



## Numerical study of the combustion process and emissions pollution in a spark ignition engine

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**Abstract-** To better understand the in-cylinder complicated physical phenomenon, Computational Fluid Dynamics (CFD) in conjunction with optical methods, has attracted increasingly popular attention in the vehicle. In this study, a numerical simulation has been developed using the CONVERGE software to perform investigation of indirect injection system into the cylinder of spark ignition internal combustion engines. The RANS approach is used. To simulate the airflow field, was achieved by the rapid distortion RNG ( $k-\epsilon$ ) model. The atomization process was computed using the model based on KH-RT models. For combustion, the SAGE model associated with Shell ignition model was used. For prediction, extended Zeldovich model was adopted. Finally the Hiroyasu soot model was used for soot prediction. The numerical results obtained by the CONVERGE computer code that takes into account interactions between chemistry and turbulence will be compared with experimental results obtained in a combustion chamber of spark ignition engines. The experimental in-cylinder pressures are used to calibrate the CFD code. The result was found to have excellent agreement with experimental and numerical results. The numerical results demonstrate that the numerical CFD tools, at their stage of development, can help the engine designers to define the more promising strategies to obtain tailpipe emission control of SI engine.

**Keywords—** spark ignition engines, combustion, pollution, CONVERGE, numerical investigation.

## I.INTRODUCTION

By focusing on the substantial improvement in automotive fuel economy, automotive engineers are working to develop engines with improved brake-specific fuel consumption (BSFC) that can also be Requirements of future stringent emissions. The objective is to combine the specific power of the gasoline engine [1] to reduce the fuel consumption and pollutant emissions of gasoline SI engines. But to bring this new concept to final industrialization, some problems are not relevant for injection concepts to be addressed by engine designers. First, improve the burning in the

room. They adversely affect the efficiency of the catalyst system after treatment, usually demonstrated for stoichiometric mixture. It is therefore important to minimize the design of pollutants in the combustion chamber. The second problem is the high sensitivity of consumption and the formation of pollutants on the parameters of design and injection of the chamber. These two problems make the design of an efficient gasoline engine a serious challenge for engineers. In this context, the numerical simulation of the combustion system by means of computer modelling makes it possible to explore combustion regimes that may be difficult and/or expensive to achieve with experiments [2].

Such modelling first started in 1950 with simple thermodynamic models for engine cycles which then were extended in 1970 to multi-zone models. Nowadays with the progressive development of computational fluid dynamics (CFD) and flow field models, it is also possible to study and predict droplet distribution, temperature, pressure and other parameters at every desired point and time within the combustion chamber.

In literature, it is reported that many research groups have been working on natural gas-fuelled engines via experimental work or through numerical simulation. For example; Wyszynski et al. [3] compared three fuels (unleaded gasoline, iso-octane, and toluene) on an optical gasoline DI engine. From high-speed combustion images, they observed soot formed in rich regions from pool fires glowing late in the engine cycle. Catapano et al. [4] also used combustion images of ethanol and gasoline blends to demonstrate that the diffusion combustion of fuel is the source of soot formation. Similar results were found by Fatouraie et al. [5]. Jiao and Reitz [6] and Naik et al. [7] performed 3D computational fluid dynamics simulations in GDI engines to show the in-cylinder soot evolution by semi-detailed soot models.

In the present study, reaction mechanisms of gasoline (C<sub>8</sub>H<sub>18</sub>) combustion in SI engine have been proposed to predict the heat release rate, cumulative heat release, temperature and fuel mass evolution and emissions profiles of pollutants including carbon monoxide (CO), carbon dioxide (CO<sub>2</sub>), oxides of nitrogen (NO<sub>x</sub>) and soot. The model based results were confronted to experimental measurements of the in-cylinder pressure measurement.

## II. In-cylinder numerical investigation

### A. Mathematical formulations

In this context, the use of the digital tool reduces costs and study time. It is very simple to modify numerically the geometry or the conditions of use (pressure, temperature ...). Investigations carried out with Computational Fluid Dynamics (CFD) codes, for example CONVERGE, KIVA, Fluent and CFX, make it possible to test a large number of solutions in order to retain only the most relevant ones for experimental tests.

In the context of the modelling of turbulent combustion, the use of a calculation code like CONVERGE CFD represents a good approach to understanding and predicting the phenomena that manifest themselves inside the cylinder of an internal combustion engine SI fuelled by a gasoline [8].

The compressible equation for species mass transport is given by:

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial u_j \rho_m}{\partial x_j} = \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial Y_m}{\partial x_i} \right) \quad (1)$$

By summing the previous equation over all species we obtain the total fluid density equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = S \quad (2)$$

$$\text{Where} \quad \rho_m = Y_m \rho$$

In the above equations,  $u$  is velocity,  $\rho$  is density,  $\rho_m$  is the species density,  $Y_m$  is mass fraction of specie  $m$ ,  $D$  is the mass diffusion coefficient, and  $S$  is the source term.

and the compressible equation for momentum transport is given by

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + S_i \quad (3)$$

Where the stress tensor is given by

The compressible form of the energy equation is given by

$$\frac{\partial \rho e}{\partial t} + \frac{\partial u_j}{\partial x_j} = -P \frac{\partial u_j}{\partial x_j} + \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left( K \frac{\partial T}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \rho D \sum_m h_m \frac{\partial Y_m}{\partial x_j} \right) + S \quad (4)$$

$e$  is the specific internal energy,  $K$  is the conductivity,  $h_m$  is the species enthalpy,  $\sigma_{ij}$  is the stress tensor, and  $T$  is temperature. Note, if a turbulence model is activated, the conductivity is replaced by the turbulent conductivity given by

$$K_t = K + c_p \frac{\mu_t}{Pr}$$

Where  $Pr$  is the *Prandtl* number and  $\mu_t$  is the turbulent viscosity.

## B. Detailed chemistry modeling

A multi-step chemical reaction mechanism can be written in the form:

$$\sum_{m=1}^M v'_{m,r} x_m \rightleftharpoons \sum_{m=1}^M v''_{m,r} x_m \quad \text{for } r = 1, 2, \dots, R$$

Where  $v'_{m,r}$  and  $v''_{m,r}$  are the stoichiometric coefficients for the reactants and products, respectively, for species  $m$  and reaction  $r$ .  $x_m$  represents the chemical symbol for species  $m$ . The net production rate of species  $m$  is given by

$$\dot{\omega}_m = \sum_{r=1}^R v_{m,r} q_r \quad \text{for } m = 1, 2, \dots, M \quad \text{With } V_{m,r} = v''_{m,r} - v'_{m,r}$$

And the rate-of-progress variable  $q_i$  for the  $r^{th}$  reaction is

$$q_r = k_{fr} \prod_{m=1}^M [X_m]^{v'_{m,r}} - k_{rr} \prod_{m=1}^M [X_m]^{v''_{m,r}}$$

With  $[X_m]$  is the molar concentration of species  $m$ , and  $k_{fr}$  and  $k_{rr}$  are the forward and reverse rate coefficients for reaction  $r$ . In SAGE configuration, the forward rate coefficient is expressed by the Arrhenius form:

$$k_{fr} = A_r T^{b_r} e^{(-E_r/R_u T)}$$

Where  $A_r$  is the pre-exponential factor,  $b_r$  is the temperature exponent,  $E_r$  is the activation energy, and  $R_u$  is the universal gas constant. In addition, the reverse rate coefficient can either be specified in an analogous mode as calculated from the equilibrium coefficient  $K_{cr}$ :

$$k_{rr} = k_{fr}/k_{cr}$$

In order to include the effects of detailed chemistry in combustion computation, the SAGE configuration has been incorporated into CONVERGE. This approach allows us to introduce a chemical kinetic mechanism into the simulation process using a set of CHEMKIN-formatted input file (GRI3.0 Mech) which have become the standard for chemical mechanisms. The chemical kinetic mechanism that has been used in this study was GRI Mech 3.0 [9]. It is an optimized chemical reaction mechanism to compute the iso-octane ( $C_8H_{18}$ ) chemical reaction process and it is the latest version. GRI 3.0 consists of 139 elementary chemical reactions with associated rate coefficient expressions and thermo-chemical parameters for the 44 species.

### C. Turbulence model

Currently, there are three Reynolds averaged Navier-Stokes (RANS) turbulence models available in CONVERGE. These turbulence models are the standard  $k-\varepsilon$ , RNG  $k-\varepsilon$ , and the rapid compression RNG  $k-\varepsilon$  model, in the present work the turbulence modeling was achieved by the RNG  $k-\varepsilon$  model.

The transport equation for turbulent kinetic energy is given by;

$$\frac{\partial \rho k}{\partial t} + \frac{\partial \rho u_i k}{\partial x_i} = \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \frac{\mu}{Pr_k} \frac{\partial k}{\partial x_j} - \rho \varepsilon + S \quad (5)$$

Where  $k$  is the turbulent kinetic energy,  $\varepsilon$  is the turbulent dissipation,  $S$  is the source term, the stress tensor is given by;

$$\sigma_{ij} = 2\mu_t S_{ij} - \frac{2}{3} \delta_{ij} \left( \rho k + \mu_t \frac{\partial u_i}{\partial x_i} \right)$$

and the turbulent viscosity is given by;

$$\mu_t = C_\mu \rho \frac{k^2}{\varepsilon}$$

The rapid distortion RNG  $k-\varepsilon$  model uses the transport equation for  $\varepsilon$  given by

$$\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial (\rho u_i \varepsilon)}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \frac{\mu}{Pr_\varepsilon} \frac{\partial \varepsilon}{\partial x_j} \right) - \left[ \frac{2}{3} C_{\varepsilon 1} - C_{\varepsilon 3} + \frac{2}{3} C_\mu C_\eta \frac{k}{\varepsilon} \frac{\partial u_k}{\partial x_k} \right] \rho \varepsilon \frac{\partial u_i}{\partial x_i} + \left( (C_{\varepsilon 1} - C_\eta) \frac{\partial u_i}{\partial x_j} \sigma_{ij} - C_{\varepsilon 2} \rho \varepsilon + S \right) \frac{\varepsilon}{k} \quad (6)$$

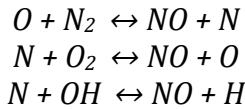
Where  $R$  is dependent on the turbulence model,  $R = 1.0$  when the turbulence is activated,  $C_{\varepsilon 1}$ ,  $C_{\varepsilon 2}$ , and  $C_{\varepsilon 3}$  are model constants, and  $S$  is a source term. More detailed information on the turbulence models can be found in the reference of *Richards K. J* [10].

### D. Spray Modeling

The CONVERGE code includes several spray breakup mechanisms, including models based on the Kelvin-Helmholtz (KH) and Rayleigh-Taylor (RT) instability mechanisms, the LISA sheet breakup model, and the Taylor Analogy Breakup (TAB) drop breakup model. In the present study the collision model along with the KH-RT breakup model are used. After injection, the liquid breakup was simulated using primary KH and secondary RT breakup models. Details of the KH-RT breakup models and coupling developed and validated by ref [10].

### E. Emission models

The extended Zel'dovich mechanism as presented by Heywood (1988) [11] is used to calculate NO<sub>x</sub> formation. This mechanism is given by the following set of reactions:



The production of soot mass  $M_s(g)$  within a computational cell can be determined from a single-step competition between the soot mass formation rate  $\dot{M}_{sf}$  and the soot mass oxidation rate  $\dot{M}_{so}$  according to Hiroyasu and Kadota (1976) [12].

$$\frac{dM_s}{dt} = \dot{M}_{sf} - \dot{M}_{so}$$

Details of these models are described in ref. [10].

## F. Engine geometry and configuration

The engine studied in the present work is a single cylinder engine fueled with a gasoline. The main engine specifications are as given in Table 1 and the section view of its cylinder head and liner is depicted in Fig.1, which shows the position of the intake and exhaust ports, intake and exhaust valves, indirect injector, spark plug and combustion chamber with the shape of piston bowl and Fig.2 shows the entire geometry of the SI engine with the above boundaries.

The specifications of injection in SI engine are listed in Table II. In order to perform modeling, single injector for cylinder type of four-hole have been used.

Table 1. Engine SI specifications

| Parameters             | Specifications  |
|------------------------|-----------------|
| N° of cylinders        | Single cylinder |
| N° of strokes          | Four-stroke     |
| Cylinder Bore          | 80.6 mm         |
| Stroke length          | 90.0 mm         |
| Connecting rod length  | 180.0 mm        |
| Squish                 | 1.0 mm          |
| Compression ratio      | 10:1            |
| Spark timing           | 15 ATDC         |
| Spark duration degrees | 5 CA            |
| Spark Energy total     | 20 mJ total     |

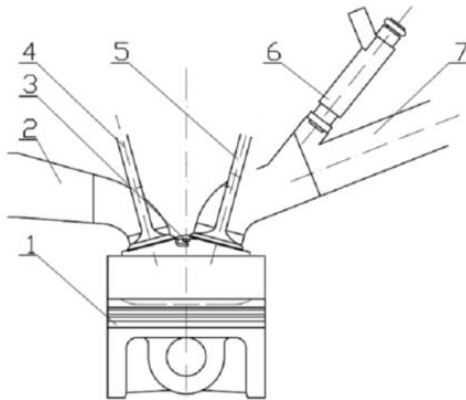


Fig 1 : The location of injector indirect fuel system

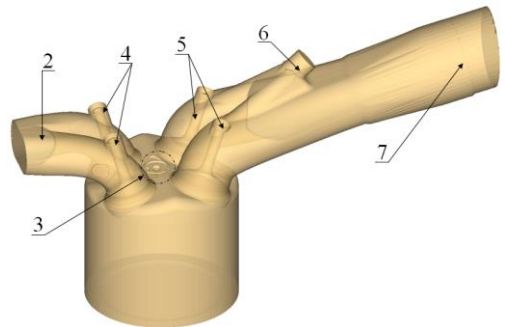


Fig 2. A 3D view of base engine geometry and ports.

1-Piston, 2-Exhaust channel, 3-Spark plug, 4-Exhaust valve, 5-Intake valve, 6-Indirect injector, 7-Intake channel.

Table 2: Specification of injection

| Fuel Injection System    |                    |
|--------------------------|--------------------|
| Fuel type                | C8H18              |
| Mode of injection        | Injector injection |
| Initial fuel temperature | 330 K              |
| Start of injection       | -390 CA            |
| Duration of injection    | 190 CA             |

## G. Computational mesh

The generation of the mesh is a very important phase in a CFD analysis, given its influence on the calculated solution, in terms of accuracy and computation time. Fig. 3 contains a structured mesh created by the

CONVERGE pre-processor. The number of cells was about 447864 at 120 CA.

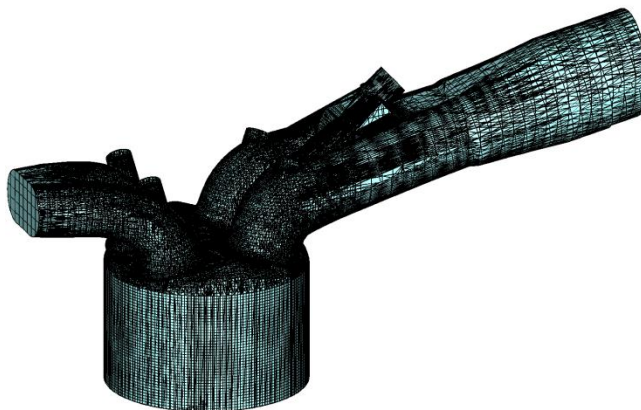


Fig .3. Three dimensional mesh in the simulation.

## H. Boundary conditions

In order to solve the previous governing transport equations, boundaries and boundary conditions must be specified for each equation. For each boundary, conditions for pressure, temperature and velocity were specified. Several types of wall boundary are chosen.

Piston wall: moving wall;  $U_{\text{gas}}=U_{\text{piston}}$ ;  $T_{\text{piston}}=450\text{K}$ ;

Cylinder head: stationary wall;  $U_{\text{gas}}=0$ ;  $T_{\text{cylinder-head}}=450\text{K}$

Valve wall: moving wall;  $U_{\text{gas}}=U_{\text{valve}}$ ;  $T_{\text{valve}}=525\text{K}$ ;

Initial conditions in the combustion chamber are:

370K gas temperature; 101544Pa gas pressure

$62.02710 \text{ m}^2/\text{s}^2$  initial turbulent kinetic energy

$17183.40 \text{ m}^2/\text{s}^2$  initial turbulent dissipation

## III. Results and discussions

### A. In-cylinder pressure and heat release evolution

The plots of in-cylinder pressure during the combustion process for several crank angles during compression can be depicted in Fig.4. There is good agreement between the measured and the calculated values. The maximum error does not exceed 4% in the combustion zone, which is an

acceptable value from the literature. As predicted, the pressure reached its maximum value at the top part of the cylinder head when the piston reached TDC position during compression stroke, which tend to appear in the side part of engine cylinder, which is near to the spark plug. This shows that the burned fuel causes the flame to propagate to the side part of engine cylinder near the spark plug instead of being distributed uniformly.

The comparison of the calculated and measured pressure shows that the SAGE model is strong enough to predict the combustion phenomenon within the combustion chamber of a gasoline engine powered by C8H18. Fig. 5 shows the evolution of the heat released as a function of the degree of the crank angle. A very rapid increase in heat release which means the start of combustion. The maximum average heat content reaches a value of the order of 41  $\text{kJ/deg}$ .

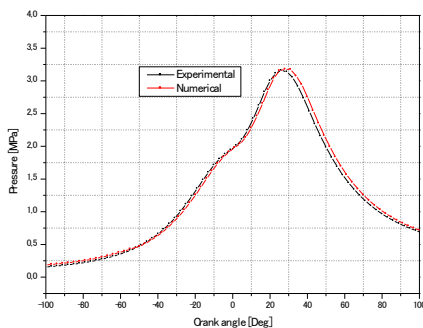


Fig.4. Comparison of in-cylinder experimental and simulation pressure

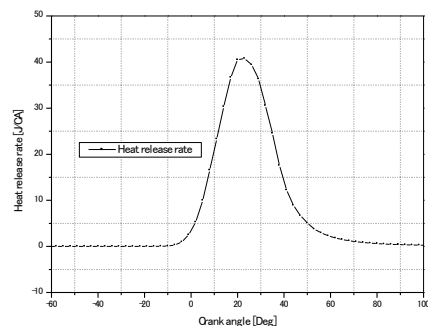


Fig. 5. The in-cylinder average heat release rate.

## B. In-cylinder cumulative heat release, temperature and fuel mass evolution

The cumulative heat release (CHR) is simulated and illustrated in Fig. 6. Results show that the cumulative heat release increases. The position of the maximum CHR represents the end of combustion. This increase in heat release is mainly due to better mixing and evaporation of gasoline, which leads to complete burning. The time (or crank angle) interval between the start of combustion and the end of combustion it is the combustion duration. The end of combustion is taken as the point where

95% of the heat release had occurred. In this study the combustion duration is 70CA.

Fig.7 presents the predicted cylinder temperature against the crank angle for the subsequent validation of the spray and combustion modelling. On this graph, we observe an increase in temperature during the compression phase (air-gasoline) until reaching a threshold of about 750 K and this at the moment of spark, followed directly by a very rapid and considerable increase in Reaction zone (rapid combustion). The maximum average temperature reaches a value of the order of 2382 K. Fig.8 presents the profile of the fuel mass  $C_8H_{18}$  as a function of crank angle.

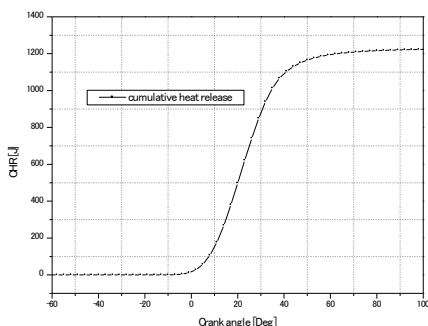


Fig.6. The in-cylinder cumulative heat release evolution.

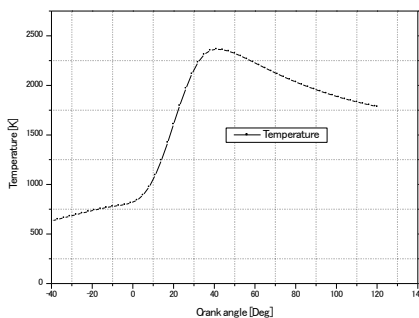


Fig.7. The in-cylinder average temperature evolution.

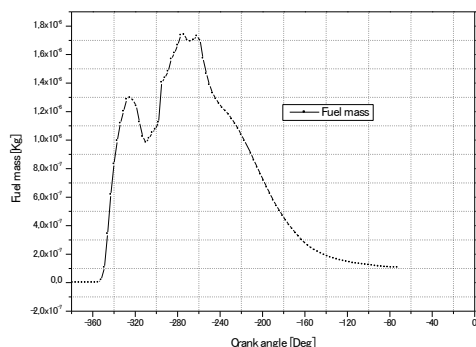


Fig.8. Evolution of the fuel mass.

### C. Pollutants gas evolution

Fig. 9 shows the formation of NO<sub>x</sub> emission inside the cylinder. More NO<sub>x</sub> formed around the spark plug due to higher temperature produced during ignition. Apart from high temperature, the amount of NO<sub>x</sub> generated depends on pressure, air-gasoline ratio and combustion time within the cylinder. The highest concentration was found around the spark plug, where the highest temperature was observed.

Fig. 10 presents the predicted cylinder soot emissions as a function of crank angle. It is seen that soot formed at early stages of combustion is oxidized up to TDC point. Fig. 11 presents the level concentration of CO for several crank angles position during and after the combustion. As seen, most of the CO concentration was located next to the cylinder liner wall and inside the piston bowl due to poor combustion, due to oxidation process from CO to CO<sub>2</sub> in the core gas and to wall quenching.

The Fig.12 above shows the evolution of carbon dioxide as a function of the crank angle. It is noted that CO<sub>2</sub> increases at the beginning of the combustion phase.

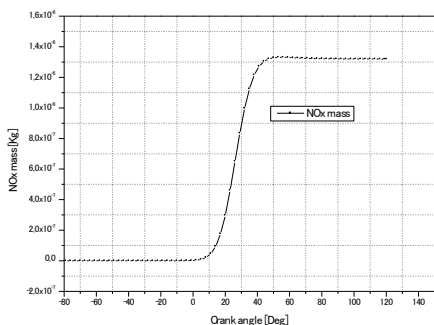


Fig 9. The prediction NOx emission.

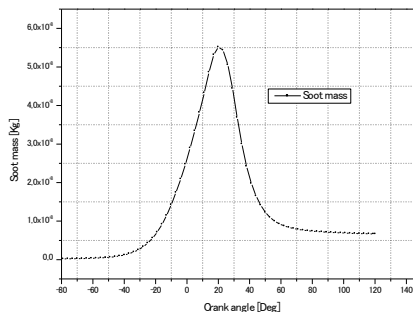


Fig.10. The prediction of soot emission.

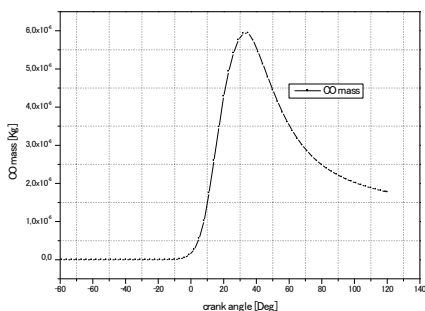


Fig.11. The prediction of CO emission.

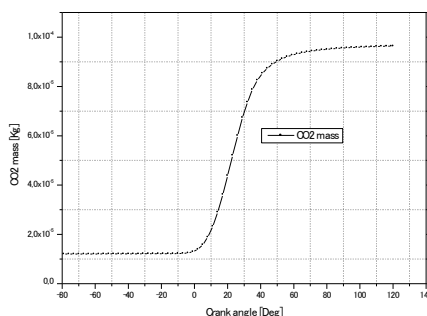


Fig.12. The prediction of CO2 emission.

## D. Flame propagation

The simulation can tell us the moment of the ignition, this is possible thanks to the continuation of the first traces of the products of the spark from the spark plug. In this section we present results concerning ignition. It should be noted that capturing the delay of inflammation is very tricky. This ignition delay can be detected roughly by analyzing the pressure curves or the heat ratio. Fig.13 shows the location of the first ignition cells approximately -15 CA.

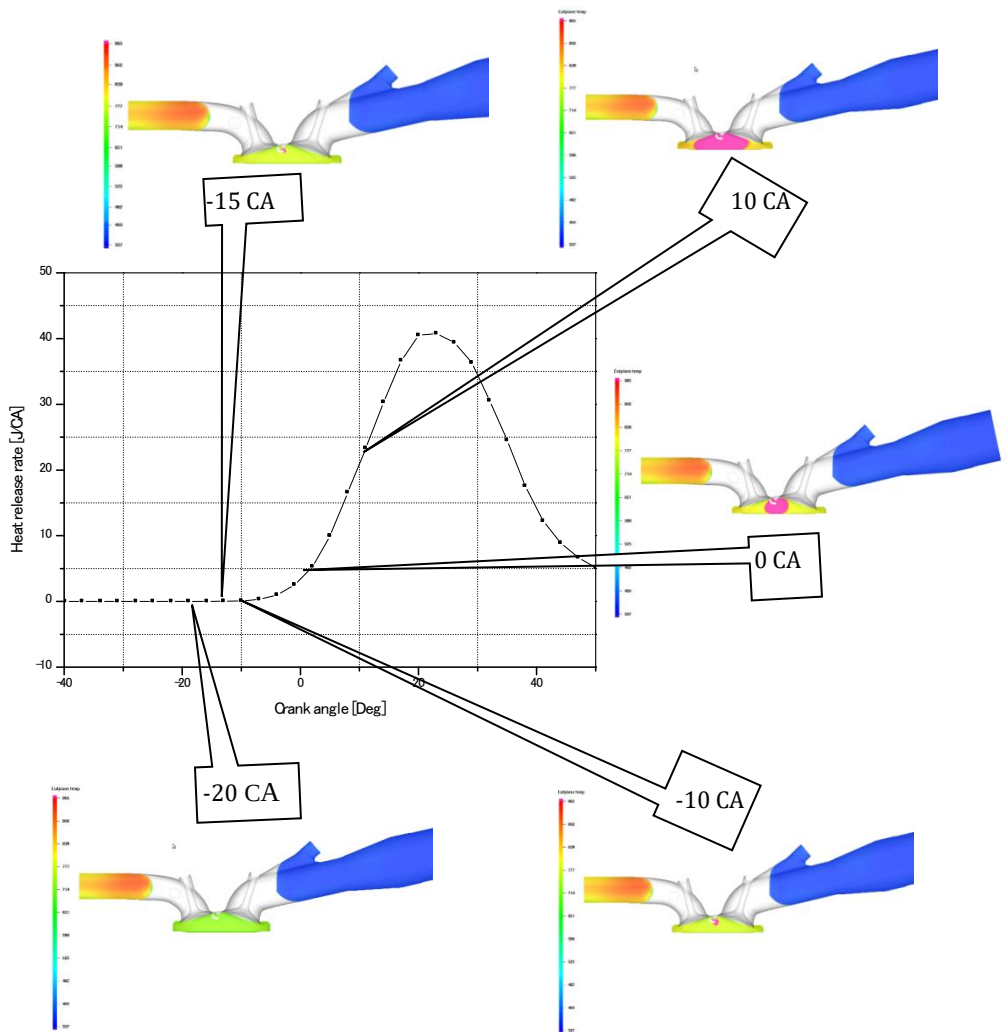


Fig.13. Propagation of the flame.

### E. Evolution of spray and temperature

Fig. 14 shows the distribution of the mass fraction and temperature of fuel in the iso-volume distribution of the cylinder in different crank angle.

The stream of fuel injected indirectly into the engine cylinder is clearly visible in Fig at -390 CA and -370 CA.

On the basis of the analysis of Fig. 15 it can be concluded that the combustion develops in the initial stage significantly faster when the mixture is formed by injector per cylinder. It can be seen that at the end of the combustion process slightly higher temperature in the cylinder.

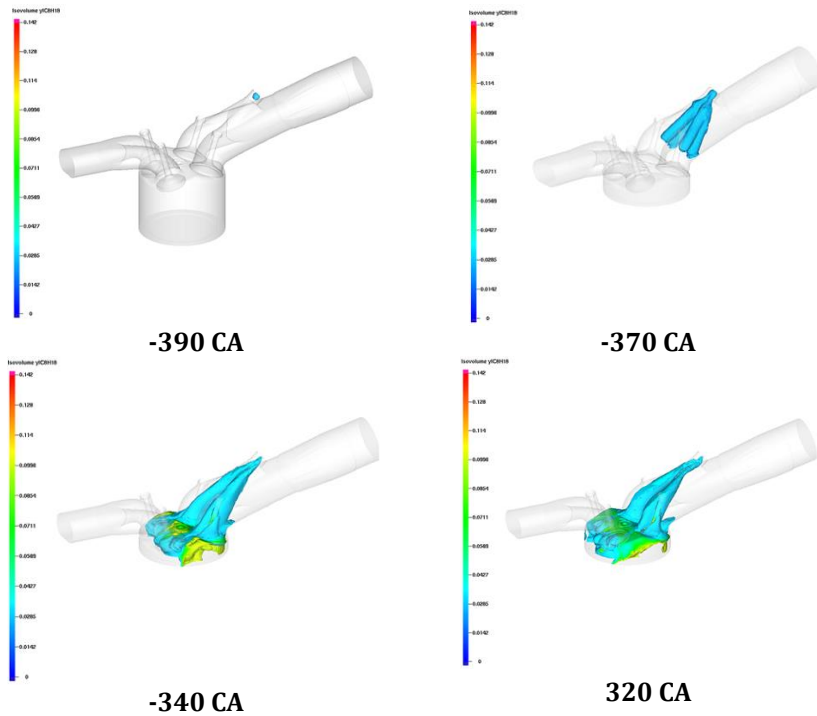
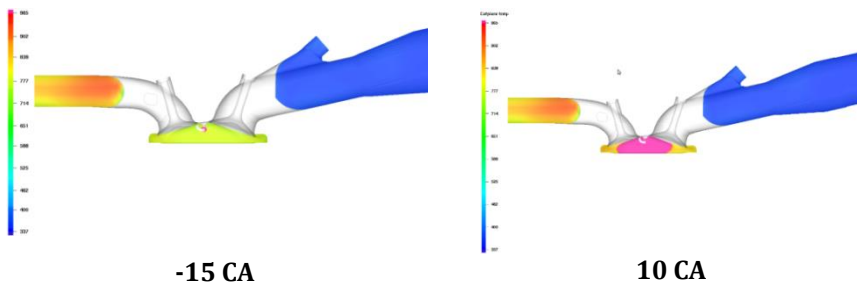


Fig.14. Fuel mass contours at different crank angle.



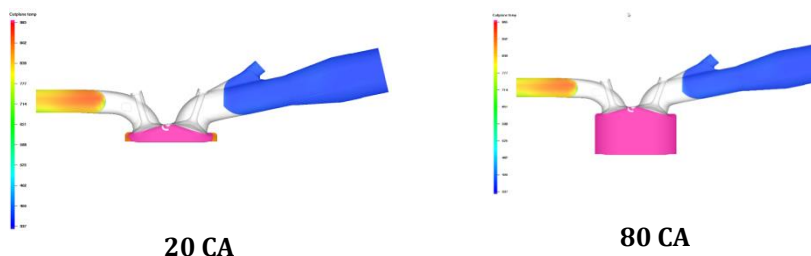


Fig.15. Temperature contours at different crank angle.

## IV. Conclusion

The work in this article is to calibrate and validate the numerical results of combustion in a gasoline engine with the CFD code CONVERGE 2.2V, the results were in good agreement with the experimental data, and the investigation resulted in the following results:

- The SAGE model is capable of predicting the combustion phenomenon within a combustion chamber of gasoline engine.
- The simulation models used in this project to represent the phenomena within the combustion chamber such as combustion, turbulence, ignition, formation of pollutants give good results.
- Numerical simulation has become one of the powerful tools to investigate the performance and emission characteristics of internal combustion engines for better understanding of the complex combustion phenomenon.
- In conclusion, the results obtained during the simulations were an important complement to the outcome of experimental tests.

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