Analyses of the Combustion Process in a Direct Injection Gasoline Engine

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ABSTRACT

The improvement of efficiency and reduction of emissions has precedence in present development and optimization of internal combustion engines. One of the internal combustion engine types is the direct injection gasoline engine. This technology provides enormous potentialities to achieve the target for low fuel consumption and low exhaust emissions.

The development of this technology requires new experimental methods and numerical models to analyze and to describe the mixture formation and combustion process which differ essentially from the premixed combustion, especially at part load. The objective of this paper is to present an attempt to simulate the in-cylinder flow, mixture formation and combustion in direct injection gasoline engines (GDI). The numerical investigation of a 4-stroke-3-valve GDI engine is discussed and compared to experimental results.

The numerical simulation of the in-cylinder flowfield and the turbulent combustion were performed with the code KIVA-3V. A flame area evolution model for homogenous-charge and turbulent combustion presented by Weller et al. [1] has been implemented and amplified for partially premixed turbulent combustion. This model expansion is based on the discussion of the burning velocity in partially premixed flames described by Peters [2].

INTRODUCTION

The gasoline direct injection (GDI) concept represents a combination of the combustion phenomena of both spark-ignition- and Diesel-engines and combines the advantages of both. Therefore, the four-stroke GDI engine offers high efficiency and low emission potential. Especially at part load conditions, unthrottled operation offers GDI engines similar fuel economy like an Diesel-engine. The combustion characteristic of a GDI engine provides a high antiknock quality and therefore a higher compression ratio. An improvement of thermal efficiency can be obtained. Furthermore the GDI method has no delay in fuel transport during cold start, warm-up, and transient mode, which leads to combustion with lean mixtures and reduced HC- and CO-emissions.

In spite of the distinct advantages, especially fuel consumption and exhaust emission, the GDI engine has certain inherent problems. The mixture preparation for stratified-charge at low load demands a well-atomized fuel spray to optimize and to accelerate the evaporation. The formation and controlling of the required stratified-charge in a wide range of operating conditions represents a central difficulty [3-7]. The injection is controlled by the parameters injection-pressure, injection-time, and injection-duration. It must be ensured that in interaction with turbulent charge motion a flammable mixture reaches the spark plug at that moment, which thermodynamically represents the best ignition time.

As the combustion characteristic at full load does not essentially differ from homogenous working SI engines, the combustion characteristics of GDI engines change significantly with combustion control strategy at part load. After combustion has started around the spark plug the flame develops rapidly into the rich mixture region. However, in the lean outer region of the stratified charge the speed of flame propagation is reduced. This early combustion may be characterized by flames as they occur in typical premixed lean or stoichiometric mixtures. The significantly lower combustion rate near the end of the combustion process is caused by high contribution of diffusively controlled combustion to the global reaction rate. Flame propagation in partially premixed flows, like the stratified charge in GDI engines, is determined by the movement of triple flames, which consist of two premixed wings and a trailing diffusion flame [8,9].

Experimental and numerical methods provide a better understanding of mixing and combustion process in GDI engines and lead to an improvement of engine efficiency and engine design. This paper represents a first attempt to describe the physical process in GDI engines numerically.

NUMERICAL MODEL

Computations were performed using KIVA-3V, a CFD code for transient reactive flows with spray. KIVA-3V uses a block-structured mesh and permits flexibility for modeling complex geometries with various boundary conditions. The equations and the numerical method are discussed in detail by Amsden et al. [10]. In the present study the original KIVA submodel for gas turbulence, hollow-cone spray atomization and vaporization was used. The submodel for turbulent combustion was replaced by a model for premixed combustion which was extended for the partially premixed combustion.
COMBUSTION MODEL

Premixed Combustion. Premixed turbulent combustion occurs mostly in spark-ignition engines. In homogeneous-charge spark-ignition engines fuel is injected into the intake manifold and mixes with the intake air. An essential foundation for numerical modeling of turbulent combustion in a homogenous SI engine is the knowledge of structure and motion of the flame inside the cylinder. There are several reports about experimental investigations which allow to describe and characterize such flames [11-13]. Based on these results a multitude of numerical schemes were developed to reconstruct the premixed combustion in an SI engine. Among others the Eddy-Break-Up Model [14], G-Equation of Peters [15] or the Flamelet-Model discussed by Duclos et al. [16] should be mentioned here.

At the International Symposium COMODIA 1994 Weller et al. [1] introduced a new model for homogeneous-charge turbulent combustion. This flame area evolution model simulates the growth of the initial flame kernel into a fully developed turbulent flame and its subsequent propagation.

The fundamental assumptions of this model can be summarized as follows:

- the flame represents a discontinuity separating burned and unburned regions
- the reaction takes place in a relatively thin layer and can be modeled in a single-step-reaction (flamelet approximation)
- turbulent structures stretch and wrinkle the flame surface
- the flamelets propagate with laminar flame speed into unburned areas
- the reaction area may be defined by a regress variable, which has the limits unity and zero in the unburned and fully-burned areas respectively.

In preinvestigations the combustion model in KIVA-3V was replaced by the Weller model in the one-equation form which defines the flame front location by an iso-surface of a scalar field of the regress variable \( \overline{c} \). If the flame is characterized by the distribution of the local ensemble-averaged regress variable \( \overline{c} \), the associated transport equation can be formulated as:

\[
\frac{\partial \overline{c}}{\partial t} + \nabla \cdot \overline{U} \overline{c} - \nabla (\overline{p} \overline{Dc} \nabla \overline{c}) = \overline{\rho}_u S_i [\nabla \overline{c}] \tag{1}
\]

The right hand side of equation (1) represents the mean reaction rate \( \overline{\omega} \).

\[
\overline{\omega} = \overline{\rho}_u S_i [\nabla \overline{c}] \tag{2}
\]

In the present investigation a semi-empirical correlation (Eq. (3)) was used to calculate the speed of a turbulent developing flame of the premixed combustion proposed by Maly et al. [17].

\[
S_f = S_l + S_l \left( \frac{u'}{u' + S_l} \right)^{1/2} \left( \frac{u'}{S_l} \right)^{5/6} \left( 1 - \exp \left[ -\frac{S_l}{u' + S_l} \frac{t}{\tau} \right] \right)^{1/2} \left( 1 - \exp \left[ -\frac{t}{\tau} \right] \right)^{1/2}
\]

\text{temporal variation of flame speed}

(3)

where \( t \) is the time after ignition and the constant \( \tau \) is related to the flame development and is set to be 1.0ms. The laminar flame speed \( S_l \) is defined in the unburned gas and depends on pressure, local temperature, and mass fraction. According to Heywood [18] it can be calculated in the following form:

\[
S_l = S_{l,\text{ref}} \left( \frac{T_u}{T_{\text{ref}}} \right)^{\alpha} \left( \frac{P}{P_{\text{ref}}} \right)^{\beta}
\]

(4)

The reference speed of laminar flames \( S_{l,\text{ref}} \) and the exponents \( \alpha \) and \( \beta \) in equation (4) represent functions of the equivalence ratio and were discussed by Heywood [18]. For the numerical simulation of the flame propagation in a homogeneous SI engine the \( \overline{c} \) field was initialized with \( \overline{c} = 1 \) for unburned conditions. Combustion was initiated by setting \( \overline{c} = 0 \) in one cell at the location of the spark plug. The results of the numerical simulation were compared with experimental investigations. The flame propagation which was detected using the optical fiber technique as well as the temperature distribution determined by spectroscopic measurements are in a good agreement with the numerical results. Details of the experimental investigations and comparisons with the simulations can be found in references [19] and [20].

![Fig. 1 A schematic graph of the triple flame structure](image-url)

Partially Premixed Combustion. The partially premixed combustion is essentially determined by the mixture fraction
because the laminar burning velocity depends on the local equivalence ratio \( \phi \) and for that reason on the mixture fraction. The maximum of laminar burning velocity is close to \( \phi = 1.0 \). Therefore, flames will propagate fastest along the surface \( \phi = 1.0 \) in a mixture field. According to Peters [2] the flame propagation in a partially premixed field with a surface \( \phi = 1.0 \) generates a flame structure that is called triple flame. The leading edge of the flame, called the triple point, propagates along the surface of stoichiometric mixture (see Fig. 1). On the lean side of that surface there is a lean premixed flame branch and on the rich side a rich premixed flame branch both propagating with a lower burning velocity. Behind the triple point on the surface of stoichiometric mixture a diffusion flame develops, where the unburned fuel from the rich premixed branch burns together with the remaining oxygen from the lean premixed branch.

For the numerical simulation of an analogous flame structure additional quantities are required to describe the inhomogeneous mixture field. For this purpose the combustion model of premixed flame was supplemented by transport equations (Eq. (5)) for the mass fractions \( \bar{Y}_i \) of fuel, \( \text{O}_2 \), \( \text{N}_2 \), \( \text{CO}_2 \), \( \text{H}_2\text{O} \) and \( \text{CO}_2 \text{ Res} \) as one component of the residual gas.

\[
\frac{\partial \bar{Y}_i}{\partial t} + \nabla \bar{U} \cdot \bar{Y}_i - \nabla \left( - \bar{p} \frac{\partial \bar{Y}_i}{\partial \bar{y}_i} \right) = \dot{\bar{Y}}_i \bigg|_{\text{chem}}
\]

with:

\[
\dot{\bar{Y}}_{\text{fuel}} \bigg|_{\text{chem}} = \dot{\bar{c}} \bar{Y}_{\text{fuel}, u} = \bar{P}_u S_i \nabla \bar{c} \bar{Y}_{\text{fuel}, u}
\]

\[
\bar{Y}_{\text{fuel}, u} = \bar{Y}_{\text{fuel}} + m\text{bco}_2 \cdot \left( \bar{Y}_{\text{CO}_2} - \bar{Y}_{\text{CO}_2 \text{ Res}} \right)
\]

Now the regress variable \( \bar{c} \) may be reconstructed from the fractions and can be defined by equation (8).

\[
\bar{c} = \frac{\bar{Y}_{\text{fuel}}^*}{\bar{Y}_{\text{fuel}} + m\text{bco}_2 \cdot \left( \bar{Y}_{\text{CO}_2} - \bar{Y}_{\text{CO}_2 \text{ Res}} \right)}
\]

\[
\bar{Y}_{\text{fuel}}^* = \min \left[ \bar{Y}_{\text{fuel}, u} + m\text{bco}_2 \cdot \bar{Y}_{\text{O}_2} \right]
\]

where \( m\text{bco}_2 \) and \( m\text{bo}_2 \) stand for the fuel-CO\(_2\)-mass-ratio and fuel-O\(_2\)-mass-ratio in stoichiometric combustion.

In rich mixture areas the local oxygen fraction limits the amount of fuel which can be burned in a premixed flame. Therefore a maximum fuel mass fraction \( \bar{Y}_{\text{fuel}}^* \) (Eq. (9)) must be used to calculate the regress variable. The inhomogeneous mixture field can be described by the local equilibrium ratio. In the presented combustion model the local equivalence ratio is used to determine the local burning velocity in the unburned area. Therefore the local equivalence ratio in front of the flame is required:

\[
\tilde{\phi}_{u} = \frac{\bar{Y}_{\text{fuel}} + m\text{bco}_2 \cdot \left( \bar{Y}_{\text{CO}_2} - \bar{Y}_{\text{CO}_2 \text{ Res}} \right)}{m\text{bo}_2 \cdot \bar{Y}_{\text{O}_2} + m\text{bco}_2 \cdot \left( \bar{Y}_{\text{CO}_2} - \bar{Y}_{\text{CO}_2 \text{ Res}} \right)}
\]

In partially premixed turbulent systems flame propagation is fastest in regions with the highest probability of the existence of stoichiometric mixture fraction. Therefore the laminar burning velocity depends on the mean mixture fraction \( \bar{Z} \) and additionally on the Favre averaged mixture fraction variance \( \bar{Z}^{\prime \prime} \). Here the laminar burning velocity has been derived in a similar manner as Peters described [2] by considering the mean value of \( S_i \) as a stochastic mean value depending on \( \bar{Z} \) and \( \bar{Z}^{\prime \prime} \).

\[
\bar{S}_i(\bar{Z}) = \int_0^1 S_i(\bar{Z}) P_2(\bar{Z}, \bar{Z}^{\prime \prime}) d\bar{Z}
\]

Here \( P_2(\bar{Z}, \bar{Z}^{\prime \prime}) \) is a joint probability density function of \( \bar{Z} \) and \( \bar{Z}^{\prime \prime} \), which is defined as follows:

\[
P_2(\bar{Z}, \bar{Z}^{\prime \prime}) = (\bar{Z}^{\prime \prime} - 1)^{\alpha - 1} (\bar{Z} - \bar{Z}^{\prime \prime})^{\beta - 1} \frac{\Gamma(\gamma)}{\Gamma(\alpha) \Gamma(\beta)}
\]

where

\[
\alpha = \bar{Z}^{\prime \prime} \gamma = \frac{\bar{Z}^{\prime \prime}(\bar{Z} - \bar{Z}^{\prime \prime})}{\bar{Z}^{\prime \prime} - 1}
\]

To reduce the enormous calculation effort equation (11) may be approximated by the function (15).

\[
\bar{S}_i(\bar{Z}) = S_i (P_{\text{Stf}} (\bar{Z}, \bar{Z}^{\prime \prime})) \sqrt{C_{\text{Stf}}}
\]

![Graph showing mean laminar burning velocity, \( p = 8\text{bar} \), \( T = 700\text{K} \), Iso-Butane](image)

In comparison between the results of equation (11) and (15), pictured in Fig. 2, a nearly constant value for \( C_{\text{Stf}} = 0.9 \) was detected. Further an additional transport equation is required for the mixture fraction variance. The source terms appearing in this equation are described by Peters [2]. The knowledge of the local laminar burning velocity in an inhomogeneous mixture field enables to determine the turbulent burning velocity corresponding to the equations (3) and (4).
**NUMERICAL SIMULATION**

**Model Verification.** In a first test the model described above was used to calculate the flame propagation in a stratified mixture field. Therefore a closed vessel in which the mixture fraction of Iso-Octan varies linear corresponding to the x-coordinates between the flammability limits was used. The charge was ignited at \( Z = Z_{fl} \). In Fig. 3 the flame structure detected by the reaction rate is pictured.

![Fig. 3 Triple flame configuration](image)

It can be seen that three flame branches were developed. A rich premixed flame propagates in the area with \( Z > Z_{fl} \) and a lean premixed flame propagates into the region \( Z < Z_{fl} \). Between both branches the remaining fuel of the rich flame and the oxygen of the lean flame react in a diffusion flame. The curvature of the premixed flames was caused by the expansion motion of the burned gas. This study verifies the ability of the discussed model to describe a partially premixed combustion. In further investigations corresponding experiments must be used to validate the model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<td>Bore</td>
<td>89,95 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>86,60 mm</td>
</tr>
<tr>
<td>Compression Ratio ( \varepsilon )</td>
<td>10 -</td>
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<tr>
<td>Intake-valve Opening</td>
<td>20 BTDC CAD</td>
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<tr>
<td>Intake-valve Closing</td>
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<td>Maximum Valve Lift</td>
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<td>Indicated Mean Effective Pressure</td>
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<td>Engine Speed</td>
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<td>Fuel</td>
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<td>Injection Geometry</td>
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<td>Sauter Mean Diameter</td>
<td>8.5 ( \mu )m</td>
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<tr>
<td>Ignition Time</td>
<td>31 BTDC CAD</td>
</tr>
</tbody>
</table>

**Table 1 Geometry and operating conditions**

**Engine and Computational Condition.** The present simulation uses the actual geometry of the intake port, moving valves and piston of an engine investigated experimentally. The engine has two intake valves and one outlet valve. At part load one intake port can be throttled to generate a swirl which stabilizes the mixture stratification. The injector is mounted in a central position. Ignition stability is maintained by positioning the spark plug at the periphery of the fuel spray. The geometry specification and the reference operating conditions are listed in Table 1.

![Fig. 4 Computational grid structure at BDC](image)

The mesh (Fig. 4) comprises about 80,000 cells. The KIVA-3V calculation started at the crank angle position representing the inlet valves opening. The boundary conditions were defined as pressures at the intake flow and outflow boundaries, which were associated with experimental values. For initial condition a zero velocity field and homogeneous pressure and temperature field in the combustion chamber were assumed.

![Fig. 5 Flow field at 90 CAD ATDC](image)

**Results and Discussion.** In Fig. 5 the velocity field in a cross section containing one inlet valve and the opposite exhaust
valve at 90 CAD ATDC is pictured. Herein the structure of the inlet flow, which generates a tumble flow with a superimposed swirl, is shown.

At 305 CAD ATDC fuel was injected into the remaining tumble flow. The injection parameters were adjusted to experimental investigation at analog engine configuration and operating conditions [21]. In Fig. 6 the resulting distribution of the equivalence ratio $\Phi$ at ignition time 329 CAD ATDC is shown. At this time 64.7% of the injected mass is vaporized. 94.45% of the combustion chamber volume is leaner and 3.76% is richer than the flammable limit regime. Only 1.78% of the charge volume is within the flammable limits. This fact signifies the difficulty of placing a flammable mixture at the spark plug location at part load operating conditions which was mentioned before. The white line in Fig. 6 belongs to the stoichiometric mass fraction. In this region the fastest flame propagation is expected.

![Fig. 6 Fuel vapor distribution at ignition time](image)

Fig. 7 shows the comparison of the pressure traces versus crank angle for the calculation and measurement at reference operating conditions. It can be seen that the simulation predicts an abrupt rise of the cylinder pressure after the ignition. This fact may be caused by a higher amount of fuel burning premixed because the simulation indicates a spray vaporization which is too fast. After TDC the absolute value of the pressure as well as the curvature of the pressure line are in good agreement. Additionally the fraction of burned fuel mass is plotted. Corresponding to the rise of pressure the burned fuel mass increases fast after ignition. At 5 CAD ATDC 75% of fuel was burned, at this point the reaction rate reduces due to an increasing amount of fuel burning diffusively controlled.

![Fig. 7 Cylinder pressure history](image)

The flame structure can be discussed in Fig. 8, in which the reaction rate is plotted at TDC in a horizontal plane. There is an inhomogeneous, cleft flame shape recognizable with high intensity regions with stoichiometric mixture fraction. In regions with very lean mixture the flame extinguishes.

![Fig. 8 Flame structure at TDC in cross section B-B](image)
In Fig. 9 the temperature distribution in horizontal planes are shown at several crank angle positions. The area of the maximal temperature propagates due to the fuel distribution and encloses the region with the rich mixture. The temperature reaches values over 2500 K. The position of the temperature maximum belongs to a quasi stationary diffusion flame. As a result of the reduced reaction rate at the end of the combustion the temperature field is inhomogeneous even at 20 CAD ATDC.

![Temperature Distribution in Cross Section B-B](image)

**CONCLUSION**

Direct injection technology gets more and more interesting in present and future development and optimization of GDI engines. This technology differs in a wide range of engine operating conditions from conventional mixing formation and combustion process. Therefore new experimental methods and numerical models are required to analyze the processes in such engines.

A simulation of the inhomogeneous combustion in a direct injection SI engine at part load was described. Therefore a combustion model for premixed flames was extended for partially premixed combustion. It was proved that the resulting model is able to describe a triple flame configuration as they are expected in direct injection SI engines.

The comparison of the results with first experimental data shows good agreement in temporal progression. Shortcomings at the beginning of the combustion seem to be caused by incorrect simulation of the fuel evaporation. However, the discussion of the flame structure provides an insight into the combustion process of GDI engines.

For additional development and understanding it is necessary to extend the research over a wide range of data and operating conditions because of the complex combination between charge motion, fuel injection and combustion. At the Institute of IC engines of the University Karlsruhe this work is currently in progress.

**REFERENCES**