).

The numerical simulations were obtained using a cluster computer with 40 cores distributed on 5 computers (named nodes), each with 8 processors Intel Xeon 5420 Quad-core 2.5 GHz/12MB with 16-GB RAM. The solution of the equations were obtained from the Second Order, with 10^{-6} residual target between iterations.

2.1 Simmetry and Periodicity

The use of symmetry conditions and periodicity are crucial for reducing the computational time employee. Initially, the simulations was performed in a full burner domain like showed in the Fig. 3a, following by a 1/16 sector analysis, according to the Fig. 3b.



(a) (b)

Figure 3. Domain detail and mesh used: (a) full and (b) 1/16 sector

Figure 4 presents a comparison between experimental and numerical values for the velocity v (considered in the main flow direction) along the central axis of the burner, both for the sector domain and the full domain. Given in Fig. 4, the numerical simulation considering the full domain, named iso3x4KESFull, was in good agreement with the experimental data, showing that the use of the sector condition can lead to errors in the results obtained. However, the computational time spent was extensive being able to make unfeasible the calculations involving more detailed reaction schemes. Regarding the analysis involving a sector, still at Fig. 4, named iso3x4KESsector, the numerical results were different from the experimental data, thus not featuring a good choice.

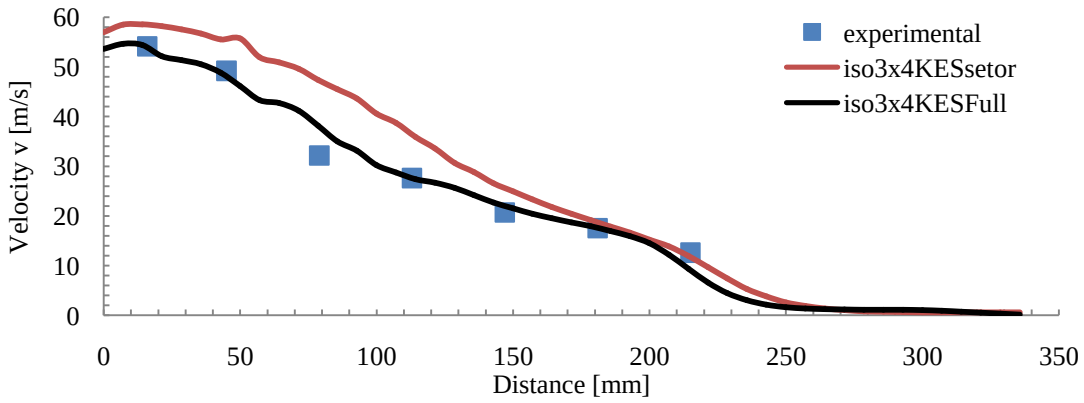


Figure 4. 1/16 sector *versus* full domain for the velocity v along the central axis.

Due to the high computational time using the complete domain, the condition involving half was evaluated, imposing the condition of symmetry. The numerical tests have been done in half burner domain. In the Fig. 5, obtained by the ANSYS Meshing® program is shown along with the defined regions. In the region named Symmetry (E) indicated, the domain symmetry condition was imposed on the ANSYS Fluent® program, in order to minimize the computational time spent in performing the calculations.

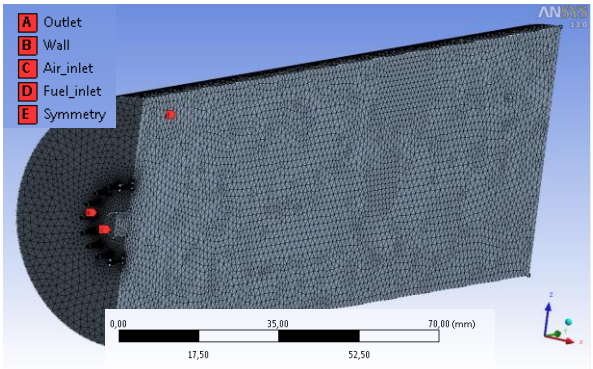


Figure 5. Mesh used in simulations involving the half burner.

In Fig. 6, the distribution of velocity v along the central axis is presented. It is noted that the behavior of the velocity v in a half domain is similar when considering the full burner, like showed in the Fig. 4, but with a lower computational effort. Furthermore, the choice of half domain reduces the enormous simplification introduced by the analysis of only a section of 1/16.

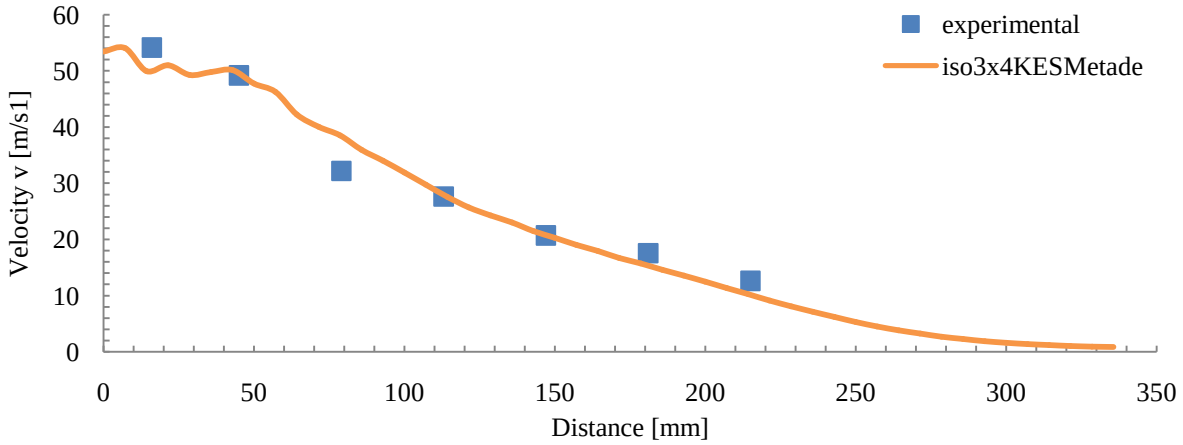


Figure 6. Vector velocity for half of the burner along the central axis.

The numerical results in a radial plane, 45 mm from the injector, are shown in Fig. 7, emphasizing the good agreement with the available experimental data.

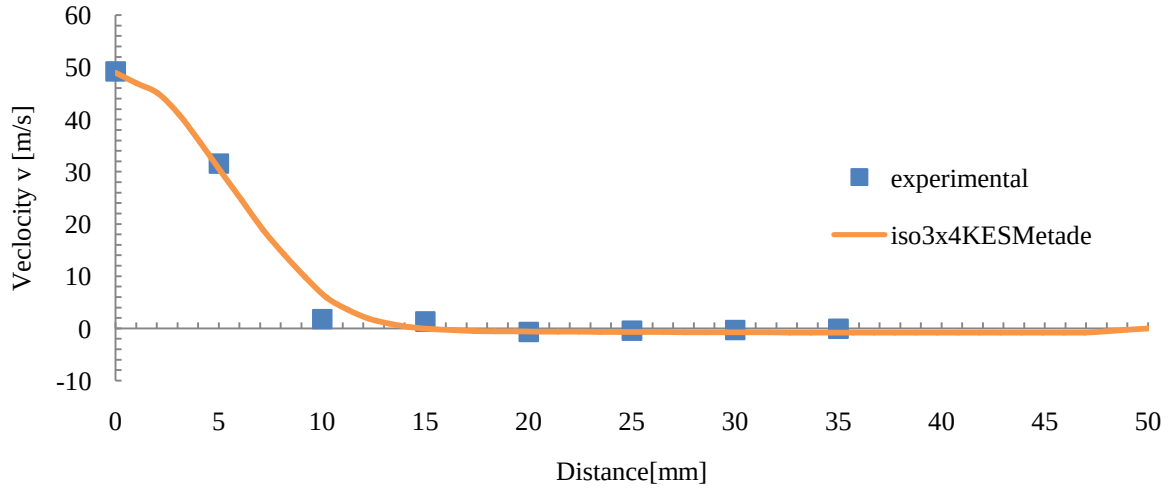


Figure 7. Velocity distribution (half domain) in the radial plane at 45 mm from the injector.

Based on the previous results, it will be used in combustion simulations a half domain and the mesh element size 3x4 totaling 97,039 nodes and 517,395 elements.

2.2 Mesh Independence

A comparison between the results obtained by varying only the size of the element used in the mesh can be seen in Fig. 8 and Fig. 9, showing the velocity v along the central burner axis. These results were obtained after the stability of parameters involved, like P-max, radiation and combustion species, using root mean square deviation distribution, RMS, and the convergence target of 10^{-6}. The mesh used was the tetrahedral type, once the construction process is simplified, besides the robustness already tested by other researchers.

It can be observed that the coarse mesh, named iso8x12KESMetade, containing 29,819 nodes and 144,956 elements its away from the experimental data, while the superfine mesh, named iso2x3KESMetade with 262,349 nodes and 1,463,431 elements had failures in the outlet region. Thus, the intermediate mesh, named iso3x4KESMetade with 97,039 nodes and 517,395 elements showed good agreement, according to the Fig. 8 and Fig. 9. Furthermore, the

computational time spent was significantly reduced. All simulations was employed k-epsilon standard turbulence model, in order to evaluated correctly the mesh element influence.

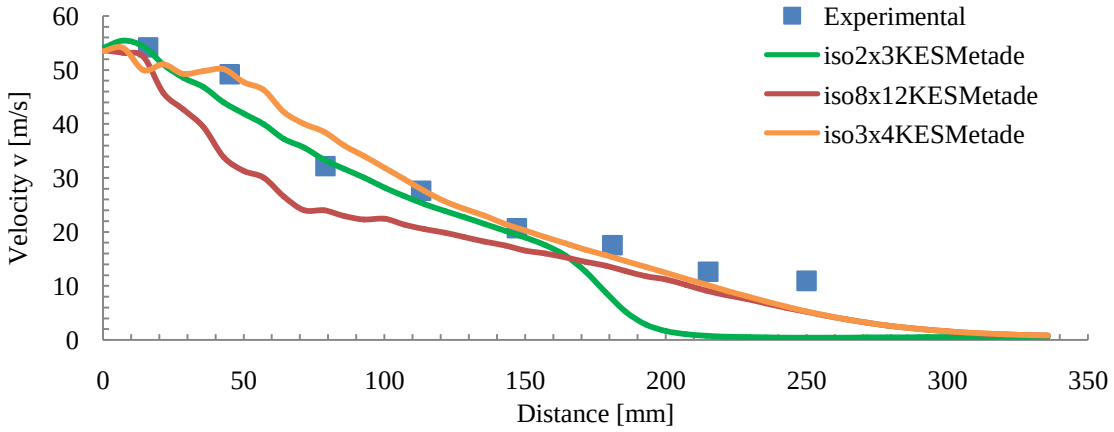


Figure 8 Comparison of velocity vectors v in the central plane as a function of mesh elements used.

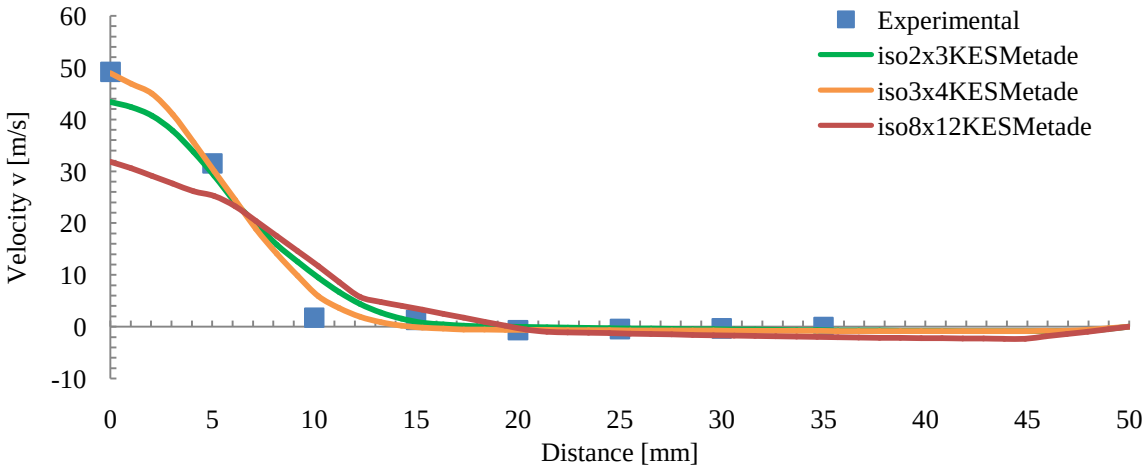


Figure 9 Comparison of velocity vectors v at 45 mm of the injector, according to the mesh elements used.

2.3 Detailed Chemical Mechanisms

The simulations involving combustion and detailed chemical kinetics employs the k-ε Realizable (KER) turbulence model, EDC Eddy Dissipation Combustion model (EDC) with detailed chemistry by GRIMech3.0 and Discrete Ordinates Model (DO) for modeling radiation. The GRIMech3.0, a chemical reaction library, is the latest version created by the Gas Research Institute, in order to collect and standardize data on chemical kinetics. In addition to the GRIMech 3.0, 325 intermediate reactions, associated to the reaction rate and Arrhenius parameters, totaling 53 different chemical species (Smith *et al.*, 2014).

Given the numerous intermediate reactions presents in the modeling with detailed kinetics, the expected result tends to be closer to the experimental data. Considering the temperature field, due to the enthalpies of formation of the various steps involved, the energy available by the combustion process tends to be consumed, reducing its global temperature.

However, the computational time for the solution of the 325 partial reactions, the flow variables and the radiation properties exceeded 380 hours of simulation. Thus, if geometry were more complex, time would certainly increase, making the whole process unfeasible. In this context, it is necessary to search for alternatives to reduce this computational time spent. One of them is the simplification of the partial reactions described in the library GRIMech3.0, where for each type of experiment are maintained those reactions and preponderant chemical elements. Therefore, it is sometimes necessary to change the Arrhenius constants in order to compensate for the elimination of the other reactions.

One of the libraries tested with flameless combustion is called KEE58 (Amniam *et al.*, 2012). KEE58 is composed by 18 chemical species and 58 intermediary reactions, which represents a considerable reduction compared to

GRIMech3.0. Next, the results obtained with the simulation involving KER / EDC_KEE58 / DO are presented. It is worth mentioning that the results presented below were obtained with 1/3 of the computational time employed in GRIMech3.0, considering a more pronounced convergence profile towards the target value of 10^{-6} for residuals.

3. RESULTS AND DISCUSSIONS

A comparison of the temperature profile along the central axis between the GRIMech3.0 and KEE58 libraries is shown in Fig. 10. Note that the profile behavior traced by the numerical data is the same for the two approaches, with a greater distance for KEE58 kinetics, possibly due to simplifications of the model in the number of species and intermediate reactions.

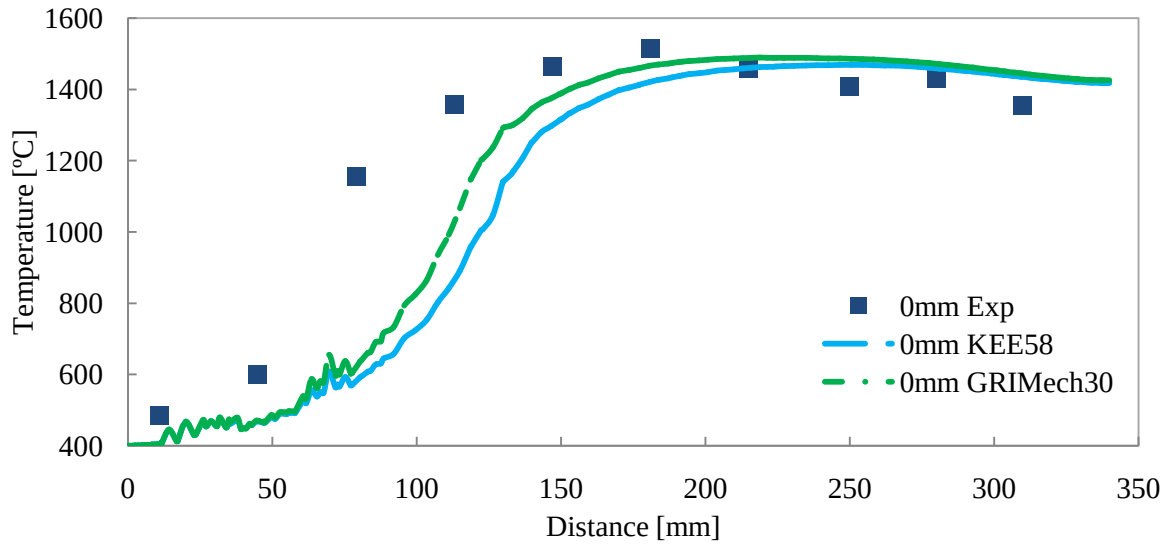


Figure 10 Comparison of temperature between KEE58 x GRIMech3.0 on the central axis.

According to Tab. 1, the deviations between the KEE58 and GRIMech3.0 mechanisms were calculated in order to facilitate the comparison between the results. The region of greatest deviations between the two kinetics is noted between 79 mm and 147 mm, but still small by the various simplifications present in KEE58 kinetics.

Table 1 Evaluation of the deviation in the temperature distribution between KEE58 and GRIMech3.0

Distance (mm)	simulation KER/EDC_KEE58/DO (ºC)	simulation KER/EDC_GRIMech30/DO (ºC)	relative deviation (%)
11	404,7	412,1	1,8
45	467,6	470,2	0,6
79	591,6	636,3	7,0
113	891,3	1066,6	16,4
147	1296,4	1374,6	5,7
181	1421,1	1466,3	3,1
215	1460,7	1488,6	1,9
250	1469,4	1486,4	1,1
280	1458,8	1471,3	0,9
310	1438,9	1445,2	0,4

The consumption of O_2 and CO_2 formation along the central axis for both KEE58 and GRIMech3.0 are shown in Fig. 11 and Fig. 12 respectively. It is observed that the profile is very similar as expected, since the formation reactions of the main chemical species were maintained during the simplification in KEE58 and, being preponderant over the others.

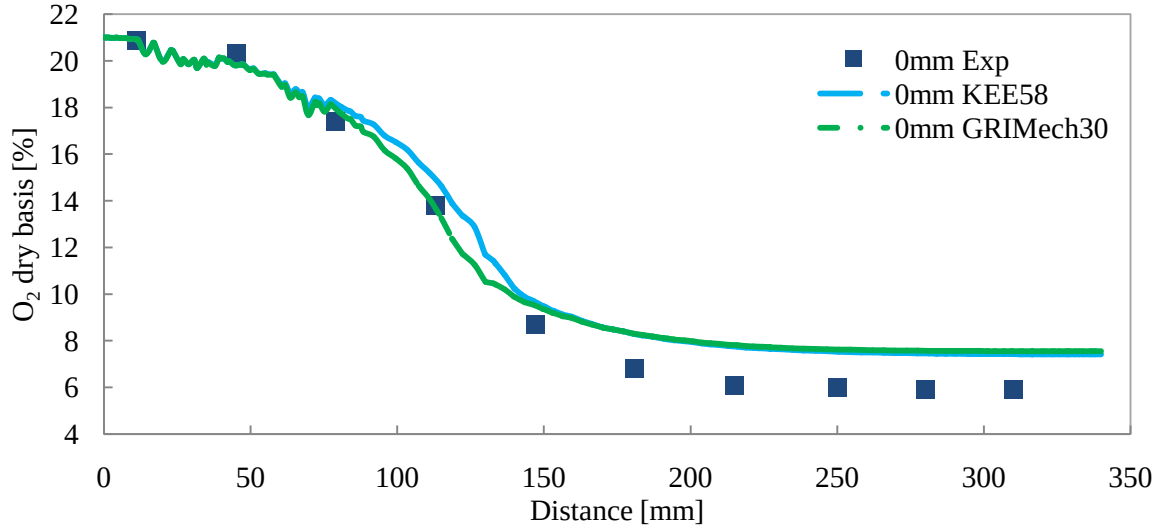


Figure 11 Comparison of O_2 between KEE58 x GRIMech3.0 on the central axis.

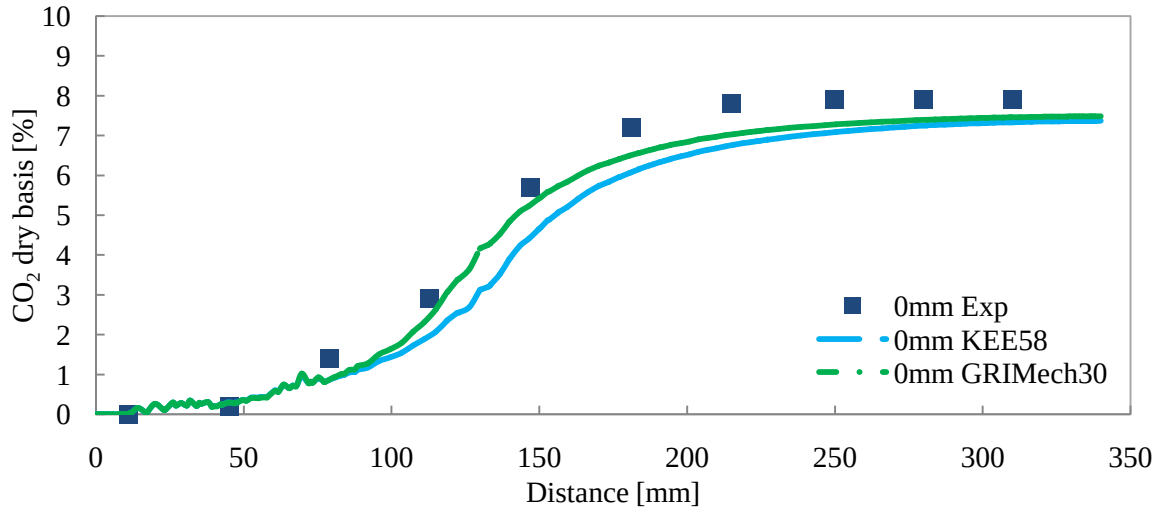


Figure 12 Comparison of CO_2 between KEE58 versus GRIMech3.0 on the central axis.

In Fig. 13 the formation of CO along the central axis between KEE58 and GRIMech3.0 is presented. It can be observed that the profile for KEE58 was displaced, approaching the experimental behavior. However, the maximum value was 15.6% higher than the GRIMech3.0 simulation, possibly due to the fact that some reactions were neglected.

Finally, a comparison of the NO_x formation between KEE58 and GRIMech3.0 kinetics along the central axis is shown in Fig. 14. Note that the KEE58 had agreement up to 1/3 of the burner length, distancing until reaching a maximum of 60 ppm. Analyzing the reactions presents in KEE58 kinetics, it is verified that those responsible for the formation of NO were eliminated, which results in less data and information for the so-called pathways present in ANSYS Fluent®. In summary, pathways are functions and equations that determine the rate of formation of the pollutant from the concentration resulting from the chemical balance. Thus, in the absence of the concentration values of a given species, the calculated training rate may be overestimated.

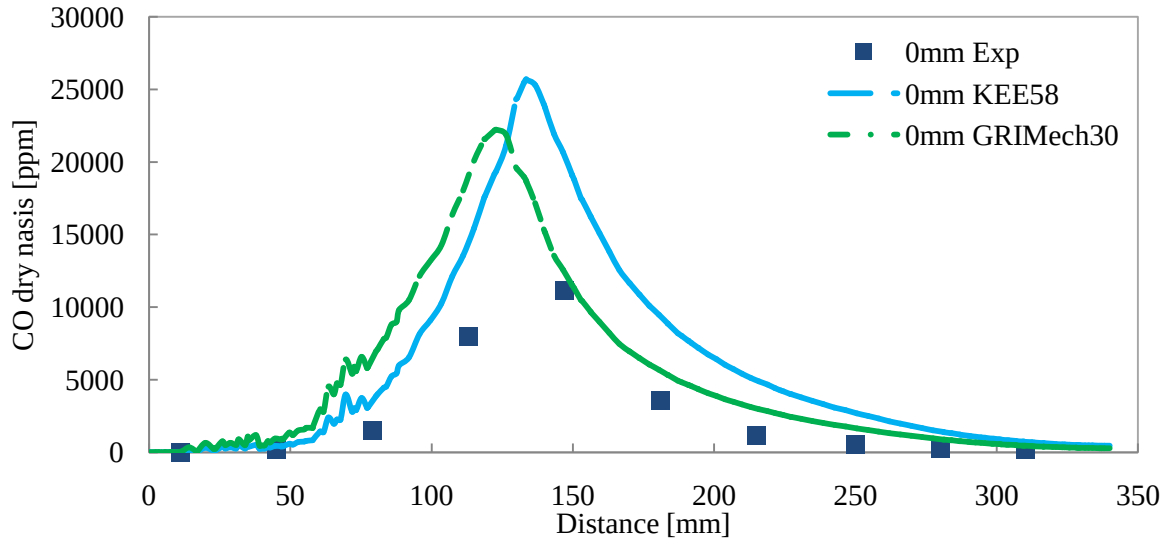


Figure 13 Comparison of CO between KEE58 x GRIMech3.0 on the central axis.

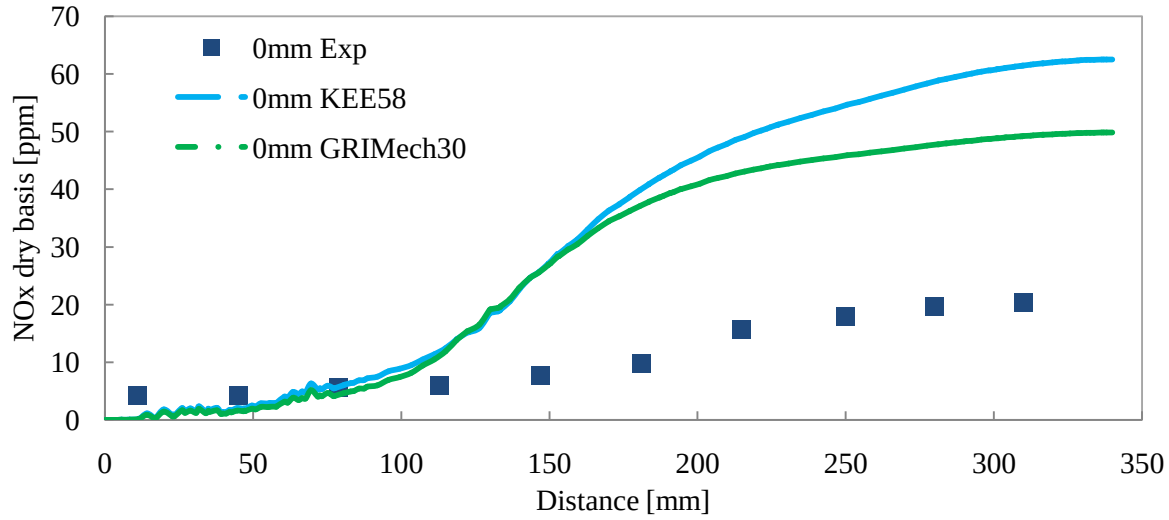


Figure 14 Comparison of NO_x between KEE58 and GRIMech3.0 on the central axis.

4. CONCLUSIONS

It can be noted by the results obtained that the use of detailed chemical kinetics guarantees better information for the combustion products generated and the flow pattern inside the combustor. Moreover, it made it possible to identify a milder temperature field, more coherent with the physical phenomenon identify. However, the computational time required was large, worsening in more complex geometries and cases involving more complex physical phenomena. In this context, it was possible to investigation the reduced mechanisms, such as KEE58, which provided good results in a shorter time interval. However, large deviations were found in the prediction of CO and NO_x formation, even using detailed kinetics. Such deviations may have a strong influence of the method used in turbulence modeling, which in this work was RANS. As discussed earlier, the runoff variables are considered averages in this case, which leads to sometimes distorted estimates of actually present fluctuations. In this case, as the NO_x content formed is very small, especially in the flameless combustion regime, such fluctuations assume a relevant role in the final value obtained. Based on this analysis, closer values can be obtained in LES or DNS type modeling, despite the excessive computational time already required by them. Regarding the formation of CO, the parameters and reaction constants used must be more investigated, in the context of being a combustion regime with many particularities, which should be evaluated in future studies.

5. ACKNOWLEDGEMENTS

The authors gratefully acknowledge the financial support given by funding agencies like CAPES, CNPq and FAPEMIG, which were essentials to the development of this work. In particular, the ESSS company, an ANSYS partner for Brazil, by the support on Chemkin program, responsible for solution the detailed chemical reactions.

6. REFERENCES

Aminian, J.; Galletti, C.; Shahhosseini, S.; Tognotti, L. Numerical Investigation of a MILD Combustion Burner: Analysis of Mixing Field, Chemical Kinetics and Turbulence-Chemistry Interaction. Flow, Turbulence and Combustion, v. 88, n. 4, p. 597–623, 2012. Disponível em: <http://link.springer.com/10.1007/s10494-012-9386-z>. Acesso em: 23/5/2014.

EDP. Conheça a origem da energia em 2012. Available in: <https://energia.edp.pt/particulareshome/apoio-ao-cliente/origem-da-energia/2012.aspx>. Acesso em: 4/10/2013.

Gomez-Garcia, M. A.; Pitchon, V.; Kiennemann, A.. Pollution by nitrogen oxides : an approach to NOx abatement by using sorbing catalytic materials. Environment International, v. 31, p. 445–467, 2005.

Quaresma, P. M. R.. Efeito da Composição do Combustível no Desempenho de uma Câmara de Combustão com Baixas Emissões de NO x para Aplicação a Turbinas a Gás, 2010. Lisboa, Portugal: 74 f. Tese (Doutorado em Engenharia Mecânica) - Instituto Superior Técnico, Universidade Técnica de Lisboa.

Skalska , K.; Miller, J.S; Ledakowicz, S.. Science of the Total Environment Trends in NOx abatement : A review. Science of the Total Environment, v. 408, n. 19, p. 3976–3989, 2010. Elsevier B.V. Disponível em: <http://dx.doi.org/10.1016/j.scitotenv.2010.06.001>.

Smith, G. P.; Golden, D. M.; Frenklach, M.; et al. GRIMech 3.0. Disponível em: <http://www.me.berkeley.edu/gri_mech/>. Acesso em: 6/1/2014.

Szego , G. G.,. Experimental and Numerical Investigation of a Parallel Jet MILD Combustion Burner System in a Laboratory-scale Furnace, 2010. Australia: PhD Thesis, School of Mechanical Engineering Faculty of Engineering, Mathematical and Computer Science, University of Adelaide.

Veríssimo, A. S. Estudo Experimental de uma Câmara de Combustão Operando no Regime de Combustão sem Chama Visível, 2011. 131 f. Tese (Doutorado em Engenharia Mecânica) - Instituto Superior Técnico, Universidade Técnica de Lisboa.

7. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.