REDUCED CHEMICAL KINETIC MECHANISM APPLIED TO 3D NUMERICAL SIMULATION OF A SINGLE-CYLINDER RESEARCH ENGINE RUNNING A BLEND OF GASOLINE AND ETHANOL IN LOW LOAD REGIMES

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Abstract*. The understanding of the combustion process in spark ignition engines is very important in the development of more efficient engines in both, fuel consumption and energy conversion. Numerical simulations are applied to engines to understand all phenomenona occurring inside it to reduce time and money costs, which would be spent through experimental procedures. Also, reduced chemical reaction mechanisms are important tools in reducing computational cost and to reproduce the combustion process. However, few studies in literature report reduced mechanism validated for GDI engines. In this paper a reduced chemical kinetics mechanism was tested in a 3D CFD simulation of a single cylinder engine running Brazilian Gasoline type C in two different operation regimes (2000 rot/min, BMEP of 0,2 MPa and 4 MPa, homogenous charge) and direct injection of fuel. The comparison*

between experimental data and the numerical results showed that, under the conditions analyzed, the mechanism tested was not able to reproduce the behavior of the fuel mixture.

Keywords: *Spark ignition engines, Gasoline direct injection, Finite volume method, Reduced chemical kinetic mechanism.*

1. INTRODUCTION

The understanding of the combustion of fossil fuels in spark ignition engines is an important tool in the development of more efficient engines in both fuel consumption and energy conversion. Since the 1960s, studies have been published in the literature relating pollutant emissions by the automotive sector with environment and human health problems due to the use of fossil fuels as energy source in internal combustion engines (Heywood, 1988). Exhaust gases from the internal combustion engines may contain nitrogen oxides, carbon monoxide, and other organic compounds such as unburned and partially burned hydrocarbons. Those pollutants, formed by the oxidation of chemical species present in fossil fuels, contribute to increase respiratory problems, heart diseases and are responsible to environmental changes such as global warming (Dallmann & Façanha, 2017). For the analysis of the combustion process in spark ignition engines, numerical simulations are applied, objecting the understanding of the phenomenon that occur inside it without the time and money costs which would be spent through experimental procedures.

Computational Fluid Dynamics Simulation (CFD) has been largely applied in tri-dimensional simulations of engines (Senecal *et al*., 2003; Tan *et.al*., 2016; Tao *et. al*., 2009; Tao *et. al*., 2005). This method allows the analysis of in-cylinder processes according to time and space (Versteeg & Malalasekera, 2007). Moreover, the chemical reaction mechanism which describes the oxidation of the fuel during the combustion plays a very important role in CFD simulations. The use of detailed kinetic mechanisms requires a great computational effort, which makes it impossible to use them in applications that require many simulations in short intervals of time. It is then necessary to use reduced kinetic mechanisms capable of representing the behavior of the fuel in the different operating conditions of the engines (Tan *et al*., 2016).

The reduced mechanisms are composed of key species that serve for different situations. The first methods applied in order to create reduced mechanism were based on time scale analysis. Computational Singular Perturbation, Intrinsic Low dimensional manifolds and Level of importance, are examples of such methods. The elimination of the species considered as unnecessary was based on considerations of quasi-steady-state or partial equilibrium reactions (Terese, 2012).

The reduced mechanism used at this work contains 204 chemical species and 1158 elementary reactions. The mechanism was obtained by reducing a detailed mechanism containing 1410 species and 6107 reactions through the Directed Relation Graph (DRG) method, associated with Sensitivity analysis, as described by Cota (2017).

In Brazil, the use of ethanol as an additive to gasoline has been shown to be an efficient alternative with a high impact in reducing dependence on fossil fuels and in mitigating

vehicular emissions of greenhouse gases (Soares *et. al.*, 2009). According to the Brazilian National Agency of Petroleum (ANP), gasoline available to consumers at Brazilian gas stations, Gasoline type C, contains 27% by volume of ethanol. The fuel injection system plays also a crucial role related to engine performance and emission formation (Baumgarten, 2006). The gasoline direct injection (GDI) is a technology that allows working with mixture stratification, which can remarkably reduce fuel consumption, especially during part load conditions and cold start. However, the charge stratification can lead to different burning velocities, misfire and increase soot and NOx emissions (Zhao *et. al.*, 2000). Due to its visibility and high consumption, as well as the impact of its use on the adequacy of national and international environmental standards, it is necessary to study the physical chemical behavior of the combustion of Brazilian gasoline type C in internal combustion engines.

This paper proposes the use of CONVERGE CFD software for numerical simulation of an internal combustion engine running Brazilian Gasoline type C in two different operation regimes (2000 rot/min, BMEP of 0.2 and 0.4 MPa, homogenous charge and average intake pressures of 38.81 kPa and 54.92 kPa, respectively) and direct injection of fuel with the objective of evaluating the reduced chemical kinetic reactions mechanism for GDI engines in low load regimes. The numerical results were compared with experimental results obtained from the database of the Center for Mobility Technology (CTM), Federal University of Minas Gerais.

2. METHODOLOGY

2.1 Kinetic mechanism

The methodology proposed to create a reduced kinetic mechanism to be used during the simulations was divided into four steps. The first one was the creation of a gasoline surrogate composed by a smaller number of components than the complete gasoline formulation, based on a chemical composition analysis. The second step was the creation of a detailed kinetic mechanism capable of reproducing the characteristics of the surrogate and its blends with ethanol. The next step was the mechanism reduction through the directed relation graph (DRG) method, by which unimportant species and reactions were removed. The final step was a sensitivity analysis used to achieve a greater reduction by removing species which do not have a significant impact on the simulation of ignition delay time data.

The parameter selected to validate the final mechanism was the ignition delay time. The ignition delay is considered, for engine simulation, as the time elapsed from the start of injection to the start of combustion. The Chemistry tool of the software CONVERGE CFD was used to simulate this parameter. The simulation proceeds by burning the fuel mixture in a constant-volume spherical bomb. The software considers the ignition delay as the time required to a temperature increasing of 400 K from its initial value, Richards et. al (2017).

The simulations were conducted for pressures of 1, 2, 4 and 8 MPa; temperatures from 600 K to 1000 K; equivalence ratio of 1; and for a gasoline blended with 27% of ethanol in volume.

2.2 Fuel composition

For the fuel composition, a chemical analysis was conducted by the Fuel testing laboratory of the Chemical department of the Federal University of Minas Gerais (UFMG). The analysis defines the fractions of Alkanes, Olefins and Aromatics of the fuel through the GS 1000 equipment, according to internal methodology. At this work, following the methodology of Cai & Pitsch (2015), a mixture of iso-octane, n-heptane, 1-heptene and toluene was chosen as a proper gasoline surrogate, representing the fractions of Alkanes, Olefins and Aromatics, respectively. With the gasoline surrogate composition defined, the fuel was blended with Anhydrous Ethanol, so that a mixture containing 27% ethanol by volume was obtained, reproducing, therefore, Brazilian gasoline type C. Table 1 presents the final fuel composition according to the gasoline surrogate obtained.

Table 1. Fuel composition

Component	Molecular formula	Mass fraction	Volume fraction
n-Heptane	C_7H_{16}	0,0774	0,0871
Iso-Octane	C_8H_{18}	0,1822	0,2031
Toluene	$C_6H_5CH_3$	0,3178	0,2819
Heptene	C_7H_{14}	0,1250	0,1380
Ethanol	C_2H_5OH	0,2975	0,2900

2.3 Mechanism creation

The complete mechanism was divided into a mixture of n-heptane and iso-octane, primary reference fuels (PRF), toluene, polycyclic aromatic hydrocarbons (PAH), heptene and ethanol. The detailed kinetic mechanism for the PRF and heptene mixture was obtained by the research group of Lawrence Livermore National Laboratory of United States, developed by Mehl *et al.* (2009). The PRF mechanism contains 878 species and 3796 elementary reactions. The toluene oxidation model was adopted from the study of Nakamura (2014). The model consists of 550 species and 2805 elementary reactions. For the Ethanol fraction the mechanism developed by Roehl (2009), was adopted. The mechanism has 38 species and 228 elementary reactions. As one of the goals of this work was to analyze the Nitrogen Oxides emissions, a Nitrogen Oxides formation model from Lamoureux (2010), was also incorporated to the final mechanism. The final mechanism obtained was composed by 1410 species and 6107 elementary reactions.

2.4 Mechanism reduction

The base detailed mechanism obtained was reduced according to the methodology described by Mehl *et al.* (2009 and 2011), following two steps. At the first one, the Direct Relation Graph (DRG) methodology was applied. Through this method, unimportant species and elementary reactions were removed based on the relation of each species with the reaction coefficient of the fuel surrogate. On the final step, a Sensitivity Analysis was used to reduce the mechanism as much as possible, without impairing the accuracy of the mechanism.

Through this method, the species, one by one, were removed from the mechanism and their impact on the ignition delay time was compared to the results obtained with the detailed mechanism. At the end, only the species with a significant impact on this parameter were maintained at the mechanism. The final mechanism obtained was composed by 204 species and 1158 elementary reactions (Cota, 2017).

2.5 Computational domain and operating conditions

A Single Cylinder Research Engine (SCRE), model AVL 5496, was used to perform the simulations of a physical engine and analyze its performance and pollutant emissions. This engine has two inlet valves and two exhaust valves located in the cylinder head. The main characteristics of the engine are summarized in Table2.

Table 2. Single-Cylinder Engine's characteristics

Characteristic	Description
Model	AVL 5496 – Single-cylinder
Displaced	454.16 cm3
Stroke	86 mm
Cylinder Bore	82 mm
Compression	11.5:1
Connecting rod	144 mm
Exhaust Valve	56º before BDC
Exhaust Valve	0 after TDC
Inlet Valve Open	0 after TDC
Inlet Valve Close	40º after BDC

The fuel injector was the multi-hole Bosch HDEV 5.1 composed by 7 holes with 0.17 mm diameter each and 20° outer cone angle for each single plume. From the work published by Reis et al. (2015), were obtained the holes positioning and the nozzles injection direction for the same injector.

From the tri-dimensional geometric model of the engine, the internal volume of the inlet and exhaust ports and the combustion chamber of the SCRE were extracted. Figure 1 presents the computational domain from the single cylinder engine and the details of the cylinder's head with respect to the intake and exhaust valves.

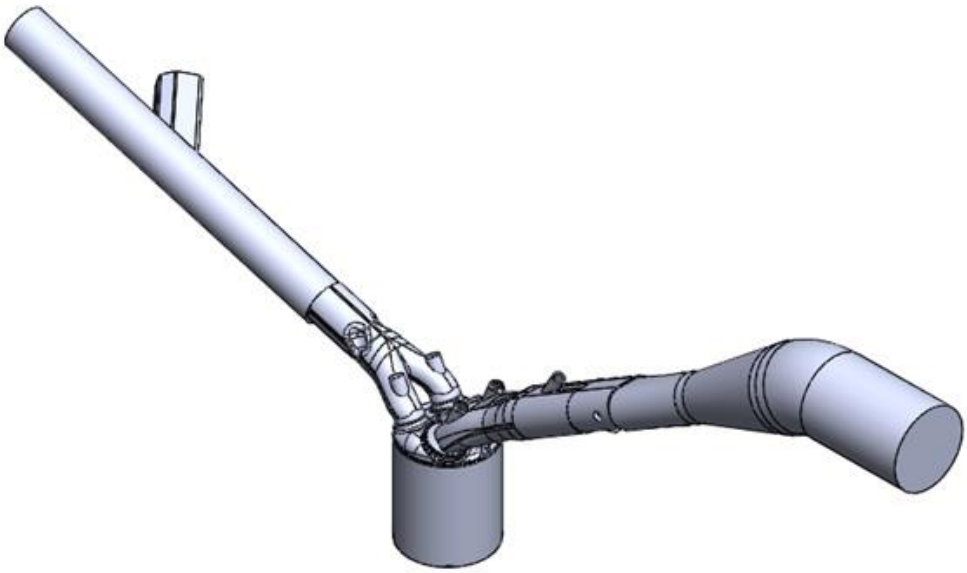


Figure 1 – Computational Domain (Source: Author)

The boundary conditions and experimental results were obtained from the Mobility Technology Center (CTM) database. The measurements were performed in wide open throttle, equivalent ratio (φ) 1 and 2000 rev/min conditions. The cases features used to compare to the results of the numerical simulations are summarized in Table 3.

Table 3. Operating conditions for the single-cylinder research SRCE

Operating mode	1	2
IMEP [MPa]	2	4
Fuel	E27	E27
Intake Temperature [K]	302	302
Start of fuel injection [° CA]	270	270
Duration of fuel injection [° CA]	11.6	17.1
Mass of fuel injected per cycle [kg/cycle]	1.1E-05	1.6E-05
Injection Pressure [MPa]	800	800

2.6 CFD modelling methodology

The computational domain was imported to the software CONVERGE CFD where the simulations using the Finite Volume Method (FVM) were performed. In the present work, sub-models for turbulence, heat transfer, spray break-up, fuel vaporization and combustion chemistry were applied for the simulations. These sub-models are presented in this section.

For turbulence, it was used the RNG k-ε model and to simulate the heat transfer the O'Rourke and Amsdem model was implemented. The wall temperatures of the subdomains (cylinder, piston, head, intake and exhaust ports, valves and spark plug) were estimated based on the engine operations conditions due to the difficulty to obtain these measurements experimentally.

The spray break-up was modeled using the combined model of Kelvin-Helmholtz Rayleigh-Taylor (KH-RT). The constants values applied in this model was based on the work published by Braga *et al.* (2017), with values 0,61; 7, 1 and 0,5 for B0, B1, Cb and C3, respectively. The vaporization of fuel was modeled using the Frossling correlation. This model calculates the time rate of change of the liquid fuel droplet radius based on the mass diffusivity of the fuel vapor (Senecal *et al.*, 2003). The SAGE model, a chemistry detailed solver, was implemented for the combustion simulation with the reduced chemical kinetic mechanism obtained at this work.

For the Mesh, a base grid size of 4mm (dx) was used together with the Adaptive Mesh Refinement (AMR) for the cylinder with 3 levels of embedding and sub-grid criterion of 1 m/s and 2.5 K for speed and temperature, respectively. The AMR for the intake region is 3 levels of embedding with sub-grid criterion of 1 m/s for speed. Fixed embedding was used encompassing the region of the cylinder with 2 levels and inlet-exhaust valves with 3 levels each. The spark plug has two fixed sphere type embedding regions with 4 and 5 levels of refinement. There are also two embedding's regions for the fuel injector: one (type injector) with 2 levels and tip of the injector (ball type) with 3 levels.

2 RESULTS AND DISCUSSION

The results for the ignition delay time obtained in a Zero-D simulation for the mechanism used at this work are shown in Fig. 2. The experimental data for each curve are represented by the dashed curves and the numerical results by the solid lines. This Fig. indicates that the mechanism presents a very good agreement with the experimental data for pressures above 4 MPa for low and high temperatures. However, for pressures below this value, it can be observed a tendency of deviation from the experimental results for intermediate temperatures.

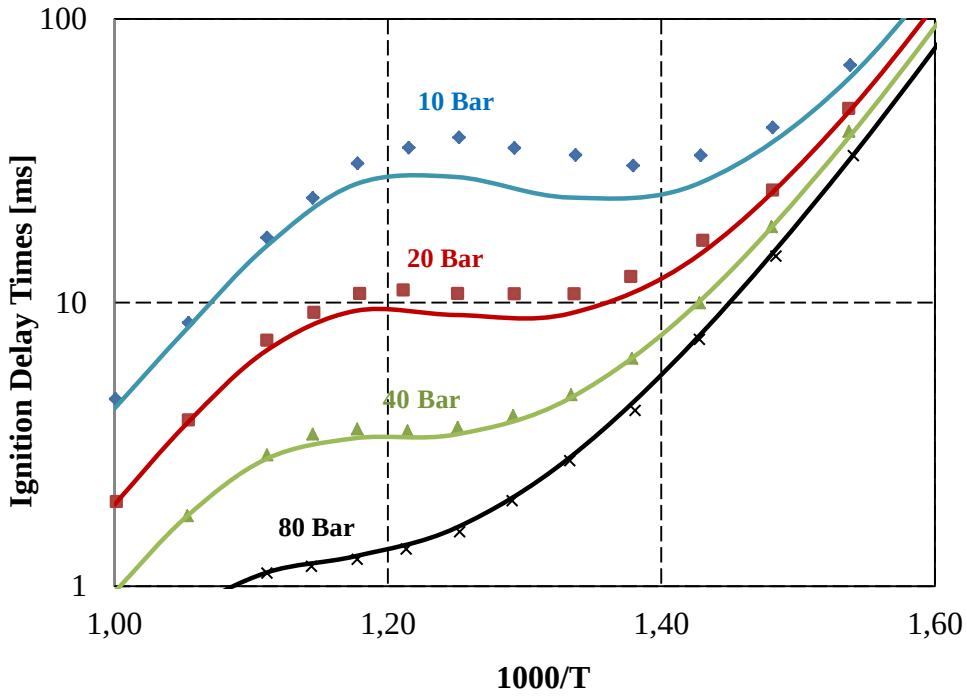
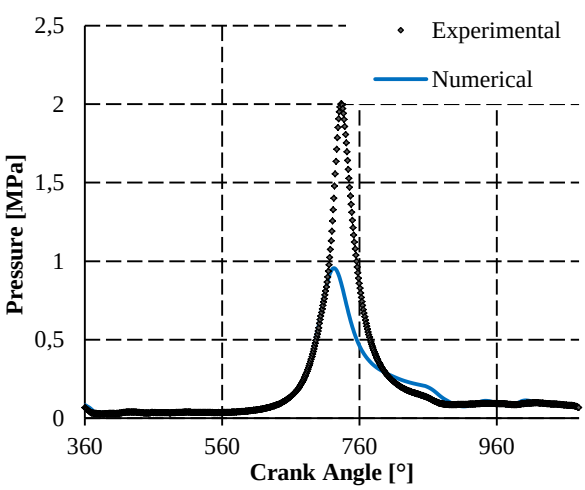


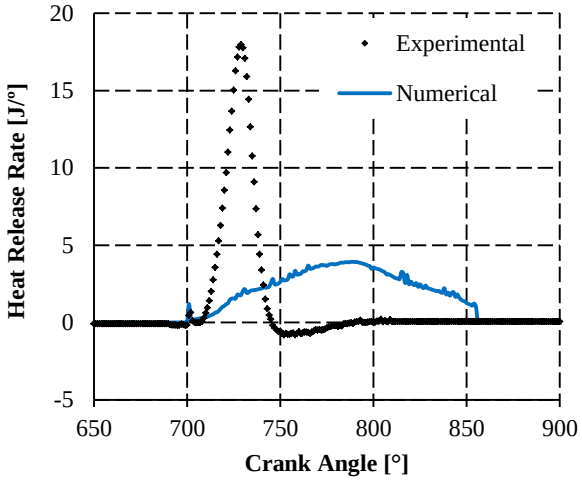
Figure 2 – Computational Domain (Source: Author)

The results obtained for the simulations for both conditions, 2000 RPM, 0,2 BMEP and 0,4 BMEP, Case 1 and 2, respectively, are shown in the Figures 3 and 4. The numerical simulations performed in this work reach in-cylinder pressures at the moment of the spark below 1 MPa. By the results obtained for the ignition delay, it could be expected that at the beginning of the combustion process, the mechanism would not correspond properly to the ignition of the air fuel mixture evaluated. Figure 3 and 4 show the results obtained for the in-cylinder pressure for Case 1 (2000 rot/min, 0,2 BMEP) and Case 2 (2000 rot/min, 0,4 BMEP), respectively.

Reduced chemical kinetic mechanism applied to 3d numerical simulation of a single-cylinder research engine running blend of gasoline and ethanol in low load regimes. C.M Martins, F.S. Cota, J.G.C. Baeta, R.M. Valle, G.Q. Hindi. UFMG-FCA, Belo Horizonte, MG, Brazil, November, 2017.

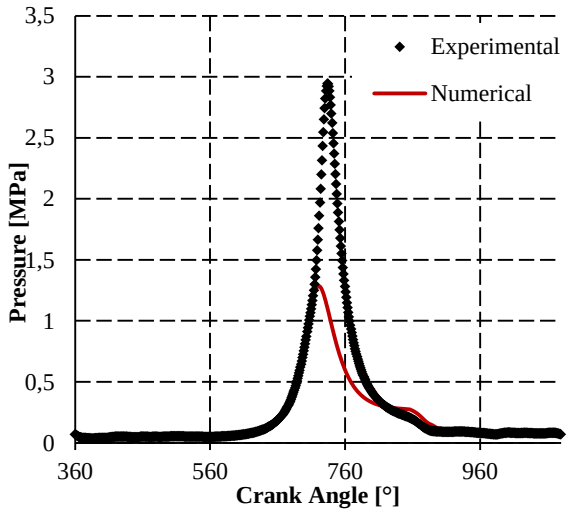


a) In-Cylinder Pressure

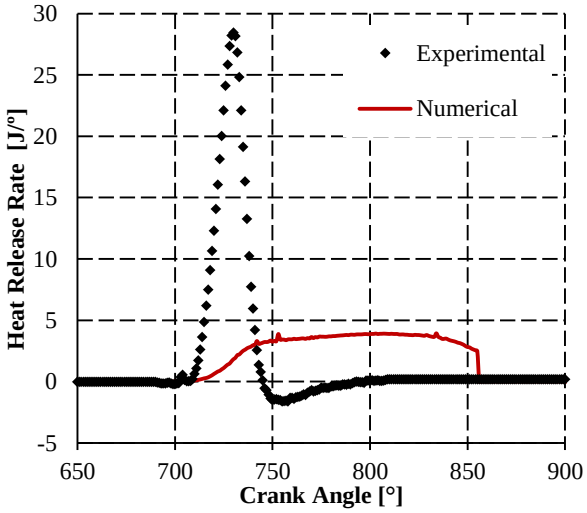


b) Heat Release Rate

Figure 3 –Case 1 (Source: Author)



a) In-Cylinder Pressure



b) Heat Release Rate

Figure 4 – Case 2 (Source: Author)

The analysis of the pressure in the cylinder and heat released rate as a function of crank angle showed a similar behavior for both conditions. The in-cylinder pressure showed good agreement with the experimental data for the regions of the intake and outflow phases, but for regions comprised between the spark moment (701º and 703º for Case 1 and 2, respectively) and the beginning of the exhaustion (136º for both cases) the pressure was underestimated by the model, indicating that the combustion process have not occurred well. The interpretation of the heat release curve corroborates with this conclusion. The discrepancy between the experimental e numerical curve's shapes indicates a slower combustion process for both cases. For better analysis of this process, Table 4 and 5 presents the comparison between the burning angles for experimental and numerical data.

Reduced chemical kinetic mechanism applied to 3d numerical simulation of a single-cylinder research engine running blend of gasoline and ethanol in low load regimes. C.M Martins, F.S. Cota, J.G.C. Baeta, R.M. Valle, G.Q. Hindi. UFMG-FCA, Belo Horizonte, MG, Brazil, November, 2017.

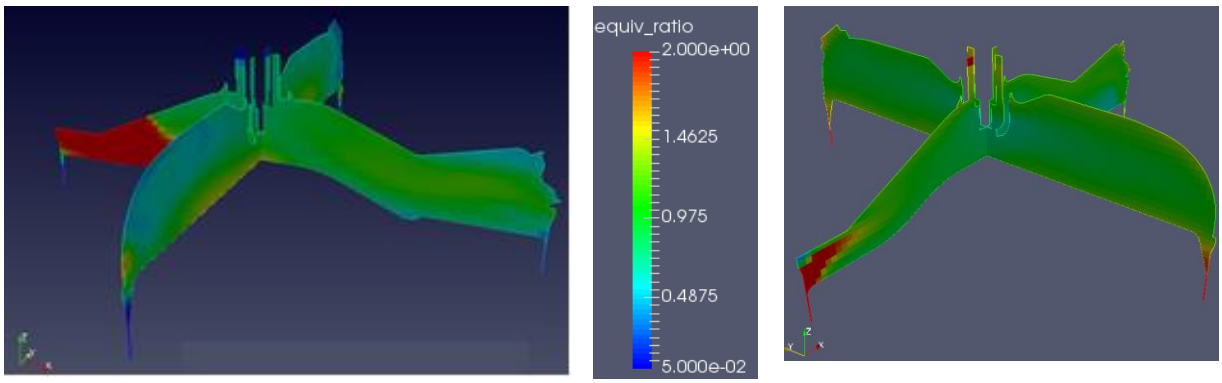
Table 4. Combustion Analysis Parameters for Case 1

MBF [º]	Experimental	Numerical
50	7,6 ± 0,1	64,1
10-90	18,8 ± 0,3	94,9
10-50	9,3 ± 0,1	47,6
50-90	9,5 ± 0,2	47,3

Table 5. Combustion Analysis Parameters for Case 2

MBF [º]	Experimental	Numerical
50	8,3 ± 0,2	72,9
10-90	18,3 ± 0,3	98,6
10-50	9,4 ± 0,1	50,9
50-90	8,9 ± 0,2	47,7

The results shown in the tables agree with assumption of a slower combustion for the numerical simulations. The MBF 50 represents the angle at which 50% of the fuel was burned, for Case 1 and 2 the difference between the numerical and experimental results are 743% and 778%. The first phase of fuel burning (MBF 10-50) also demonstrates a large discrepancy between the numerical and experimental results: 397% for Case 1 and 436% for Case 2. For the second phase of fuel burning (MBF 50-90) it can be seen the same tendency: 397% of difference for Case 1 and 436% for Case 2. To confirm that the main reason for the results observed in this work was the reduced mechanism it is important to analyze the mixture formation. Figure 5 shows de equivalent ratio parameter for the angles: 700º for Case 1 and 70º for Case 2.



a) Case 1

b) Case 2

Figure 5 – Local equivalent ratio (φ) (Source: Author)

Figure 5 demonstrates that for both cases, next to the spark plug the mixture is close to stoichiometric conditions, which was expected for the homogeneous charge. Then, it is confirmed that the reduced chemical kinetic mechanism used in this study was not able to correspond properly to the ignition of the air fuel mixture in the load regimes evaluated. That could be the reason for the slow combustion, taking to small pressure peaks and broad heat release curves.

3 CONCLUSION

In this study, CFD analyses using reduced chemical mechanism on a single-cylinder research running Gasoline Type C were carried out. Two load regimes were evaluated: 2000 rpm, BMEP of 0,2 MPa and 0,4 MPa and the numerical results were compared with experimental data obtained from the database of the CTM-UFMG laboratory.

According to the analysis of the results, as well as the bibliography used, it was concluded that the model tested was not able to reproduce the experimental data obtained for the single-cylinder engine tested, operating at low load conditions. The chemical kinetic mechanism was identified as the main reason, due to the error demonstrated in the Ignition Delay analysis for pressures below 40 bar and intermediate temperatures. For both load regimes, the local equivalent ratio (φ) demonstrates a good formation of the air-fuel mixture near the spark plug before the ignition time. Tan *et al*. (2016), points out in their studies the lack of studies for reduced chemical mechanisms validated for GDI engines. This research will serve as base for further studies aiming the development of a reduced chemical kinetic mechanism able to represent the combustion process for operating conditions of low and high charges.

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DEFINITIONS/ABBREVIATIONS

DI	Direct Injection
GDI	Gasoline Direct Injection
KH	Kelvin-Helmholtz
RT	Rayleigh-Taylor
AMR	Adaptive Mesh Refinement
B1	KH model time constant
B0	KH model size constant
C1	KH model velocity constant

$C\tau$	RT breakup model time
C3	RT breakup model size
FVM	Finite Volume Method
CTM	Centro de Tecnologia da Mobilidade
φ	Equivalent ratio
NSC	Nagle and Strickland-Constable model