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ANALYSIS OF MERGED REACTION MECHANISMS IN AN INTERNAL COMBUSTION ENGINE USING C GASOLINE

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Abstract. *The main objective of this paper is to study a set of reaction mechanisms applied in engine simulations, focusing in making the simulation more reliable, since this is crucial to make the process practicable in the design of new engines. The experimental and numerical tests were obtained in an Otto engine using C gasoline, the initial and contour conditions from the tests were acquired in a dynamometer. The engine tested was 1.6 Flex, 4 cylinders and 16 valves. This engine works with PFI and has a compression ratio of 11:1 and the fuel used was E27 with lambda 1,0 and the engine speed used was 3500 rpm. The simulations cover mechanisms that apply for gasoline and anhydrous ethanol, which have to be combined to make the simulation run. A tool to combine them was employed in Converge-CFD and tested in a 3D engine simulation. The first mechanism used had 66 species and 215 reactions, the second 80 species and 422 reactions and the third 63 species and 380 reactions. The simulations were run in the Converge-CFD software with RANS turbulence model to model the turbulence. The results showed that two of the mechanisms had good convergence between them but one of them had a low pressure peak. Comparing with the experimental results the flame speed and consequently the pressure peak had low values, to overcome this problem the ignition advance was increased and then the results of the simulation were validated.*

Keywords: Reaction mechanism, CFD, Internal Combustion Engines, Three dimensional simulations.

1. INTRODUCTION

China and others countries are suffering from severe air pollution and it is associated to public health impacts (LIU, Jun et al., 2006). This way the governments of each country are imposing new and more severe rules to restrict the major pollution sources, such as vehicles, so alternative ways to adapt engines in the new rules are receiving more attention from the Engineers. One way to improve the engines is through numerical simulations using computational fluid dynamics (CFD). To make the CFD simulations practical in the concept of new components, it is necessary to make it faster and keep it reliable. So the main objective of this paper is to validate a 3D simulation of an engine, to make this process reliable and helpful in future engine concepts.

2. EXPERIMENTAL AND COMPUTATIONAL PROCEDURE

The engine used for this work was the Ford Sigma 1.6 Flex, 4 cylinders and 16 valves. This engine works with PFI and has a compression ratio of 11:1 and the fuel used was E27 with lambda 1,0. The engine speed used was 3500 rpm.

2.1 Experimental procedure

The experimental procedure and data acquisition for the three dimensional simulation is explained in "Couto, 2017" as follows.

The dynamometer was equipped with systems to control the temperature of the room and the engine coolant. It also controlled pressure and temperature of the lubricant and fuel.

Two K-type thermocouples were installed in the exhaust manifold and crankcase, respectively, for the measurement of the exhaust gas and oil temperatures. The temperature of the cooling fluid is measured at the inlet and outlet of the engine by the installation of two platinum bulb resistance thermometers (PT-100).

The engine speed is measured by an inductive sensor mounted on the crankshaft pulley and the mass flow of fuel is measured by a Coriolis type mass flow transmitter of the Metroval brand, model RHM03, which is indicated by an electronic unit of the same type brand, model RHE08.

The identification of the position of the throttle and acceleration pedal is made by two resistive sensors. In addition, this subgroup is also composed of pressure gauges, ambient temperature and relative humidity to monitor environmental conditions.

The amount of air entering the motor is measured by an air flow sensor which provides a voltage signal that varies according to the amount of air passing through the sensor. Other signals received by the UCE are from the wide-band lambda probe, allowing the monitoring of the air-fuel ratio, and the signal coming from the control potentiometer of the butterfly valve.

The air temperatures in the intake manifold and the engine coolant are measured by two NTC type sensors, and the air pressure in the intake manifold is measured by a Manifold Air Pressure sensor.

The measured pressure is show in Figure 1 for the intake and exhaust manifold.

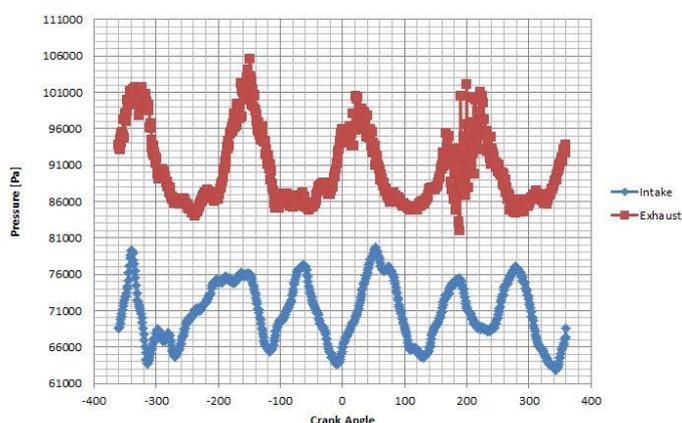


Figure 1. Intake and exhaust pressure

To measure the pressure data in the cylinder, a piezoelectric pressure transducer of the brand AVL model GH14P was used. This sensor was installed in the combustion chamber of the first cylinder through a hole machined in the head according to dimensions and inclination specified by the sensor manufacturer. As this pressure transducer measures pressure variations, an absolute pressure sensor of the brand AVL, model LP11DA, was installed in the intake manifold.

An optical encoder type angular position meter has also been installed on the motor, which provides a digital pulse-shaped signal for crankshaft angle indication. The electrical signal from the pressure transducer passes through an amplifier for signal conditioning and amplification prior to processing and scanning in an analog-to-digital converter. The amplifier used is the AVL brand, Micro IFEM model. A combustion data measurement system of the AVL brand, model IndiModul XTension, was used for treatment and recording of pressure data in 0.1° crank angle intervals. The data used in the results were calculated from the average of 100 cycles collected for each test condition with this sensor.

2.2 Computational Procedure

Computational Fluid Dynamics, CFD, is the analysis involving heat transfer, fluid mechanics, and other phenomena, such as chemical reactions, within a system. Mathematical modeling of differential equations that represent the physics of the system under study have to be used. (VERSTEEG & MALALASEKERA, 2007)

Turbulent flow generates vortices in the fluid, which are responsible for more efficient energy, mass and momentum changes. The larger vortices draw energy from the stream and carry that energy into smaller vortices until it is converted into thermal energy. The methods that exist for the turbulence calculations and consequently the vortices can be grouped into three groups, DNS (Direct numerical simulation), LES (Large eddy simulation) and RANS (Reynolds-averaged Navier-Stokes equations). the lowest computational cost, this model was chosen for the simulations performed in this work.

In order to simulate turbulent flows with the mean Reynolds and Navier-Stokes equations it is necessary to add the turbulent viscosity models to model the Reynolds tensions as well as the scalar transport terms and close the mean flow system. One of the most used and validated methods today are the k-models models, they are based on the assumption that there is an analogy between the viscous voltages and the Reynolds voltages in the average flow.

According to (Barros 2003), the modeling of chemical kinetics for a mixture of n chemical species (A_i), where simultaneously occurring m reactions, the general equation representing all reactions of the kinetic mechanism is represented in Equation 1.



The coefficients v'_{ij} and v''_{ij} are the stoichiometric coefficients of the reactants and the products, respectively, and k_{fj} and k_{bj} represent the reaction constants of the reaction j in the forward and reverse directions, respectively.

The fuel used was gasoline C, a combination of 27% anhydrous ethanol with the remainder of gasoline A. Thus it was necessary to make a combination between the chemical kinetics mechanism of gasoline and ethanol. Reaction mechanisms were combined using the software Converge-CFD. The model was used -60 degrees from the crankshaft up to 150 degrees, to save calculations during simulation.

For the three-dimensional modeling the internal geometry of the engine was inserted in the commercial software "Converge Studio", along with the initial and contour conditions necessary for the simulation. The SAGE chemical kinetics model was used to solve the combustion model. To solve the turbulence the RANS model RNG k - ϵ was used.

The mesh used has a base size of 4mm which is recommended by "Richards, K. J. et al, 2015". Converge Studio has a mesh optimization algorithm that automatically generates the mesh according to local parameters. This adaptation mechanism was used in regions where the speed or temperature are high. In addition to this mechanism, some regions have a fixed refinement criterion, such as the region of the ignition that is refined at the moment of electric discharge, the valves are refined at the time of opening and closing, and the combustion chamber within the range of combustion occurs.

For the simulation the computational domain of the engine was exported to the Converge-CFD software as show in Figure 2, on the right are the intake parts, on the left the exhaust. Then the contour conditions were set using the temperature and pressure sensors coupled in the engine in the dynamometer.

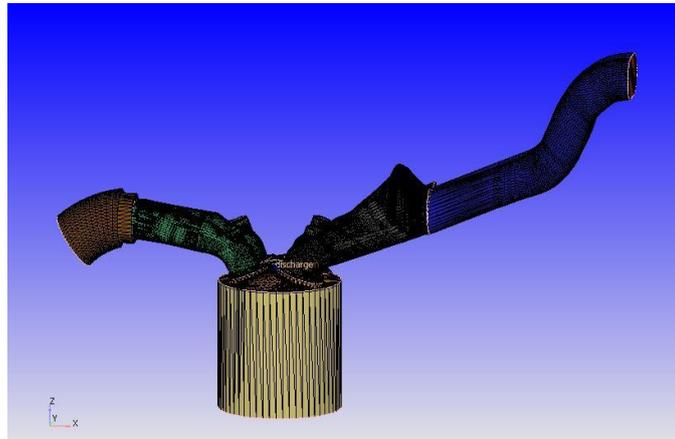


Figure 2. Computational domain

As the engine is PFI, to simplify the simulation the injection of fuel was considered pre-mixed. To calculate the partial fractions of the air/fuel mixture the data in Table 1 was used and Table 2 shows the results.

Table 1. Data used for the calculus of partial fraction

Nitrogen percentage in air	78,1	%
Alcohol percentage in gasoline	27	%
Water percentage in alcohol	0,4	%
Lambda	1,0	

Table 2. Partial fractions

Partial fraction	
0,203119859	O2
0,724368082	N2
0,052933803	Gasoline
0,019499943	Ethanol
7,8313E-05	H2O

Table 3 shows important parameters of the engine that were inserted in the simulation.

Table 3. Engine parameters

Cylinder bore:	<input type="text" value="0.079"/>	m
Stroke (2 * crank radius):	<input type="text" value="0.0814"/>	m
Connecting rod length:	<input type="text" value="0.137"/>	m
Wrist pin offset:	<input type="text" value="0e+00"/>	m

To solve the chemical reactions in Converge CFD the first step is to choose the elements that are going to be in the simulation, the elements chosen for both the gasoline and ethanol were H, C, N and O. The second step is to choose the species that participate in the reactions, this time different species were chosen for each fuel, this choice was based on past works that used this kind of fuel. After choosing the species is time to choose the reactions, and again it was chosen using the same method of the species. The next step was to combine both mechanisms so they can work in the simulation.

For combustion modeling the chemical kinetics model SAGE with three different reactions mechanisms was used. These mechanisms were a combination from mechanisms used for gasoline and ethanol.

The first reaction mechanism had 66 species and 215 reactions, this mechanism was developed by the combination of ethanol from the Lawrence Livermore National Laboratory (LLNL) which uses the mechanism from “Marinov, 1999”, and gasoline by “Liu, Yao-Dong, et al. 2013”. The second mechanism used was composed by 80 species and 422 reactions, the gasoline and NOx mechanisms were taken from “Converge Studio” and the ethanol from “Marinov, 1999”. The third mechanism had 63 species and 380 reactions and was composed by the same gasoline and NOx as the second mechanism but with a reduced ethanol mechanism derived from “Marinov, 1999”.

3. RESULTS AND DISCUSSION

The fuel flow measured in the experimental procedure was 10247,6 g/h, this represents 0,0244 grams per cycle for an engine which has 4 cylinders at 3500 rpm. Figure 3 shows the amount of fuel trapped in the cylinder for the numerical procedure.

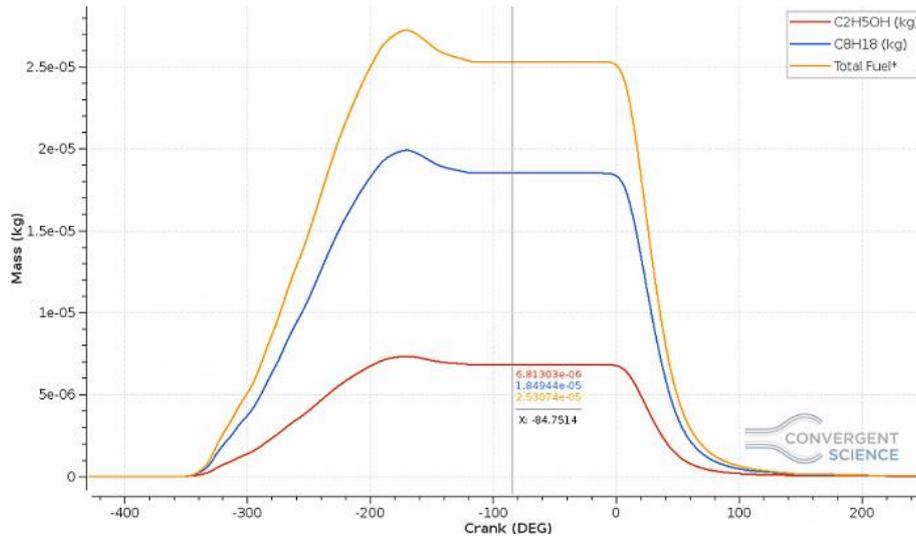


Figure 3 - Amount of fuel trapped in the cylinder

The total fuel trapped inside the cylinder was 0,0253 grams. The difference between them is only 3,6%. This shows good agreement.

The air mass flow measured by the experimental procedure was 146 kg/h which gives 0,347 grams per cycle. Figure 4 shows the amount of air trapped in the cylinder for the numerical procedure.

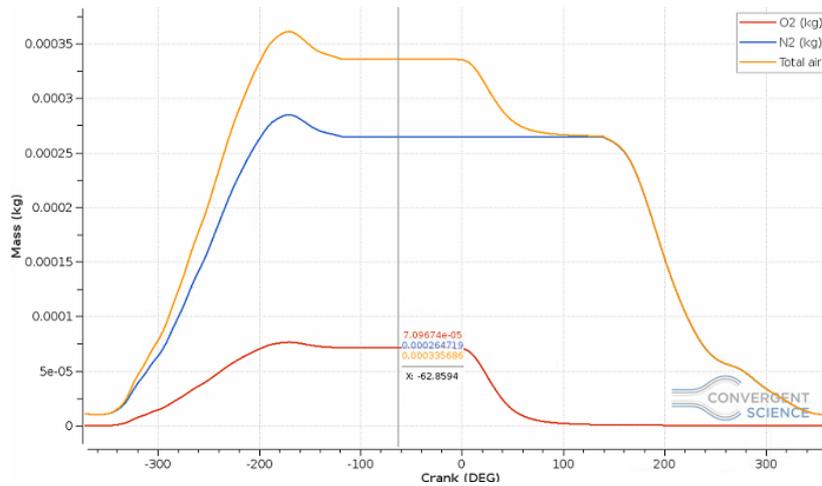


Figure 4 - Amount of air trapped in the cylinder

The total mass of air was 0,336 grams. The difference between them is only 3,6%. This also shows good agreement.

Figure 5 shows the integrated heat release for the three different reaction mechanisms as well as for the experimental procedure.

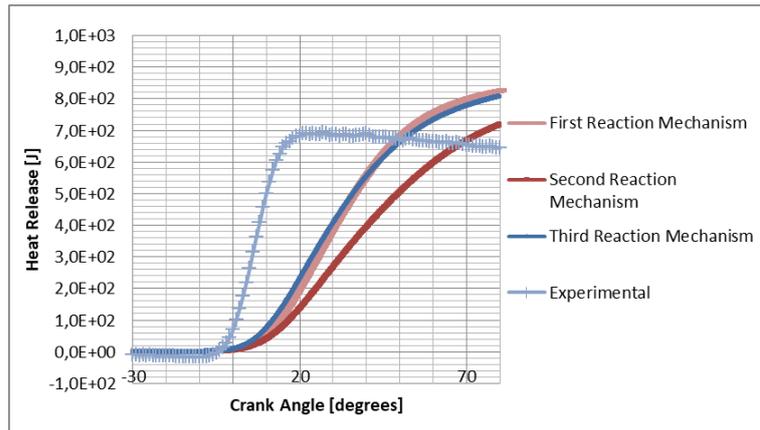


Figure 5. Heat release

Figure 6 shows pressure for the three different reaction mechanisms as well as for the experimental

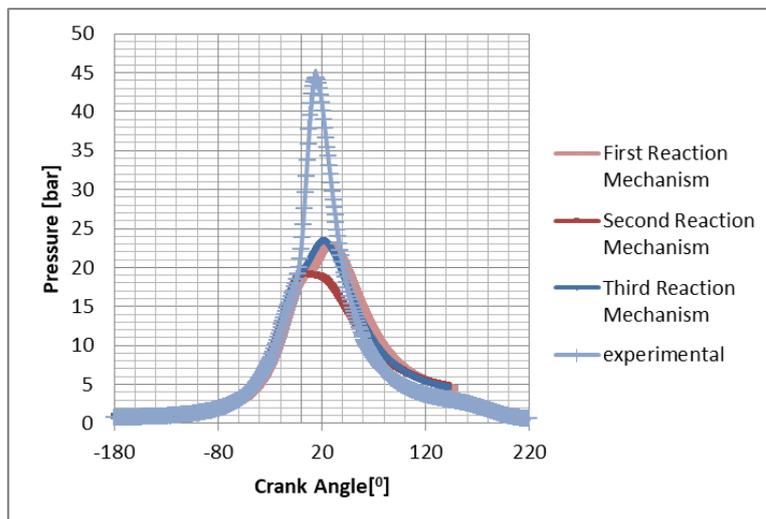


Figure 6. Pressure inside the cylinder

Comparing these results we can see that all three mechanisms released their heats too slow compared to the experimental procedure, and is also notable that the second mechanism is the slowest of the three. This delay caused what Figure 6 shows, all the pressure peaks were too low.

According to Converge-CFD's Manual the mechanism resulted from the merging can have different paths from the original, it can change quantities such as flamespeed and ignition. To compensate these problems the ignition advance was increased by 5, 10, 15, 20 and 25 degrees for the third mechanism. Figures 7 and 8 show the results of heat release and pressure for this simulations. In the Figures, o_e represents the experimental results, o₀ represents the ignition in the same time as the experimental procedure, o₅ having five degrees more of advance, o₁₀ having ten more degrees and so on.

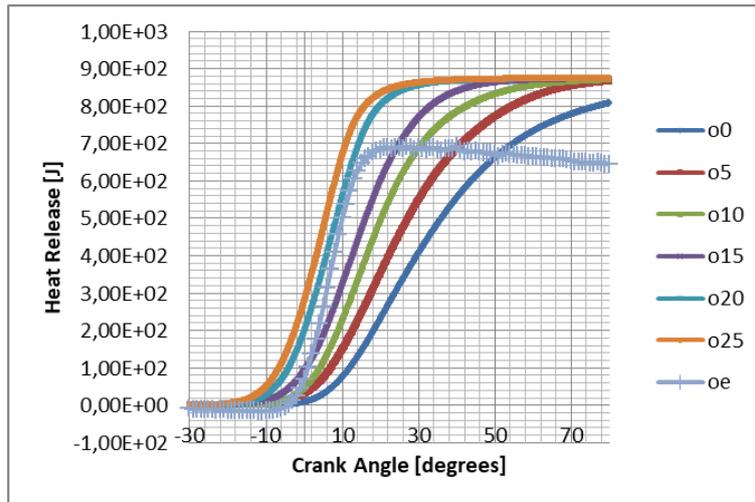


Figure 7. Heat release for ignition advance test

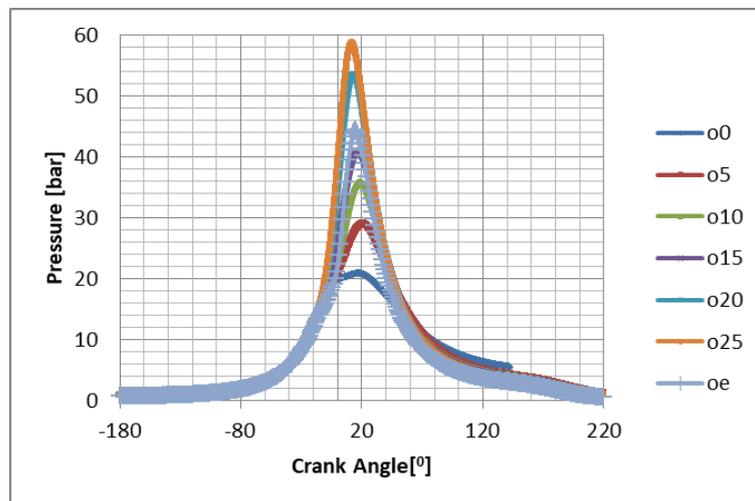


Figure 8. Pressure inside the cylinder for the ignition advance test

Figure 9 shows a zoom in the peak pressures for a better comparison.

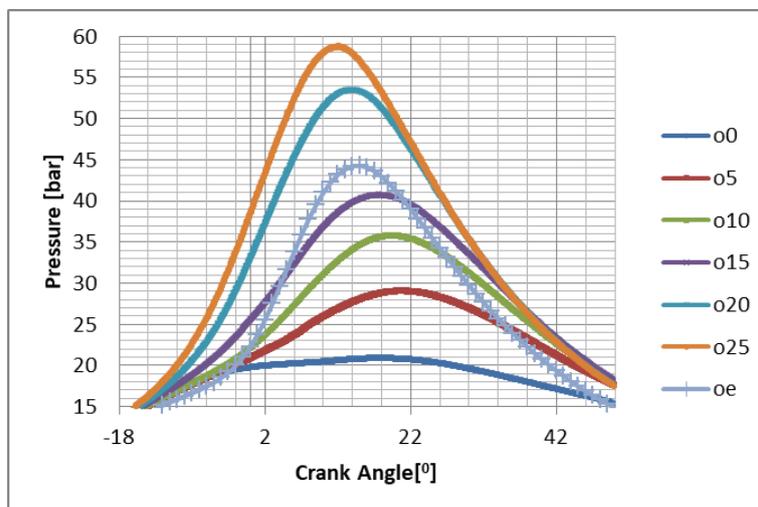


Figure 9. Pressure inside the cylinder for the ignition advance test

Table 4 shows the peak pressures for these simulations.

Table 4. Peak pressure with percentage different

	o0	o5	o10	o15	o20	o25	experimental
Pressure [Pa]	23,41963	29,00503	35,71121	40,69072	53,45435	58,66625	44,2557
% difference	47,08111	34,46036	19,3071	8,055419	-20,7852	-32,562	-

By analyzing the heat release data it is possible to see that the simulations were releasing more heat than in the experiment, this is related to some facts such as the estimation of wall temperature and the amount of fuel that has entered. Analyzing the data in the table and in the Figures 8 and 9, the simulation that best fits had fifteen additional degrees of advance. The best simulation will also be between this simulation and the one with twenty degrees of additional advance.

4. CONCLUSIONS

This paper presented three dimensional simulations for an engine using the CONVERGE CFD software, in which the developed methodology for the engine simulation was able to meet the objectives, making the simulation more reliable, proving that it can be used to help in new engine concepts. This can help future users to improve their simulations and make the engine optimization process better and faster.

The Converge-CFD reaction mechanism merging process still has to improve, since after its use it became necessary to change the ignition advance timing.

5. REFERENCES

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6. RESPONSIBILITY NOTICE

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