

Zero-Dimensional Modeling of Combustion and Heat Release Rate in DI Diesel Engines

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ABSTRACT

Zero-dimensional heat release rate models have the advantage of being both easy to handle and computationally efficient. In addition, they are capable of predicting the effects of important engine parameters on the combustion process. In this study, a zero-dimensional combustion model based on physical and chemical sub-models for local processes like injection, spray formation, ignition and combustion is presented. In terms of injection simulation, the presented model accounts for a phenomenological nozzle flow model considering the nozzle passage inlet configuration and an approach for modeling the characteristics of the Diesel spray and consequently the mixing process. A formulation for modeling the effects of intake swirl flow pattern, squish flow and injection characteristics on the in-cylinder turbulent kinetic energy is presented and compared with the CFD simulation results. The applied combustion model accounts for the turbulence-controlled as well as the chemistry-controlled combustion. The effects of EGR on ignition delay and combustion are described as well. This model is validated using measurement data of different Diesel engines applying EGR and various injection strategies. The results of heat release rate and center of combustion are compared with measurement results over the entire engine map of a heavy-duty Direct Injection Diesel engine.

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INTRODUCTION

Numerical simulation is a decisive tool for further powertrain optimization and development towards fulfilling future emission standards, fuel consumption reduction and improved safety and drivability. A predictive engine model that accounts for several engine processes such as gas exchange, injection, combustion and emission formation provides a simulation platform for virtual powertrain development. It can be used to perform parametric studies or optimizations of engine components such as a turbochargers. Additionally, this can work as a virtual engine for testing and evaluation of different EGR (Exhaust Gas Recirculation) and injection control strategies. Furthermore, there is increasing need to utilize such sophisticated models within vehicle simulation software like VeLoDyn [1] to model transient engine behavior on real driving cycles. One important part of any engine model is the combustion model. The main task of a combustion model is to describe the effect of different engine operating conditions on combustion and subsequent emission formation.

Combustion models are classified according to computational time and model complexity into three major categories. First, the empirical or thermodynamic models,

which are principally a mathematical approximation of heat release rate by a compensatory burning rate function. For instance, the proposed formulation of Vibe [2] is one of the simplest approaches. These models are computationally very fast and after calibration of parameters with measurement data, can then be used to describe the burning rate. The disadvantage of such simple models is that they can only be used to simulate the heat release rate near the calibration points and are not able to predict the combustion when the operating conditions deviate from that calibration point. The phenomenological models employ simple physical and chemical sub-models, describing several in-cylinder processes like injection, air-fuel mixing, ignition and combustion. In contrast to empirical models time-dependent engine parameters, such as injection rate, should be given as an input vector. Based on applied physical models, they provide a certain capability to predict the combustion process while the operating conditions deviate from the calibration point. Depending on the modeling approach - if it is a zero-dimensional, one or two-zone model, more information about temperature and composition of each zone can be delivered. These models could be used in the subsequent steps as a foundation for modeling the emission formation.

All empirical and phenomenological models are incapable to completely resolve the spatial distribution of air-fuel mixture and consequently its effect on combustion and emissions. The multi-dimensional CFD (Computational Fluid Dynamics) models give a detailed insight into the combustion phenomenon and enable a detailed study of important effects like the in-cylinder swirl flow in-homogeneity and stability, which has a great influence on combustion and emission formation [3]. However, the computational effort of CFD models are too extensive, which makes it impractical for use in many applications (e.g. in combination with a vehicle simulation tool), where computational time is the limiting parameter.

Phenomenological combustion models use physical and chemical sub-models that are practical for combustion modeling with minimal simulation effort. In recent years, multiple modeling approaches have been studied by various investigators. The approach proposed by Chmela et al. [4,5] is a global model based on a single-zone description of the combustion chamber. It does not require the subdividing the combustion chamber into zones of different compositions and temperatures. Therefore, it offers a fast and computationally efficient model. However, it is categorized as a phenomenological combustion model, since it relates the burn rate to the engine characteristics parameters (e.g. the injection rate as a time-dependent input parameter) [6,7]. The main issue of this model is the hypotheses that the rate of fuel combustion is determined by the rate of air-fuel mixing. The rate of air-fuel mixing depends on the injection rate as well as turbulent kinetic energy. In this model, the injection spray is the main source for the generation of the turbulent kinetic energy. It is assumed that the turbulent kinetic energy of intake flow as well as the turbulent kinetic energy generated by the squish flow can be neglected. However, CFD modeling of intake and compression stroke show a considerable influence of the swirl flow and squish flow on the in-cylinder turbulent kinetic energy [3]. Furthermore, the effect of oxygen concentration, which is an important parameter that limits the combustion rate, especially for high load points, is not considered in the diffusion combustion model. For engines using EGR, concentration of the oxygen has an important effect on the combustion rate.

Constien and Woschni [8] proposed another simple global model. The main idea of this model is the assumption that fuel conversion rate is determined by ignition delay and fuel vaporization. The injected fuel is divided into multiple segments and the vaporization is calculated by a diffusion equation. This is not a multiple-zone model such that the temperature and concentration of each zone is individually considered. Limitation of fuel burning rate due to the air-fuel mixing is not considered. It should be noted that the diffusion combustion is controlled not only by the rate of fuel vaporization but also by the air-fuel mixing and the turbulent kinetic energy, which is not considered here. Ignition delay is modeled and the pre-mixed combustion is considered as well. However, for operating points with early start of pilot

injection and hence long ignition delay, only a part of the injected mass can be burned in the pre-combustion phase. Modeling such effects could be a limitation of this model. According to the model each fuel segment burns after the ignition delay and therefore for cases with very early fuel injection, after the start of combustion all fuel mass will be burned completely.

Hiroyasu et al. [9,10] proposed a so-called packet model that is used as a conceptual basis for many similar models, e.g. [11,12,13]. During the compression stroke, there is only one zone, which is modeled as an ideal mixed gas. The injection spray is discretized to small packets in axial and radial directions. The number of packets in axial direction depends on the amount of injection mass. Each packet has its own temperature and composition history and is treated as a thermodynamic control volume to solve the mass and energy conservation equations. After spray break-up, air is entrained into the spray packets. No mass and energy exchange between the various packets is modeled. Combustion and fuel conversion are controlled by vaporization as well as air entrainment. The penetration length is calculated in both radial and axial directions. After ignition, burning of the vaporized fuel is controlled by available air in each packet.

The phenomenological combustion model presented by Stiesch [13] is based on the Hiroyasu model [9,10]. One modification of this model is that the maximum burning rate of each packet depends not only on the vaporized fuel and the available air but also on the maximum chemical reaction rate. Thoma et al. [14] extended the packet model to account for the pilot injection. The packets of the main injection penetrate into the pilot injection spray zone. This zone consists of pilot injection packets and has the mass-averaged properties from the former packets. The entrainment will be from this pre-zone instead of the fresh gas.

Barba [7] proposed an empirical and a phenomenological combustion model. The phenomenological combustion model accounts for pre-mixed as well as the diffusion combustion in combination with an ignition delay model. A simple evaporation model is also employed. It is assumed that the evaporated fuel before start of combustion burns as a pre-mixed flame with the calculated flame speed and the vaporized fuel after start of combustion burn as a mixing-controlled combustion. The mixing-controlled part of the combustion employs a characteristic frequency model such that the reaction rate is controlled by a characteristic mixing time scale [7].

A phenomenological combustion model for Diesel engines, which accounts for numerous pilot and post injection events, is presented by Rether et al. [15]. Each pilot injection event is modeled as an air-fuel mixture cloud with air entrainment. The ignition delay is calculated separately for each injection event. The heat release rate of the pilot injection is simulated as a function of flame propagation and local excess air ratio. A slice modeling approach is used for main- and post-injection modeling. Pre-mixed and diffusion combustion are calculated. The model has been integrated

into the 'cylinder module' developed by Grill [16] for modeling the in-cylinder processes of internal combustion engines. More detailed modeling of the effect of piston movement, squish flow and intake flow motion on the turbulent kinetic energy based on the project 'cylinder module' [16] is in progress [17].

MODEL FORMULATION

The developed model in this study applies a single-zone modeling approach as used by Chmela et al. [4,5] and does not subdivide the combustion chamber into zones of different compositions and temperatures. However, the model can be employed within a two- or multi-zone description of the cylinder thermodynamics. A phenomenological nozzle model based on a measurement database and the model of von Kuensberg Sarre et al. [18] is used for calculation of the injection rate of pilot, main and post injection events. In order to minimize the computational time, instead of using a packet model, the simple approach of Chmela et al. [5] is selected for injection and spray formation.

For more accurate simulation of turbulent kinetic energy, a model based on the work of Chmela et al. [4] is developed. The ignition model considers both the physical and the chemical ignition delays. The combustion model is principally a characteristic time combustion model accounting for the pre-mixed, diffusion and burn-out combustion. The combustion is controlled mainly by the rate of air-fuel mixing, turbulent kinetic energy as well as the oxygen concentration.

SPRAY MODEL

In contrast to the empirical models, injection rate is a time-dependent input vector of the phenomenological combustion models. The injection rate mostly affects the in-cylinder turbulent kinetic energy and the rate of air-fuel mixing which finally determines the combustion rate.

In the present study, the applied methodology for determining the injection characteristics is based on experimentally measured data at the IAV hydraulic test bench, combined with the phenomenological nozzle model of von Kuensberg Sarre et al. [18]. Injection measurements carried out for several representative durations of injection and rail pressures are given to the model as a measurement database. However, hydraulic measurements are not performed for all engine operating points on the engine map with different injection durations. Therefore, based on the available database, first, an injection rate is estimated and then the estimated injection rate is corrected by employing the phenomenological nozzle model [18].

The nozzle model [18] is used to calculate the nozzle discharge coefficient and injection pressure at the nozzle hole as well as the cone angle and the effective injection velocity for a given injection rate. This model is originally developed for CFD codes in order to simulate the effect of nozzle geometry on fuel injection and spray process. Flow losses,

nozzle inlet configuration as well as combustion chamber conditions are taken into account in a simplified manner. The parameter r/d used in the nozzle model, which determines the ratio of the roundness of nozzle inlet passage to the hole diameter is calibrated by using the measured injection rate. The discharge coefficient of the injector and injection pressure at the nozzle hole are calculated dynamically during each injection event.

For each point of operation, the injector opening and closing behavior as well as the time delay between start of electric activation and start of fuel injection are directly taken from the measurement database. For operating points with relatively high injection quantities, first an injection rate is estimated using the available database. Next, the injection pressure at the nozzle hole exit is calculated by the nozzle model [18]. By comparing the calculated value to the rail pressure, the duration of injection is adjusted in an iterative manner until it reaches the desired pressure. For low load operating points with small injection quantities, the injector needle cannot be completely opened and hence the injection pressure at the nozzle hole is much lower than the rail pressure. In this case, given the duration of activation and the rail pressure, the duration of injection is determined from the measured database included in the model.

The next step after calculation of injection rate is simulation of the spray and subsequently the mixing process. The simple model proposed by Chmela et al. shows good agreement compared to CFD results [5]. Hence, it is selected here for modeling the spray and mixture formation. The time evolution of spray characteristics are governed by mass and momentum conservation equation of the spray control volume. The spray tip penetration, $s(t)$, is derived [5] as:

$$s(t) = \left[\int_0^t \frac{4M(t)}{k^* \rho(t) \frac{\pi}{3} \tan^2(\theta/2)} dt \right]^{1/4} \quad (1)$$

Where $p(t)$ is taken here as in-cylinder air density, k^* is a constant parameter which is not adapted here and set to the proposed value of 0.6514. θ is the spray cone angle calculated by the nozzle model [18] with considering the effect of rail pressure and nozzle geometry, and $M(t)$ stands for the volume integrated momentum flux of injection spray equal to:

$$M(t) = \int \dot{M}(t) dt = \int \rho(t) u(t) dV \quad (2)$$

The mass fraction of the mixed fuel above a certain air-fuel ratio, $m_{f,mix}(t)$ to total injected fuel mass, $m_{inj}(t)$, is defined as:

$$Y_{f,mix}(t) = \frac{m_{f,mix}(t)}{m_{inj}(t)} \quad (3)$$

Mass fraction of the mixed fuel above a certain air-fuel ratio is calculated by the formulation proposed by Chmela et al. [5] as a function of spray tip penetration $s(t)$, cone angle θ and other spray parameters.

Fig. 1 illustrates the fuel mass distribution for pre-mixed and diffusion combustion. It is assumed that the prepared mixture before start of combustion is used for pre-mixed combustion. Mixture preparation for diffusion combustion begins with the start of combustion, Fig. 1.

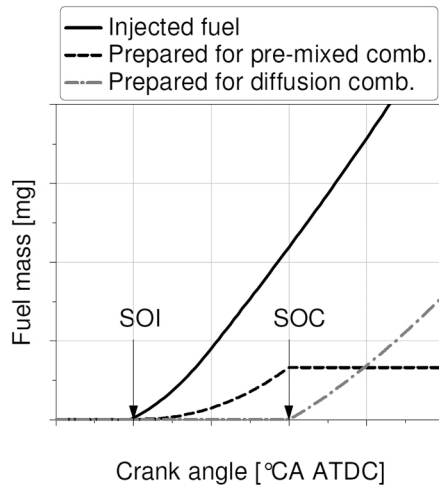


Figure 1. Fuel mass distribution for pre-mixed and diffusion combustion

It is assumed that the first part of the prepared mixture for the pre-mixed combustion is above a certain air-fuel ratio, λ_1 , as given by [5]:

$$m_{spray,pre,1} = m_{inj} Y_{f,mix,1} \quad (4)$$

The rest of the fuel mass in the combustion chamber, $m_{f,2}$, is calculated as:

$$m_{f,2} = m_{inj}(1 - Y_{f,mix,1}) \quad (5)$$

The prepared mass for diffusion combustion is introduced by Chmela et al. [5] as:

$$m_{spray,diff} = m_{f,2} Y_{f,mix,2} - m_{f,2} Y_{f,mix,2}|_{SOC} \quad (6)$$

where $Y_{f,mix,2}$ is the mass fraction of the mixed fuel above another air-fuel ratio, λ_2 , used as a threshold for diffusion combustion. Chmela et al. [5] assumed that the total fuel mass prepared at SOC is earmarked for the premixed

combustion phase and preparation of mass for diffusion combustion begins with the start of combustion, Fig. 1.

Therefore, prepared mass for the pre-mixed combustion is given by:

$$m_{pre,mix} = m_{spray,pre,1} + m_{f,2} Y_{f,mix,2} = m_{inj} Y_{f,mix,1} + m_{f,2} Y_{f,mix,2} \quad (7)$$

It is assumed that the mixture for the pre-mixed combustion is prepared only before start of combustion and will be consumed later by the pre-mixed combustion.

TURBULENCE MODEL

Turbulent kinetic energy plays an important role for air-fuel mixing, combustion and emission formation. The applied model for simulation of the in-cylinder turbulent kinetic energy is based on the model proposed by Chmela et al. [4] with several developments. The main formulation is based on the general idea that in an internal combustion engine three sources are principally responsible for production of turbulent kinetic energy. The first source is the kinetic energy of the inlet flow generated through intake ports as swirl or tumble motion during the intake phase. Squish flow resulting from piston movement is another production source. The most important source is the kinetic energy of the high-pressure fuel injection. CFD simulations of intake and compression phase show that the contribution of first two sources in the total amount of turbulent kinetic energy is considerable. Therefore, a formulation for modeling both sources are proposed and evaluated here.

In this study, the kinetic energy associated with the inlet flow is modeled as an initial condition at Intake Valve Closes (IVC). Assuming a constant swirl ratio for a specific port layout and valve strategy for all engine speeds, the tangential velocity of the in-cylinder is proportional to the engine speed. Therefore, the kinetic energy associated with the intake flow is considered as:

$$E_{kin,IVC} = C_1 m_{air} n^2 \quad (8)$$

Where m_{air} is the intake flow mass, n is the engine speed and C_1 is a constant parameter, which depends on port layout and the generated swirl ratio.

Production rate of kinetic energy resulting from squish flow depends on piston velocity as well as its position from the cylinder head during the compression or expansion stroke. The rate of kinetic energy production increases as the piston approaches the Top Dead Center (TDC). The cube root of the in-cylinder volume is taken as a measure of the distance between the piston and the cylinder head. The proposed equation for modeling the kinetic energy because of squish flow is proposed as:

$$\frac{dE_{kin,prod,squish\ flow}}{dt} = C_2 n^2 V_{cyl}^{-1/3} \quad (9)$$