A Simplified Model for Description of Triple Flames in Stratified Charge Gasoline Engines

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ABSTRACT
A simplified and numerically efficient model for spark ignition and partially premixed flame propagation in direct injection spark ignition (DISI) engines is developed and implemented into an enhanced KIVA-3V code. Based on the general idea of the discrete particle ignition kernel model by Fan et al. [1] the ignition kernel developing after spark onset is represented by Lagrangian marker particles. However, in this new model the propagation of the premixed flame front of the so-called triple flame is estimated by marker particles as well, even after the end of the spark duration. Moreover, the effect of the supplied spark energy on the flame kernel development and the interaction of the turbulent flow field with the self-sustained flame front is modeled in detail. The diffusion part of combustion that can take place behind the premixed flame front in case lean and rich residuals mix because of turbulence is described by an adjusted version of the characteristic time scale combustion model known from diesel engine modeling. The new submodels are validated by comparison to experimental data and the complete model is then applied to simulate an ignition timing variation in a stratified charge DISI engine. Generally, a good accordance between predictions and measurements is found.

INTRODUCTION
Partially premixed combustion in DISC engines can take place in so-called triple flames as shown in Fig. 1 [2]. At the spark plug a flame kernel starts to develop due to the energy transferred to the mixture by spark discharge. This initiation of combustion is comparable to conventional spark ignition engines, with the exception that the air-fuel ratio at the spark plug might not be stoichiometric in the stratified charge case. Once the flame kernel has reached a critical size, a self-sustained premixed flame front starts to spread into the combustion chamber. The speed and the amount of energy released by this flame front is significantly influenced by turbulence and temperature, and even more by the local equivalence ratio of the mixture. Thus, it propagates fastest along a line of approximately stoichiometric air-fuel ratio and it will eventually quench if the mixture becomes too lean at the periphery of the fuel cloud. Behind the premixed flame front a diffusion flame similar to the flame type known from diesel combustion can develop if residuals from the lean and rich flame branches mix due to turbulence. Thus, at the leading edge of the flame, the so-called triple point, three different flame types are present: lean and rich premixed flame fronts as well as a diffusion flame.

MODEL FORMULATION
Marker Particle Concept: Based on the ignition model by [1] the propagation of the developing ignition kernel is described by Lagrangian marker particles that track the position of the flame front but do not model the chemistry within the flame front directly. The particles are distributed uniformly around the two main steradians and initially describe a sphere. However, several modifications to this concept have been applied in the present study. Firstly, the particles which have zero mass can now be convected freely by the cylinder gases [3]. Therefore, it is achieved that the propagation due to chemical effects becomes relative to the flow field. Moreover, not only the ignition kernel but also the subsequently developing self-sustained premixed flame is tracked by the marker particles in the new model. Hence, throughout the entire combustion process the position of the premixed flame front is described by particles. The heat release by chemistry is then modeled separately for the premixed flame, i.e. within the grid cells containing flame marker particles, and for the diffusion flame taking place behind the premixed flame front. The governing equations for flame propagation

Fig. 1: Schematic of triple flame structure [2]
and chemical reactions will be described in the following sections.

**Ignition Kernel Growth:** According to [4] the breakdown phase of the spark discharge takes place in extremely short time scales (ms-range) that are typically not resolved in CFD-engine modeling. In contrast, most of the spark energy is transferred to the gas phase in the glow discharge mode [5] which continues over a much longer period (ms-range) and which is characterized by smaller energy transfer efficiencies because of heat losses from the gas to the spark plug electrodes. To account for these effects and in order to simplify the model it is assumed that an initial ignition kernel is present after \( \Delta t_0 = 1 \) \( \mu \)s which is in the range of a typical computational time step. Its initial radius \( r_{k,0} \) depends primarily on the spark system and the air-fuel-ratio at the spark gap. It can be derived from an energy balance assuming that the energy necessary to heat the gas within the kernel from unburned to approx. adiabatic flame temperature is supplied by the electrical energy \( W_\text{el} \) of the spark plug and the chemical energy released within the kernel:

\[
\frac{4}{3} \pi \rho_k r_{k,0}^3 \rho_c \varepsilon_c (T_{ud} - T_u) = W_\text{el} \Delta t_0 + \frac{4}{3} \pi \rho_k \varepsilon_c LHV_{\text{max}}
\]

(1)

\[
\Leftrightarrow r_{k,0} = \left[ \frac{3W_\text{el} \Delta t_0}{4\pi\rho_c \varepsilon_c (T_{ud} - T_u) - LHV_{\text{max}}} \right]^{1/3}
\]

(2)

where \( \rho_k \) and \( \varepsilon_c \) are the kernel density and specific heat, respectively, \( LHV_{\text{max}} \) represents the lower heating value per gram mixture and subscript \( u \) refers to the unburned gas state.

In the early stages the growth of the ignition kernel is primarily governed by electrical energy supply to the spark gap and by heat conduction within the gas. As in Eq. 1, it is again assumed that the chemical energy stored within the ignition kernel is immediately released once it is heated to approximately adiabatic flame temperature. Hence, an energy balance for the growing ignition kernel can be established in analogy to Eq. 1. However, in this case the volume change of the kernel is the product of the kernel surface area and the change in kernel radius \( dr_k \), and the energy transfer efficiency from the spark plug to the gas \( \eta_{sp} \) is significantly less than unity in the glow discharge mode. The kernel growth rate \( \frac{dr_k}{dt} \) is commonly referred to as plasma velocity \( v_p \).

\[
4m_k \frac{dr_k}{dt} \rho_c \varepsilon_c (T_{ud} - T_u) = \eta_{sp} W_\text{el} + 4m_k \frac{dr_k}{dt} \rho_k \varepsilon_c LHV_{\text{max}}
\]

(3)

\[
\Leftrightarrow \frac{dr_k}{dt} = \frac{\eta_{sp} W_\text{el}}{4m_k \rho_c \varepsilon_c (T_{ud} - T_u) - LHV_{\text{max}}}
\]

(4)

Since the spark duration is typically short (< 1 ms) and the ignition kernel / developing flame front is still approximately spherical during this period, the plasma velocity is assumed to be equal in all spatial directions. It is inversely proportional to \( r_k^2 \) (Eq. 4) and thus, decreases rapidly as the kernel is growing. The energy transfer efficiency \( \eta_{sp} \) is the only “tuning” parameter in the ignition model and ought to be chosen between 0.3 and 0.5 according to [5].

**Premixed Flame Front Propagation:** In contrast to the plasma velocity, the speed of the self-sustained flame front which develops from the ignition kernel has to be calculated separately for each particle position, since it strongly depends on local conditions and the particles are no longer in the immediate vicinity of the spark gap. The laminar flame speed \( s_f \) is calculated based on the relation by [6] for iso-octane

\[
s_f = \left( 1 - 2.1R \right) \left( 26.32 - 84.72 \cdot \phi - 1.13 \right)^{0.28} \left( \frac{p}{101.3kPa} \right)^{-0.16 + 0.22/\phi},
\]

(5)

where \( R \) is the residual mass fraction and \( \phi \) the fuel-air equivalence ratio. The effect of turbulence on the burning velocity by flame straining and wrinkling is expressed following [7]:

\[
s_f' = I + \left( I_0 + u'/u' + S_f \right)^{1/2} \left( 1 - \exp \left[ \frac{r_f}{L} \right] \right)^{1/2}
\]

(6)

where \( I_0 \) is the strain rate, \( u' \) the isotropic turbulence intensity, \( I \) the turbulence integral length scale, \( r_f \) the flame radius and \( T_{ud} \) is a characteristic time scale calculated as \( T_{ud} = l/u' + S_f \). Equation 6 has the effect that the ratio \( s_f'/s_f \) is close to unity shortly after ignition, and increases as the flame surface grows and is fully affected by turbulent wrinkling. In order to ensure a smooth transition from ignition to self-sustained flame front propagation the effective flame velocity \( s_{eff} \) is calculated as

\[
s_{eff} = \frac{P_{\text{cell}}}{P_k} \cdot \max(r_{f,cell}, s_f)
\]

(7)

where the unburned to burned density ratio accounts for thermal expansion effects of the hot combustion products.

**Flame Front Heat Release:** For simplicity, a one-step reaction mechanism from fuel and O\(_2\) to CO\(_2\) and H\(_2\)O is assumed within the premixed flame front. The reaction rate per computational cell is based on the product of fuel density within the gas mixture, flame speed and flame surface area \( A_{p,cell} \) within the cell. The latter is approximated in terms of the mean distance \( r_{p,cell} \) between the cell particles and the spark gap and the number of particles \( N_{p,cell} \) contained within that particular grid cell.

\[
\frac{dm_f}{dt} = \rho_{f,cell} s_f A_{p,cell} = \rho_{f,cell} s_f 4\pi r_{p,cell}^2 N_{p,cell} \frac{N_{p,cell}}{N_{p,cell}}
\]

(8)
Balancing the enthalpies of formation of the species involved in the reaction then yields the heat release and the new cell temperature.

**Diffusion Flame:** The diffusion flame taking place behind the premixed flame front is modeled by the often applied time scale combustion model, e.g. [8-10], which specifies the temporal changes in species densities $d\rho_i/dt$ by dividing the deviation from the equilibrium composition by a characteristic time scale $\tau_{turb}$ which is composed of a laminar (chemical) $\tau_{lim}$ and a turbulent (mixing) $\tau_{rob}$ time $\tau_{turb}$

\[
\frac{d\rho_i}{dt} = -\frac{\rho_i - \rho_i^{eq}}{\tau_c} = -\frac{\rho_i - \rho_i^{eq}}{\tau_{lim} + \tau_{rob}}.
\]

Details about the definition of the laminar and turbulent time scales can be found in the above references. It should be noted though, that in order to account for the greater knock resistance of gasoline compared to diesel fuel, the time scale model for diffusion combustion becomes active only in cylinder areas that have already been passed by the premixed flame front or where an onset-temperature has been reached that is greater than the one usually chosen for diesel combustion (1300 K in this study).

**Spray Model:** In the engine simulations performed in this study the LISA sheet atomization spray model [11, 12] has been applied in order to describe the mixture formation established by a pressure swirl injector.

**MODEL VALIDATION**

The new ignition and combustion model was implemented into the CFD-Code KIVA-3 [13] and initially tested by comparing calculated flame kernel growths shortly after ignition to experimental data as presented by [14]. Figure 2 displays the development of the kernel radius for three different spark energies and durations in a quiescent propane-air mixture of fuel-air equivalence ratio of 0.7. The initial temperature and pressure within the constant volume bomb are 300 K and 101.3 kPa, respectively. The energy transfer efficiency ($\eta_{sp}$ in Eqs. 3 and 4) was adjusted to a value of 0.46 in order to fit the 11.5 mJ case and the two other spark energies have been precalculated without further parameter adjustment. The error bars of the experimental data represent an uncertainty of ± one standard deviation. Even though the kernel growth for the 2.0 mJ case, which is close to the minimum ignition energy, is slightly underpredicted, the overall agreement between simulations and experiments is very good. The effect of ignition energies and durations on kernel growth speed can be predicted satisfactorily by the model. The influence of the plasma velocity in the early stages of ignition is clearly visible by the rapid growth speed. It then quickly decreases as the flame kernel becomes larger, and after the end of spark duration the kernel grows with constant speed (straight line in Fig. 2) which equals the laminar flame velocity.

![Fig. 2: Calculated and experimental flame kernel growth](image)

In order to test the model’s capability of describing the structure of a partially premixed flame, ignition and early stages of combustion were calculated in a constant volume bomb filled with stratified octane-air mixture (Figs. 3 to 6). The initial conditions within the bomb are $T_0 = 700$ K, $p_0 = 101$ kPa, and the initial equivalence ratio varies from $\phi_0 = 0.5$ to $\phi_0 = 2.0$ in vertical direction as indicated in the figures. The ignition location is at stoichiometric mixture approx. in the middle of the elliptical flame shape indicated by the black particles and the turbulence level is artificially set to a value which resembles typical turbulence intensities in DISC engines. Thus, turbulent diffusion is enabled. In addition to the premixed flame front positions, Figs. 3 to 6 show the distributions of the fuel-, CO$_2$- and CO-mass fractions and of temperature at a timing of 1 ms after ignition. The elliptical shape of the flame front indicates that the local flame speed is fastest along a horizontal line of approx. stoichiometric mixture whereas it decreases perpendicular to this direction as the local equivalence ratios become leaner or richer (upwards or downwards in the figures, respectively).

The fuel mass fraction shown in Fig. 3 is zero in most parts within the flame kernel. However, it can be seen that as expected there is some unburned fuel left even behind the flame front in areas of rich combustion where the O$_2$-concentration is the limiting factor. The distribution of the CO$_2$ mass fraction in Fig. 4 indicates the completeness of combined premixed and diffusion combustion. As expected it has a maximum at the leading edges of stoichiometric premixed combustion (left and right hand sides of the kernel) where a one step mechanism from C$_8$H$_{18}$ to CO$_2$ is assumed. The mass fraction in the upper (initially lean) part of the kernel is also large since diffusion combustion has already started.
and there is enough oxygen available to convert all the fuel to CO\textsubscript{2}. Only in the lower (rich) part of the kernel a smaller CO\textsubscript{2} mass fraction is observed even though diffusion combustion is taking place in this region as well. This corresponds to the CO mass fraction distribution displayed in Fig. 5 which has a maximum at this exact position. The diffusion combustion model considers a two step mechanism from fuel via CO to CO\textsubscript{2} and stops at CO in case there is too little oxygen for complete burning. The temperature distribution in Fig. 6 indicates that the maximum temperature occurs in stoichiometric or slightly rich mixture where the adiabatic flame temperature has its maximum as well.

The visible fact that the species mass fractions are clearly affected by combustion outsight the flame kernel as well can be explained by two phenomena. Firstly, the heat release within the flame kernel causes an expansion which then results in a radial displacement of the unburned mixture. This explains the deviations in some distance outside the kernel, e.g. the 0.034 to 0.051 fuel mass fraction band above the flame kernel in Fig. 3. The second type of deviation surrounds the kernel by about the size of one computational grid cell. It is an artifact because the mean composition of a grid cell starts to change as soon as it is entered by the first flame front particles. This effect is accounted for in the model by calculating the local burning velocities and reaction rates of the flame front based on the unburned cell properties that existed at that point in time when the first particles entered the particular cell. Therefore, the flame propagation is hardly affected by this artifact.

**ENGINE SIMULATION**

**Test Engine:** The investigated engine is a DISI two-stroke single-cylinder research engine with a 0.4-liter displacement volume and a dome shaped cylinder head. It is equipped with a centrally mounted pressure swirl injector and a spark plug that reaches about 10 mm into the dome on the exhaust port side of the cylinder. Its location is indicated on the cross-sectional view of the cylinder in Fig. 7 which also shows the air-fuel-ratio distribution at the ignition timing of the baseline case (-31° ATDC). At this timing the fuel cloud is – in spite of the central injector position and orientation – deflected towards the right hand side (exhaust port side) of the combustion center by a clockwise tumble induced by the intake ports. The engine is operated at 2000 rpm with a fuel injection quantity of 7.3 mg (approx. 20% load). The injection timing is fixed at -85°ATDC and an ignition timing variation has been performed with ignition settings at -41°, -31°, -21° and -16°ATDC.

**Results:** In Fig. 8 the experimental and calculated pressure traces are compared for the varying ignition timings and Fig. 9 displays the respective NOx concentrations at the time the exhaust port opens (95°ATDC). The model constants have been coarsely adjusted for the ignition timing of -31°ATDC and the other cases have been pre-calculated with the same set of parameters.

![Fig. 3: Fuel distribution 1ms after ignition](image3)

![Fig. 4: CO\textsubscript{2} distribution 1ms after ignition](image4)

![Fig. 5: CO distribution 1ms after ignition](image5)

![Fig. 6: Temperature distribution 1 ms after ignition](image6)
It can be seen from the pressure results in Fig. 8 that the new model is capable of predicting the influence of the ignition timing on combustion in the investigated direct injection stratified charge engine well. The characteristic trend that an earlier ignition timing causes a higher peak pressure at a timing closer to top dead center is clearly visible. In the baseline and late ignition cases the quantitative agreement between simulation results and experimental data is excellent, too. Only for the earliest ignition case (-41° ATDC) the predicted pressure trace exceeds the experimental data noticeably. However, the overall agreement is still very satisfying considering the above calculations represent the first model test and no extensive parameter adjustment has been performed yet.

The comparison between estimated and measured NOx concentrations in Fig. 9 indicates that the model does predict the increasing NOx emissions for earlier injection starts that are caused by the higher pressures and especially temperatures encountered under these conditions. However, this effect seems to be over predicted by the model as the calculated NOx concentration is too small for the late ignition cases and too high for the earliest ignition case (-41° ATDC) as the predicted pressure trace exceeds the experimental data noticeably. However, the overall agreement is still very satisfying considering the above calculations represent the first model test and no extensive parameter adjustment has been performed yet.

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In general however, the results obtained with the new combustion model are very promising such that there is confidence that the important characteristics of partially premixed combustion in stratified charge gasoline engines can be simulated with this relatively simple and easy to handle model. Hence, after a more thorough model adjustment, a more detailed chemical reaction scheme will be applied to further enhance this new combustion model in future work.

**CONCLUSIONS**

A new computationally efficient combustion model for spark ignition and triple flame propagation has been developed and implemented into KIVA-3. The submodels for ignition as well as premixed and diffusion combustion have been validated by comparison to experimental data obtained in a constant volume bomb. The results indicate that the new model is capable of predicting the structure of partially premixed flames typical for direct injection spark ignition engines. Hence, the model is applied to simulate an ignition timing variation in a small DISC engine. Good accordance between calculated and measured cylinder pressure histories and reasonable agreement between the respective NOx emissions is achieved for all investigated ignition settings.
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