

Experimental and Numerical Study of Flame Kernel Formation Processes of Propane-Air Mixture in a Pressurized Combustion Vessel

Xiucheng Zhu
Michigan Technological University

Lorenzo Sforza
Politecnico di Milano

Tejas Ranadive, Anqi Zhang, Seong-Young Lee, and Jeffrey Naber
Michigan Technological University

Tommaso Lucchini and Angelo Onorati
Politecnico di Milano

Muniappan Anbarasu
General Motors Co.

Yangbing Zeng
General Motors LLC

ABSTRACT

Fuel lean combustion and exhaust gas dilution are known to increase the thermal efficiency and reduce NO_x emissions. In this study, experiments are performed to understand the effect of equivalence ratio on flame kernel formation and flame propagation around the spark plug for different low turbulent velocities. A series of experiments are carried out for propane-air mixtures to simulate engine-like conditions. For these experiments, equivalence ratios of 0.7 and 0.9 are tested with 20 percent mass-based exhaust gas recirculation (EGR). Turbulence is generated by a shrouded fan design in the vicinity of J-spark plug. A closed loop feedback control system is used for the fan to generate a consistent flow field. The flow profile is characterized by using Particle Image Velocimetry (PIV) technique. High-speed Schlieren visualization is used for the spark formation and flame propagation. To support the experimental activity and to better understand the effects of local flow and turbulence on the combustion process, CFD simulations were carried out at both reacting and non-reacting conditions using the OpenFOAM code with suitable libraries (Lib-ICE) developed for combustion modeling. The full vessel geometry was considered and the rotation of the fan, used to generate turbulence and velocity fields, was modeled. In this way it was possible to identify the expected combustion regimes and to clarify the effects of the spark-plug geometry on the flame propagation process.

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INTRODUCTION

The transportation sector accounts for 28% of US greenhouse gas emissions and is the second largest contributor to the greenhouse gas emissions [1]. There has been 18 % rise in the greenhouse gas emissions since 1990. This is partly due to the limited increase in fuel efficiency compared to the surge in vehicle and transportation sector growth [1]. Fossil fuels are proven for high energy density, low cost and easy availability. Currently no technology looks set to completely replace the proven and tested internal combustion engines. With the depleting reserves of fossil fuels and the growing

concern of emissions, it is of pressing importance to improve the fuel economy and reduce emissions. With the US federal law setting the target of 54 mile per gallon for 2025, it is of further importance to increase the IC engine efficiency.

Tremendous efforts have been devoted to increase the spark ignited (SI) engine combustion efficiency. The theoretical thermodynamic SI engine cycle is more efficient than combustion ignition (CI) cycle, however CI engines run on much higher compression ratios making it more fuel efficient than SI engine. SI engines are often operated at lower compression ratios to avoid knocking in

combustion. SI engines are characterized by lower nitrous oxide (NO_x) and particulate matter (PM) emissions than CI engines, however, CO₂ and CO emissions are still a concern. Also, the inherent structure of SI engines with a throttle body adds to the pumping losses, further reducing the efficiency. SI engines, unlike their CI counterparts, have to be run at stoichiometric conditions for effective working of the catalysts [2].

To account for all these losses, efforts have been devoted to run the SI engines fuel diluted. Dilution of fuels can be achieved either by running the engines fuel lean or by diluting with exhaust gases (EGR) or both. Diluting the fuel by exhaust gases has several benefits. Firstly, adding EGR reduces the peak temperature of combustion thereby reducing the NO_x emissions, as the NO_x formation is highly dependent on temperature. Other advantage of adding EGR are reduced heat loss to cylinder walls, increased expansion work and reduced pumping losses [2].

However, there are limitations in the SI engine for increasing EGR and fuel dilution. If the engine is run with either excessive lean mixtures or high EGR, it increases the combustion instability and can lead to misfire. This can cause an increase in coefficient of variation of IMEP which can be detrimental to the engine structure. It is therefore important to know the maximum levels of dilution that could be achieved in practice. Furthermore, there is always a turbulent flow field in the vicinity of the spark plug during engine running conditions. This flow field stretches out the flame kernel, which results in greater area of the spark channel and its interaction with the combustible mixture. The combustible mixture also needs a certain minimum amount of energy from the spark plug for the flame to be self-sustaining and propagating. The flow velocity around the spark plug needs to be in a certain optimum range. If there is no flow near the spark plug, the spark channel area will be small and the flame may not self-sustain, leading to misfire. If the velocity around the spark plug gap is too high, the spark channel may be extinguished before an adequate amount of energy is transferred to the combustible matter, also leading to misfire.

SI engines also face the problem of knocking under high pressure and high temperature conditions. The flame speed of an SI engine combustion is an important design factor in engines. Dilution of fuel with EGR and running fuel lean is bound to reduce the flame speed. However, the higher the turbulent intensity, the higher will be the turbulent flame speed [3].

In the current study, the combustion of propane-EGR mixture is analyzed for different low turbulent velocities in a pressurized constant volume combustion vessel. The experiments are carried out for lean mixtures with equivalence ratio of 0.7. The mixture is diluted with 20% mass-based EGR. The low turbulent velocities are generated by a shrouded fan design. Particle image velocimetry (PIV) is used to characterize the flow field around the spark plug. The visualization images are then post-processed for measuring the flame front propagation rate.

METHODS AND EXPERIMENTS

Experiments are performed in an optically accessible constant volume combustion vessel. The turbulent flow field is generated in the vicinity of the spark plug by a shrouded fan. There are two types of tests in this study: PIV test and combustion test. PIV technique is used to characterize the flow field and relate the flow field to the fan speed. Ignition combustion tests of pre-mixed propane-air mixtures with 20 percent mass-based EGR are performed under different turbulence flow. The combustion near the spark plug is visualized using high speed Schlieren technique.

Combustion Vessel

The combustion vessel (CV) in the Alternative Fuels Combustion Laboratory (AFCL) of Michigan Technological University (MTU) is used to perform the experiments. The vessel is a 1.1 liter constant volume chamber with over 95% of optical coverage. The chamber has six windows which can be either used for optical access, or for mounting experimental instruments (the spark plugs, injectors, and fans). There are total eight corners on the cubical chamber, which allow intake valve, exhaust valve, and pressure transducer accessing to the chamber. The CV also has temperature control which can maintain CV body at a stable temperature up to 453 K. The vessel can withstand maximum temperature of about 2100 K and the pressure up to 345 bar during the combustion event [4].

PIV Tests

The PIV test is a non-intrusive technique used to characterize the flow field and measure the instantaneous velocity [5, 6]. The flow with proper seeding particles is illuminated by the laser. The particles need to be small enough in order to follow the fluid velocity [7]. Di-Ethyl-Hexyl-Sebacat (DEHS) liquid is used as the particle seeding in this test [8]. DEHS has several advantages which are no soluble, colorless, the small uniform size (below 1 μm), and the long life time. DEHS can evaporate completely after use.

DEHS oil and a seeder tank with Laskin nozzle inside are used to create seeding particles as shown in Figure 1. Pressurized nitrogen is pumped into the seeder tank containing DEHS oil which created small droplets of around 1 μm diameter and infused into the CV through the intake valve. Figure 2 shows the detailed schematic diagram of the PIV system used. Two Nd-Yag lasers of 532 nm were used to continuously generate laser sheet into CV to illuminate the seeding particles. The two laser sheets are synchronized with a camera which captures two consecutive images. The time interval between the two continuous laser pulses varied from 10 ms to 50 ms according to different fan speeds. By comparing the two consecutive images, an instantaneous velocity profile is generated. Insight 3G software is used for synchronizing the laser and the camera, and also used to process the two consecutive images and measure the velocity in the flow field. For each test condition, a series of 100 consecutive image pairs are taken and the average velocity profile over these 100 images is obtained.

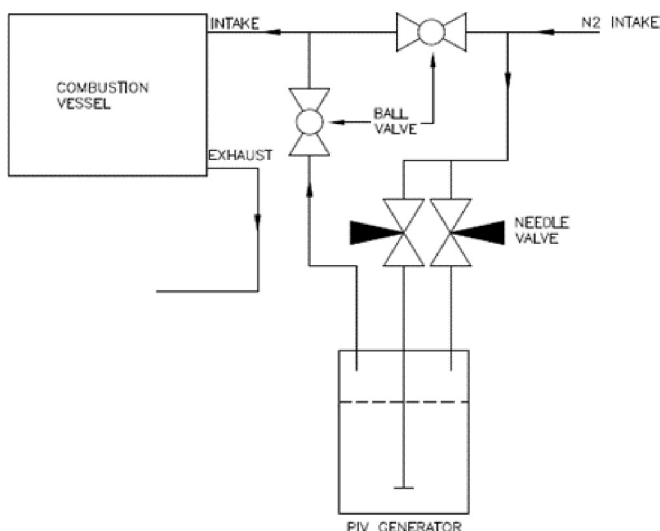


Figure 1. Schematic diagram of the PIV seeding particle generator.

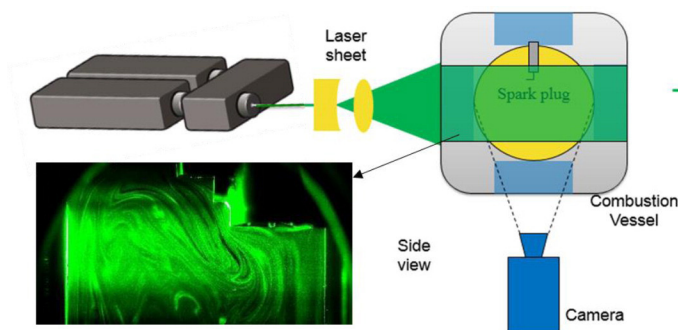


Figure 2. The detailed schematic diagram of the PIV system and a sample image of laser sheet.

A shrouded fan is designed to generate the turbulence flow field in the vicinity of the spark plug, as shown in Figure 3. The fan has a 25.4 mm outer diameter with eight straight vanes with 30 deg attack angle. The fan is connected to a 12V brushed DC motor, and it is controlled by a closed loop feedback control system. The control system contains a control board, an optical encoder, and a control software. Therefore, the fan speed can stay constant regardless the variation in pressure of the combustion vessel.

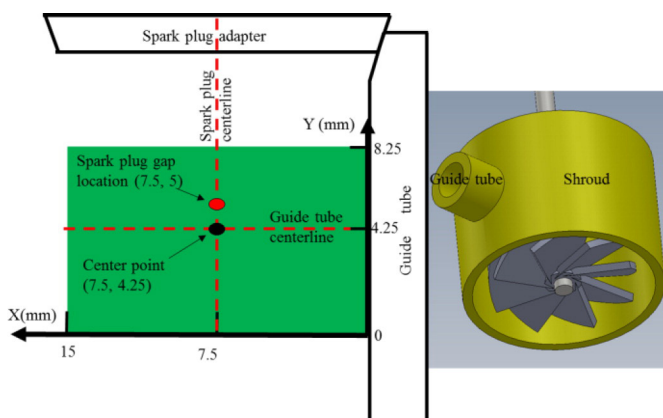


Figure 3. 3-D drawing of the shrouded fan (right) and the interested region of the PIV tests (left). Spark plug gap will be located in (7.5 mm, 5 mm).

From the PIV tests, the flow velocity corresponding to the fan speeds of 3000, 6000 and 9000 RPM are characterized. The pressure and the temperature are varied to obtain similar levels of fluid density which will be present during the ignition tests. Note that in the PIV test, the spark plug is not installed, and a solid spark plug adapter is installed at the spark plug location. The spark plug centerline is 7.5 mm from the exit of the guide tube. The centerline of the guide tube is located on 4.25 mm of y-axis.

Ignition Tests

For the ignition tests, the premixed mixture of propane-EGR is taken into the CV and ignited by the spark plug mounted on the top of the vessel. The ignition is visualized by Z-shape schlieren technique [9], shown in Figure 4. The pressure data is recorded by a dynamic pressure sensor located in the combustion vessel. The lab's data acquisition system is used to log the pressure data at 100 kHz.

Exact engine like conditions cannot be replicated in the combustion vessel. However the conditions are tried to be kept as similar as possible. Equivalence ratio (ϕ) of 0.7 is tested (compositions as shown in Table 1). The combustion vessel is kept at a constant temperature of 453 K. Four different levels of fan speeds, 0, 3000, 6000, and 9000 RPM are tested. For quiescent conditions, there is no turbulence in the chamber. Three different levels of dwell time are also tested. The detailed test matrix is shown in Table 2. Two different ambient pressures are used to explore the pressure effect on flame kernel development. During the ignition tests, secondary current, secondary voltage, and capacitance of electrical circuit were measured to calculate the discharge energy. The schematic of the electric circuit is shown in Figure 5. A voltage probe and a current probe were added in the secondary circuit. The spark plug and probes are connected to a common ground.

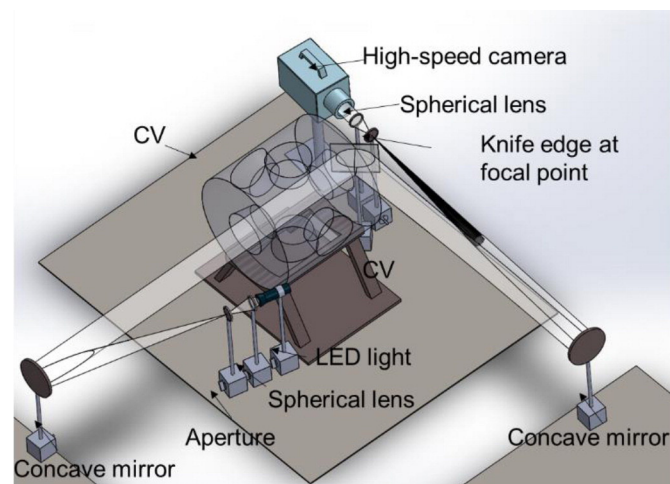


Figure 4. Schematic of Z-shape high-speed schlieren technique experimental setup.

Table 1. Mixture Compositions of ER 0.7 propane-air mixture.

Mixture Composition					
Φ	EGR	C ₃ H ₈	O ₂	CO ₂	N ₂
0.7	20.0%	2.4%	17.5%	2.8%	7.3%

Table 2. Test Matrix for ignition tests

Propane with 20% EGR					
Test No.	Φ	CV pressure (bar)	CV temp (K)	Flow velocity (m/s)	Dwell time (ms)
1	0.7	8	453	0	6
2	0.7	8	453	1	6
3	0.7	8	453	2	6
4	0.7	8	453	3	6
5	0.7	16	453	0	6
6	0.7	16	453	1	6
7	0.7	16	453	2	6
8	0.7	16	453	3	2,4,6
9	0.9	8	453	2	4

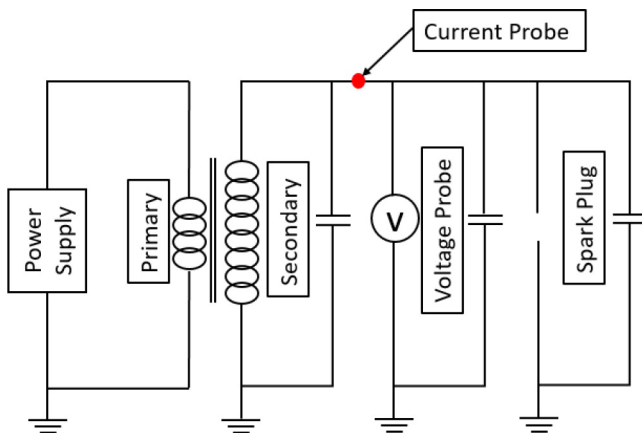


Figure 5. Ignition coil circuit.

NUMERICAL INVESTIGATIONS

To support the experimental activity, CFD simulations were performed on:

1. non-reacting setup, in order to clarify the influence of the fan rotation speed on the flow velocity and turbulence intensity fields nearby the spark-plug; in this context some numerical simulations were also carried out to match PIV measurement results;
2. reacting setup, with the purpose to identify and describe in more detail the expected combustion regimes.

All simulations were carried out with the open-source platform OpenFOAM and involving a 3-D finite volume discretization. Transport equations of mass, momentum and chemical species were solved with the RANS approach and the $k-\epsilon$ model was used for turbulence. In the following sub-sections, firstly, the numerical models used for premixed SI combustion simulation will be described. Then important details such as the adopted meshes and the technique used to simulate fan rotation will be shown. Finally, numerical results from both non-reacting and reacting simulations will be deeply analyzed in the light of the available experimental findings.

Numerical Models

The approach used for premixed SI combustion description is mainly the one adopted and already validated by Lucchini et al. [10]. It can be summarized as follows: a set of Lagrangian particles, each one

representing a possible location for an ignited kernel, is introduced along the spark-gap centerline in order to model the plasma channel. The evolution of these particles is mainly controlled by convection, due to local flow field conditions, thermal expansion, because of the energy transferred from the electrical circuit, and flame speed. A model for the secondary electrical circuit is applied to estimate the amount of energy transferred to the particles, while the heat conduction equation is solved to compute the plasma channel expansion velocity in the 5000 - 50000 K temperature range, accounting for real gas properties.

The flame surface density distribution, computed from particles position and size, is then used for fuel reaction rate computation, allowing thus to group all the flame kernel evolution effects into a single source term. The fuel reaction rate is, finally, used by the adopted Eulerian combustion model, namely the Coherent Flame Model.

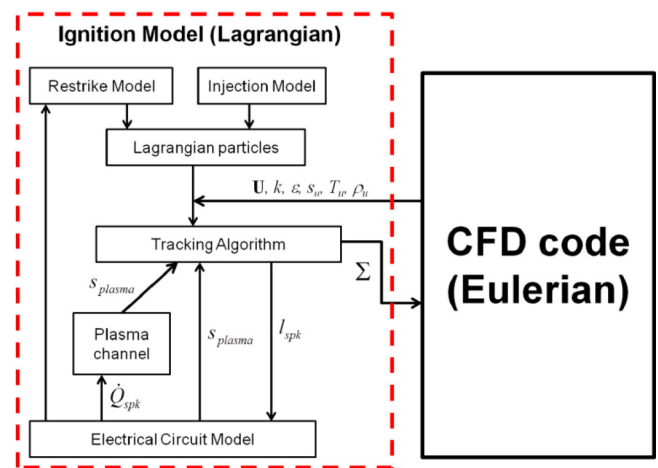


Figure 6. Lagrangian Ignition Model, with its six sub-models, and Eulerian CFD code coupling scheme [10].

In other words, the following Lagrangian models of

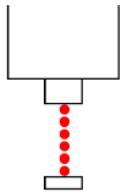
1. Injection
2. Particle evolution
3. Plasma channel
4. Electrical circuit
5. Restrike
6. Flame surface density calculation

interact among each other and exchange information with the main Eulerian CFD code during the initial flame kernel development process (Figure 6).

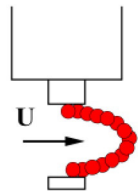
Nevertheless some little improvements were adopted, in particular:

1. the flame stretch description of the initial Lagrangian flame kernel was performed through the approach proposed by Bradley, Lau and Lawes [11];
2. the coupling between Lagrangian particles, whose role is to simulate the initial stage of combustion, and Eulerian CFD code, which is able to describe a fully turbulent flame, was achieved via a particle radius threshold value of $r_p = 2 \text{ mm}$.

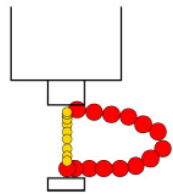
This last choice was adopted following the observations made by Falfari and Bianchi [12] about transition of flame kernel properties to that of fully turbulent flames. In the next sub-sections a detailed description of the listed Lagrangian sub-models and of the adopted improvements will be carried out.



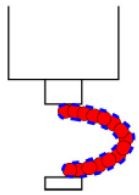
a.



b.



c.



d.

Figure 7. Details of the Lagrangian Ignition Model [10]: (a) plasma channel formation at spark discharge; (b) contemporary channel growth, due to thermal expansion and flame speed, and elongation, due to local flow field; (c) restrike; (d) flame surface density calculation.

Particles Injection Model

Three stages characterize the ignition process in SI engines: breakdown, arc and glow discharge. Because of the very small characteristic time scale of breakdown stage (nanoseconds), only arc and glow discharge were modeled. In particular, at spark-time and after any possible restrike event (Figure 7a and Figure 7c), a set of 10 Lagrangian particles were introduced along the spark-gap centerline in order to reproduce as better as possible the cylindrical shape of the generated plasma channel without too high computational costs. Consequently these particles were initialized considering all the phenomena related to the breakdown stage only as initial conditions. With this purpose we followed the approach

proposed by Refael and Sher [13], and used by Song and Sunwoo [14], where the temperature and diameter of the introduced particles at the beginning of the arc stage are:

$$T_i = \left[\frac{1}{k} \left(\frac{T_{bd}}{T_u} - 1 \right) + 1 \right] T_u \quad (1)$$

$$d_i = 2 \left[\frac{k-1}{k} \frac{E_{bd}}{p d_{gap} \left(1 - \frac{T_u}{T_i} \right) \pi} \right]^{1/2} \quad (2)$$

Here, $k = 1.66$ is the plasma channel specific heat ratio, considering plasma as an ionized monoatomic mixture, T_u the unburned gas temperature, p the gas pressure and d_{gap} the inter-electrode distance. For the breakdown temperature T_{bd} , the value of 60,000 K was chosen, considered as a reasonable value [13]. The breakdown energy E_{bd} was calculated through the following expression [15]:

$$E_{bd} = \frac{V_{bd}^2}{C_{bd}^2 d_{gap}} \quad (3)$$

where C_{bd} is a constant ranging from 4.6 to 5.4 kV/(mJ^{1/2} mm^{1/2}) and that was set according to the measured breakdown energies, while the breakdown voltage V_{bd} was computed as in [10] and [12].

Particle Evolution Model

The particles introduced by the injection model need to be evolved considering (Figure 7b):

1. the flow field conditions nearby the spark-plug
2. the heat conduction from the hot plasma channel to the unburned mixture
3. the heat transfer from the electrical circuit
4. the chemical reactions, whose speed is function of the local conditions of air/fuel mixture (equivalence ratio and EGR) and turbulence (stretch and wrinkling phenomena).

About this last point, it is also important to consider that each Lagrangian particle represents a possible location for an ignited kernel; in fact, for each of them, the conservation equations are solved. In particular, both mass conservation equation

$$\frac{dm_p}{dt} = 4\pi r_p^2 \rho_u \left(S_T + \frac{\rho_k}{\rho_u} S_{plasma} \right) \quad (4)$$

and radius variation equation

$$\frac{dr_p}{dt} = \frac{\rho_u}{\rho_k} S_T + S_{plasma} + S_{therm} \quad (5)$$

include thermal expansion (S_{plasma} , S_{therm}) and turbulent flame speed (S_T) contributions. Here m_p , r_p and ρ_k are the particle mass, radius and density, respectively, while ρ_u is the unburned mixture density at

particle position. Regarding the energy conservation equation, it is necessary to distinguish between two different mechanisms governing particles growth:

1. expansion due to heat conduction from the hot plasma channel to the unburned mixture, in which temperature distribution inside the kernel is not uniform;
2. expansion due to both heat transfer from the electrical circuit and chemical reactions, in which temperature distribution can be considered uniform and composition at chemical equilibrium inside the particle.

A temperature threshold value of $3T_{ad}$, where T_{ad} is the adiabatic flame temperature, is chosen as switch condition between the two mechanisms. When particle temperature T_p is greater than $3T_{ad}$, the expansion is governed by the first mechanism and the plasma channel model (Figure 6) computes the heat conduction inside the channel, the growth velocity s_{plasma} and other particle properties (T_p , ρ_k , r_p). On the other hand, when $T_p < 3T_{ad}$, the second mechanism controls kernel expansion, so the energy conservation equation can be written as

$$\frac{dT_p}{dt} = -\frac{\dot{m}_p}{m_p} (T_p - T_{ad}) + \frac{\dot{Q}_{spk_p}}{m_p c_p} + \frac{1}{\rho_k c_p} \frac{dp}{dt} \quad (6)$$

where c_p is the specific heat and $\dot{Q}_{spk_p}$ the energy deposition rate from the electrical circuit to the particle, reduced of the heat losses. In fact, considering $\dot{Q}_{spk}$ the total heat transfer rate from the electrical circuit to the gas phase and η_{eff} the efficiency of this energy deposition, $\dot{Q}_{spk_p}$ is $(\dot{Q}_{spk} \eta_{eff})/n_{particles}$. Moreover, because T_p is low with respect to its initial values, s_{plasma} can be neglected and

$$s_{therm} = \frac{V_p}{A_p} \left(\frac{1}{T_p} \frac{dT_p}{dt} - \frac{1}{p} \frac{dp}{dt} \right) \quad (7)$$

is introduced in Eq. 5 to consider particle expansion due to heat transferred from the electrical circuit.

In Eqs. 4 and 5 the turbulent flame speed s_T is computed as

$$s_T = \Xi s_{u0} \quad (8)$$

where Ξ is the flame wrinkling and s_{u0} the unstretched laminar flame speed at the particle position. However, differently from [10], the flame stretch phenomenon was additionally considered in turbulent flame speed computation. Hence, Eq. 8 became

$$s_T = \Xi s_u \quad (9)$$

where the actual laminar flame speed s_u was computed at particle position using the approach for flame stretch description proposed by Bradley, Lau and Lawes [11]:

$$s_u = s_{u0} \frac{1-K Ma}{1+\frac{c}{R} \delta_l Ma} \quad (10)$$

where s_{u0} is the unstretched laminar flame speed, K the dimensionless Karlovitz stretch factor, δ_l the laminar flame thickness, R the flame curvature total radius and $c = 1$ is the parameter that allows to adapt Eq. 10 to a cylindrical flame shape. The Markstein number Ma is computed through the following expression [16]

$$Ma = \frac{1}{\gamma} \ln \left(\frac{1}{1-\gamma} \right) + \frac{1}{2} Ze (Le - 1) \frac{1-\gamma}{\gamma} \int_0^{\frac{\gamma}{1-\gamma} \frac{\ln(1+x)}{x}} dx \quad (11)$$

obtained by the asymptotic analysis of Clavin and Williams [17] for an overall single-step reaction, where $\gamma = (\rho_u - \rho_k)/\rho_u$ is the expansion ratio, x is a dummy variable of integration, while Le and Ze are respectively the Lewis and the Zel'dovich number. Here, the Lewis number was assumed equal to 1, a value considered reasonable in absence of a more detailed prediction, therefore Eq. 11 reduced to

$$Ma = \frac{1}{\gamma} \ln \left(\frac{1}{1-\gamma} \right) \quad (12)$$

According to the proposed approach for the computation of the flame speed in Eq. 10, misfire occurs mainly due to the too high flame stretch rate which reduces the s_u value. For this reason, the model can properly predict the onset of misfire and how it is affected by near spark-plug turbulence, equivalence ratio and EGR levels.

Plasma Channel Model

This model [10] was created to describe the plasma channel evolution when the particles temperature is greater than the threshold value of $3T_{ad}$. In fact at these high temperatures (5000 - 50,000 K) the heat conduction effects cannot be neglected in the gas surrounding the ignited kernel; consequently the temperature distribution and its effects on plasma channel expansion velocity need to be modeled in deep.

Electrical Circuit Model

After the breakdown stage, the energy provided by the engine electrical system to the ignited plasma channel could significantly affect the early flame kernel development, especially in presence nearby the spark-gap of: lean mixtures, high flow field velocities and high turbulence-laminar flame speed ratios. Typical electrical systems of SI engines are characterized by a primary and a secondary circuit. During charging time a certain amount of energy, which can be experimentally measured, is stored in the primary circuit; at the spark-time, this energy is transferred to the secondary circuit and then dissipated as heat provided to the gaseous phase. This electrical circuit model [10] describes in detail, after the breakdown phase, the evolution in time of current and voltage inside the secondary circuit, accounting for its equivalent resistance, equivalent inductance and voltage falls due to gas column, anode and cathode.