Numerical analysis of gasoline fuel with laser ignited spark ignition

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Abstract. Laser ignition overcomes the problem of faster degradation of electrodes using high energy required for lean burn and reduced heat loss to the electrodes. A number of investigations have been carried out on laser ignition of gaseous fuels but the work, on laser ignition of liquid fuels is indeed very limited. In present work, a Multi-dimensional CFD model using ANSYS Fluent 17.2 was developed for constant volume combustion chamber (CVCC) to characterize laser ignition combustion phenomenon from the start of plasma formation to end of combustion. The combustion and emission characteristics of gasoline-air mixture ignited by laser-induced spark were studied using numerical simulation. It was predicted from results obtained from numerical results that peak pressure goes on increasing with the increase in equivalence ratios from 0.8 to 1.4. The numerical simulation results obtained were in good agreement with experimental results of literature with 10.6 % percentage error, which demonstrates that the model developed is valid for the combustion process. The trends of the NOX, CO, CO2, emissions were analyzed using a numerical model.

1. Introduction
The experimental studies on laser ignition of various fuels have been tried by some researchers, but very few researchers have worked on numerical simulations on the laser ignition of the gasoline-air mixtures. Numerical simulations can give important insight into the phenomena occurring in the combustion chamber, where measurement access is very limited. While in experiments quantitative data is mainly restricted to pressure and temperature measurement at selected points, simulations can provide data of the flow field and temperature distribution. Laser ignition is becoming the more attractive field of research, as it has many potential advantages, such as extended flammability limits, lack of heat loss from flame kernels to the electrodes, the flexibility of ignition location and absence of electrode degradation [1]. The experimental data on laser ignition of the gasoline-air mixture of Xu et al. [2] have been used as benchmark data for numerical simulation.

In laser ignition method, a nanosecond pulsed laser beam is concentrated using a set of lenses which results in the formation of a plasma having the intensity of the order of $10^{12}$-$10^{13}$ W/cm². The plasma generated acts a source of ignition to initiate combustion process. Laser ignition mechanisms are laser thermal ignition, laser-induced photochemical ignition, laser-induced resonant breakdown ignition, and laser-induced spark ignition [3]. The non-resonant breakdown mechanism is used to adopt laser ignition to initiate combustion due to its laser wavelength flexibility and high implementation feasibility [4]. The conventional ignition techniques and fundamentals of laser-induced ignition with gaseous and liquid fuels have been reviewed extensively [4,5]. There is need of time to carry out research on laser ignition application for internal combustion engines and gas turbine
with liquid fuels. Previous studies on laser ignition of various liquid fuels kerosene [6], gasoline [2] wet ethanol [7], absolute ethanol [8,9], has justified the potential advantages of laser ignition. Moesl et al [10] studied the applicability of laser ignition by conducting the tests with premixed natural gas and kerosene. The lean combustion and location of the flame kernel in the combustion chamber is one of the most important parameters for overall performance. Successful laser ignition was observed for $\phi_{global}=0.23$ which is a significant aspect for aero engines because of the high potential for emission reduction and re-ignition in high altitudes. Whereas the study carried out by Gebel et al [5] predicted various droplet breakup mechanisms for Jet A1 kerosene fuel. The results revealed that the breakup models observed under lab conditions will also appear in aviation gas turbines at high altitude conditions.

Investigations of the effect of water concentration on combustion characteristics of wet ethanol ignited using Nd: YAG laser in constant volume combustion chamber was carried out by Kazi et al. [6]. From the spectroscopic analysis, the optimum stirring period for all water concentrations was found 40 min to obtain a premixed ethanol-water mixture. Flame growth images predicted that, flame luminosity, flame propagation speed, flame growth rate, all increases with the addition of 10% to 20% water. However, with 40% addition of water, the flame becomes darker and contains granular orange luminescence, which causes a reduction in flame propagation velocity due to dilution effects and chemical influence of water. For the equivalence ratios, ranging from $0.7 \leq \phi \leq 1.2$ formations of front lobe was found evident which indicated that laser ignition can generate a consistent spark and flame kernel. The flame propagation study for absolute ethanol was also carried out by Jiang et al [7] in optical GDI engine using laser ignition and spark ignition for air-fuel equivalent ratios ($\lambda$) of 0.9 to 1.3. It was observed that the For lean mixtures ($\lambda=1.1, 1.2$ and 1.3) laser ignition can enhance the flame more significantly than spark ignition. Image processing analysis revealed that for richer mixtures; the flame starts earlier and developed faster which indicated a shorter ignition delay. The flame propagation analysis of ethanol carried out by Xu et al.[9] predicted that the laminar speed of ethanol-air mixtures with LISI is faster than SI at lean mixtures but slower at stoichiometric and rich mixtures. Study of transition from plasma breakdown to a flame kernel, subsequent growth, and flame propagation from the kernel location to the entire combustion zone has been carried out by A. Singh et al. for the ethanol-air mixture[11].

Study of engine operating parameters using laser spark induced ignition system was carried out by Nicolae et al. [12]. They also studied cycling variability, specific emissions, brake specific fuel consumption at various speeds and loads on Renault Dacia vehicle with gasoline. There was an improvement in coefficient of variability of maximum pressure by 15 % with laser ignition was observed compared to spark ignition. With laser ignition the CO, HC emissions were lowered by the range of 18% to 25% and 14% to 17% respectively compared to the classical engine. The combustion of gasoline-air mixtures in a constant-volume combustion chamber with an initial condition of 0.1 MPa pressure and 363 K temperature was experimentally investigated with laser ignition generated by a Q-switched Nd: YAG laser (wavelengths of 532 and 1064 nm) by Xu et al.[2]. It was observed that, for equivalence ratios of 0.8 to 1.4, the pressure rise rate and peak pressures of the laser ignition were significantly higher than spark ignition.

In this paper numerical model developed for investigation of combustion and emission characteristics of laser ignited gasoline which was validated with experimental results obtained through literature. Combustion peak pressure, temperature, combustion duration and NOX, CO, CO2 emissions of gasoline fuel were investigated for a constant volume combustion chamber using ANSYS 17.2 (Fluent) simulation tool. The initial conditions were set to 0.1MPa pressure and 363K CVCC temperature for simulation. The study was carried out for equivalence ratios of $\phi=0.8, 1, 1.2, 1.4$. We have developed the combustion model and compared the predicted combustion pressure and combustion duration with the experimental results of literature [2]. This validated model was used to determine NOX, CO and CO2 emissions.
2. Numerical Simulation

The combustion and emission characteristics of gasoline-air mixture ignited by laser-induced spark were studied numerically using commercially available software package ANSYS Fluent 17.2.

2.1. Governing equations

The equations of continuity, momentum, energy, turbulence, and transport were solved using ANSYS Fluent solver. The standard k-ε model was used for modeling turbulence.

2.1.1 Turbulence model. Currently, the most popular numerical method is the Reynolds Averaged Navier-Stokes (RANS) in which the local fluctuations and turbulence structures are integrated into the mean quantities. To close the Reynolds stress term, the most commonly used approach is the k-ε two-equation turbulence model. The Standard k-ε [13] model is the most widely used complete RANS model and it is incorporated in most commercial CFD codes. It solves two transport equations for two turbulent quantities, the turbulent kinetic energy k and ε for the rate of dissipation of the turbulent energy. The k-ε turbulence model solves the flow based problems where wall impingement effects are not considered.

\[
\frac{\partial}{\partial t}(\rho k) + \nabla \cdot (\rho u_i k) = \frac{\partial}{\partial x_j} \left( \mu + \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_j} \right) + G_k + G_b - \rho \varepsilon - \rho_M \tag{1}
\]

\[
\frac{\partial}{\partial t}(\rho \varepsilon) + \nabla \cdot (\rho u_i \varepsilon) = \frac{\partial}{\partial x_j} \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_j} \right) + C_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} + S_\varepsilon \tag{2}
\]

2.1.2 Flame propagation model. Reaction progress from unburnt to burnt is denoted by a scalar variable c. The transport equation for c describes the spatial and temporal evolution of the reaction progress in a turbulent flow field. In unburnt reactants i.e. ahead of flame, c is zero, whereas for burnt products behind flame it is unity. Within the flame, brush c varies between zero and one. The flame front propagation is modeled by solving a transport equation for the density-weighted mean reaction progress variable \( \bar{c} \) as,

\[
\frac{\partial (\rho \bar{c})}{\partial t} + \nabla \cdot (\rho \bar{c} \vec{v}) = \nabla \cdot \left( \frac{k}{C_p} + \frac{\mu_t}{S_{CT}} \right) \nabla \bar{c} + \rho S_C \tag{3}
\]

Where, \( S_{CT} \) is the turbulent Schmidt number, \( S_C \) is the reaction progress source term, k is the laminar thermal conductivity of the mixture and \( C_p \) is the specific heat of the mixture. From Zimont et al. model the default value of \( S_{CT} \) is taken as 0.7 [14].

2.1.3 Modelling of NOX. In laminar flames and at the molecular level within turbulent flames, NOX formation can occur in four different chemical kinetic processes namely thermal NOX formation, prompt NOX formation, fuel NOX formation, and intermediate N2O. For thermal and prompt NOX mechanisms, only the species transport equation is needed.

\[
\frac{\partial (\rho Y_{NO})}{\partial t} + \nabla \cdot (\rho \nabla Y_{NO}) = \nabla \cdot (\rho D \nabla Y_{NO}) + S_{NO} \tag{4}
\]

The formation of thermal NOX is determined by a set of highly temperature-dependent chemical reactions known as the extended Zeldovich mechanism. The rates of reactions involved are modeled using the Arrhenius equation. The rate constants are given by Hanson and Salimian [15].

2.2. Computational model

A model of the cubical constant volume combustion chamber was used in which a mixture of gasoline-air is ignited using a central laser spark. Fig. 1 shows the cut section of the computation domain with dimensions of CVCC. The geometrical dimensions used in numerical simulation resembles with CVCC specifications used for experimental work [2]. Initial conditions of pressure and temperature in CVCC are kept as 1 bar and 363 K respectively. The equivalence ratio of the gasoline-air fuel mixture is varied from 0.8 to 1.4 for simulation work. Combustion and emission characteristics of the gasoline-air mixture were carried out for a selected range of equivalence ratios using simulation. The gasoline-air mixture was ignited using a laser spark with the energy of 15 mJ which was identical with the literature [2], the initial radius of spark was 10 microns and duration of 5 ns.
The simulations were started by keeping the initial computational mesh size roughly 1mm. To check the grid independence, test simulations were performed with mesh size 1mm, 0.5mm, 0.2mm, 0.1mm and 0.08 mm. The difference in combustion peak pressure was found to be less than 3.32% when the mesh size was changed from 0.1mm to 0.08mm. Hence the simulations were carried out for 0.1mm mesh size.

Table 2 shows the input parameters required for Ansys Fluent simulation for the gasoline-air mixture, which was synonymous to the experimental input conditions of literature [2].

### Table 2. Boundary conditions used in ANSYS Fluent

| Parameter                          | Value                                      |
|------------------------------------|--------------------------------------------|
| Initial Wall Temperature           | 363K                                       |
| Operating Pressure                 | 0.1MPa                                     |
| Solver                             | Pressure based                             |
| Time                               | Transient                                  |
| Viscous                            | k-ε model                                  |
| Species                            | standard wall function                     |
| Flame propagation model            | C equation (Turbulent flame speed – Zimont Model) |
| Spark                              | (x,y,z) = (0.05965, 0.05965, 0.05965) in meters |
| Energy                             | 0.015Joule                                 |
| Material                           | Gasoline –air mixture                      |
| Laminar flame speed (cm/s)         | 36.22 @ $\phi=0.8$                        |
|                                    | 51.88 @ $\phi=1$                          |
|                                    | 50.82 @ $\phi=1.2$                        |
|                                    | 33.95 @ $\phi=1.4$ [16]                   |
|                                    | 0.0504 @ $\phi=0.8$                       |
|                                    | 0.0623 @ $\phi=1$                         |
|                                    | 0.0681 @ $\phi=1.2$                       |
|                                    | 0.0850 @ $\phi=1.4$                       |
| Mean mixture fraction              |                                            |

### 3. Results and discussions

The formulated model is validated for the combustion duration and peak pressures obtained for different equivalence ratios of the gasoline-air mixture and are compared with experimental results from literature [2] and discussed in following sections combustion and emission.
3.1. Combustion characteristics

Reaction progress. The contours of reaction progress obtained for $\phi=0.8$, 1, 1.4 at various time intervals are shown in fig.2. The reaction progress appears to be circular in the two-dimensional case before it interacts with the wall. It is observed that for stoichiometric conditions reaction progress is rapid and completes at 20ms, due to higher laminar flame speed.

| Time   | $\phi=0.8$ | $\phi=1$  | $\phi=1.4$ | Time   | $\phi=0.8$ | $\phi=1$  | $\phi=1.4$ |
|--------|------------|-----------|------------|--------|------------|-----------|------------|
| 3 ms   |            |           |            | 20 ms  |            |           |            |
| 10 ms  |            |           |            | 25 ms  |            |           |            |
| 12 ms  |            |           |            | 27 ms  |            |           |            |
| 15 ms  |            |           |            | 35 ms  |            |           |            |

Figure 2. Contours of reaction progress of gasoline-air mixture in centre cross-sectional plane for initial pressure = 0.1 MPa, initial temperature = 363 K and equivalence ratio = 0.8, 1 and 1.4.

The laminar flame speed of gasoline at various equivalence ratios was calculated using analytical correlations given by R. Amirante et al. (2017). Figure 3 indicates the variation of laminar flame speed for various equivalence ratios. At $\phi=0.8$ and $\phi=1.4$ the laminar flame speed was 36.22 cm/sec and 33.95 cm/sec respectively. These lower values of laminar flame speeds were due to the oxygen contents in the gasoline-air mixture, which increases the time required for complete reaction progress. The time required for complete reaction progress was 35ms and 27 ms for $\phi=0.8$ and $\phi=1.4$ respectively.

3.1.1 Combustion pressure. The simulation results obtained and experimental results from literature [2] of combustion pressure of gasoline-air mixture for various equivalence ratios are shown in fig.4. Combustion pressure goes on increasing with increase in equivalence ratio from $\phi=0.8$ to $\phi=1.4$ which was in good agreement with experimental results from literature [2]. It was observed from obtained simulation results that pressure rise takes place quite earlier than the experimental results from
literature [2]. The reason behind this can be the laminar flame speed of gasoline-air mixture during the actual combustion process is varying but in simulation, it is constant which may lead earlier rise of combustion pressure.

The location of the pressure sensor in CVCC during experimentation plays an important role in acquiring the pressure-time data. In the current study, the information regarding the location of a pressure sensor in CVCC was not mentioned. Hence because of this also there may deviation in simulation results obtained and experimental results from literature [2].

The peak pressure and combustion duration of the gasoline-air mixture is obtained for an equivalence ratio of 0.8 to 1.4. At $\phi = 1.4$ highest peak pressure value obtained was 0.65MPa with experimental results from literature [2] and 0.67MPa with simulation results. 3.43% error was found in both results.

3.1.2 combustion duration. It is observed from fig. 6 that at lean and rich conditions of the gasoline-air mixture the combustion duration was more as compared with the stoichiometric condition. For $\phi=0.8$, 1 and 1.4 the obtained combustion duration was 41.5ms, 31.5ms and 34ms respectively. This was because of the less thermal energy liberated from the leaner mixture which slows down the flame propagation.

![Figure 4. Experimental combustion pressure results from literature [2] and simulation combustion pressure trends for various equivalence ratios. [2] of the gasoline-air mixture.](image)

![Figure 5. Experimental and simulation peak pressure comparisons for various equivalence ratios](image)

![Figure 6. Combustion duration comparisons in experimental results from literature[2] and simulation results obtained for various equivalence ratios of the gasoline-air mixture.](image)
The incomplete combustion due to oxygen deficiency at rich gasoline-air mixtures also had an adverse effect on laminar flame speed which leads to increased combustion duration. During simulation laminar flame speed was constant as it was calculated from R. Amirante et al. Correlations [16], which was not the case for the actual combustion process in CVCC. This may be the reason behind 3% to 7% increase in combustion duration obtained with simulation results than experimental combustion duration of literature[2].

Figure 7 gives percentage error of peak pressure and combustion duration between experimental results from literature [2] and simulation results obtained. The maximum error in the computation of peak pressure obtained was 10.60% and in combustion duration, was 7.93%. The reasons behind the error may be the computation of average thermophysical properties of the gasoline-air mixture, laminar flame speed calculations through correlations available in literature and consideration of purity of gasoline in the simulation was 100%.

3.2 Emission characteristics.
The Verified simulation model is further used to predict the quantitative results of gasoline emissions. Emissions of CO and NOX gases generally takes place due to incomplete combustion of the air-fuel mixture. To consider the high knocking threshold in engines, there is a need of special engine developments with laser ignition system. As per the literature, there is no such engine development is carried out to consider the knocking due to a laser ignition. The effect of knocking was not considered for simulation work.

3.2.1 Variation of CO.
CO emissions at $\phi=0.8$ were less by 93% compared with the stoichiometric condition. At lean condition, the combustion duration was high, which allows more time for the gasoline combustion to complete and apart from that the excess oxygen was available for combustion which leads to complete combustion reducing the CO emissions. Whereas at $\phi=1.4$, the CO emissions were 2.57 times greater than $\phi=1$ as the quantity of oxygen available was less causing incomplete combustion.

3.2.2 Variation of NOX. The variation of NOX emissions for the gasoline-air mixture is shown in fig.9. For stoichiometric air-fuel ratio, NOX emissions were maximum. The growth of reaction progress was rapid at stoichiometric conditions which may lead to rapid pressure rise and hence the combustion temperature. At $\phi=0.8$, the combustion duration was higher, which can reduce the peak burned and unburned temperature and therefore the formation of NO was reduced. On the other hand, less combustion duration of $\phi=1.2$ and $\phi=1.4$, reduced the concentration of NO because of the less time of exposure of products of combustion to cylinder’s peak temperature. In rich mixtures, sufficient oxygen was not available for combustion. So, less amount of oxygen was available for oxidation of nitrogen in the combustion chamber. For lean mixtures, NOX emissions were reduced due to lower combustion temperature thereby reducing thermal NOX. From this numerical model, it can be concluded that laser combustion allows the burning of a lean air-fuel mixture of $\phi=0.8$ with fewer NOX emissions.

3.2.3 Variation of CO2. CO2 was formed as a product of complete oxidation of carbon from the fuel. The variation of CO2 emissions for the gasoline-air mixture is shown in fig. 10. The CO2 emissions were maximum for the stoichiometric condition. It was decreased at $\phi=1.2$ and 1.4, due to deficiency of oxygen required for complete combustion. As the air-fuel mixture becomes lean, the mass of fuel and thereby the mass of carbon in the mixture decreases. It resulted in a decrease in CO2 emissions for lean mixtures.

4. Conclusion
The combustion and emission characteristics of gasoline-air mixture ignited by laser spark are studied using ANSYS Fluent software. Mixtures with an equivalence ratio of range $\phi=0.8$ to $\phi=1.4$ can be completely burnt using laser spark.
At $\phi=1.4$ rich mixture, the peak pressure with experimental results from literature [2] and simulation results obtained was 0.65 MPa and 0.67 MPa respectively with 3.43% error. Minimum combustion duration was obtained at stoichiometric conditions which are 31ms and 31.5 ms for experimental and numerical results obtained respectively with 1.61% error. The maximum percentage errors in peak pressure and combustion duration are 10.6% and 7.93% respectively which indicates that the model is valid for the combustion process with prescribed conditions.
At $\phi=0.8$ CO emissions are 93 % less than $\phi=1$, whereas $\phi=1.4$ it is 2.75 times greater than $\phi=1$.
At $\phi=1.4$, NOX and CO2 emissions are decreased by 82.73% and 41.29 % respectively compared to stoichiometric mixtures. Thus, laser combustion has the ability to be implemented in the future as a substitute for electric spark. Furthermore, it is foreseen to extend the model to other liquid fuel laser ignition.
5. References

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