

Development and Validation of a Quasi-Dimensional Dual Fuel (Diesel – Natural Gas) Combustion Model

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ABSTRACT

This paper presents a newly developed quasi-dimensional multi-zone dual fuel combustion model, which has been integrated within the commercial engine system simulation framework. Model is based on the modified Multi-Zone Combustion Model and Fractal Combustion Model. Modified Multi-Zone Combustion Model handles the part of the combustion process that is governed by the mixing-controlled combustion, while the modified Fractal Combustion Model handles the part that is governed by the flame propagation through the combustion chamber. The developed quasi-dimensional dual fuel combustion model features phenomenological description of spray processes, i.e. liquid spray break-up, fresh charge entrainment, droplet heat-up and evaporation process. In order to capture the chemical effects on the ignition delay, special ignition delay table has been made. Additionally, to capture the effect of entrained methane on the chemical reaction rate, special table that features chemical reaction time scale has also been made. The start of flame propagation is calculated through the newly developed sub-model based on knock integral calculation. The existing $k-\epsilon$ turbulence model has been extended to account for the effect of diesel pilot injection on the increase of in-cylinder turbulence level. Since in the conventional dual fuel combustion process multiple flames propagate through the combustion chamber, multiple flame propagation model has been developed. This model can describe arbitrary number of flames that propagate through the combustion chamber. The validation data for the developed quasi-dimensional dual fuel combustion model have been acquired on a 2.0 liter Diesel engine, which has been modified to operate in the conventional dual fuel combustion mode. The presented model has been validated at different loads and diesel substitution ratios, and there is a good fit between the measured and cycle-simulation data.

KEYWORDS: dual fuel combustion, quasi-dimensional model, cycle-simulation

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INTRODUCTION

Although in recent years there is a significant penetration of vehicles that use some form of renewable energy, the majority of transport will depend on fossil fuels for a number of years to come [1, 2]. Majority of that fuel is derived from crude oil, but the share of natural gas in transport is expected to rise. The use of natural gas as a fuel in transport has environmental, political and economic benefits. From political standpoint it is an alternative energy source compared to crude oil products, and its use provides diversity in the energy supply. The economic benefit depends on the country of use. For example U.S. is expected to be an exporter of natural gas [2] while in Europe although both oil and natural gas are generally imported the ratio of import versus local production of natural gas is much lower [3]. The environmental potential of use of natural gas relates to ever growing concern regarding the greenhouse gas emissions from combustion of

fossil fuels. In that area the use of natural gas has the potential of reducing CO₂ emissions by 25% because of the favorable C/H ratio [4]. The above mentioned facts imply that in order to make the transport sector more sustainable in the years to come the combustion process of IC engines has to be further optimized so that the use of fossil fuels is reduced and share of use of alternative fuels such as natural gas is increased.

In IC engines natural gas can be utilized in both spark ignited (SI) and compression ignited (CI) engines. In SI engines natural gas can be used as single fuel and can completely subsidize conventional liquid fuel. Due to better mixing properties of natural gas compared to liquid fuel, the fuel mixture can be prepared easier, but at the same time because of the lower molecular weight the fuel displaces more air and therefore by using natural gas the volumetric efficiency

decreases. The octane rating of natural gas is much higher than gasoline and therefore the compression ratio can be increased which will lead to the increase of engine efficiency. However, the laminar flame speed is lower compared to gasoline which means that the spark timing has to be changed in order to compensate for longer burn duration. There are two options with respect to the air-natural gas mixture in SI engines. One is to have stoichiometric mixture which will enable the use of 3-way catalyst that can lower the increased NO_x emissions formed by natural gas use in SI engine. However, running the engine with stoichiometric mixture leads to lower efficiency compared to diesel CI engines; Diesel like efficiency can only be achieved with very lean mixtures [5]. Additionally, if one takes into account that storing natural gas on passenger cars is a challenging task, the use of stoichiometric natural gas SI engine in commercial transport is not likely. The SI natural gas engine with lean mixture can achieve much higher efficiency, but now NO_x emissions are too high. In order to reduce the NO_x emissions the mixture can be extremely lean [5], but then because of the lower laminar flame speed misfires can occur. For running the extremely lean mixtures the special ignition designs are required, such as pre-chamber ignition system [6]. Such designs are usually made so that the engine runs only on natural gas and therefore are applicable to solutions where natural gas is always available, e.g. large stationary engines.

The use of natural gas in CI engines is somewhat difficult because of the high octane rating and low cetane rating of natural gas. Therefore in standard CI engines the natural gas will not auto ignite [4] and needs an additional ignition source. The usual application of natural gas in CI engines is in so-called dual fuel combustion process [7] in which natural gas is the main energy source that is ignited by a small amount of diesel fuel. In general, there are different types of dual fuel operation that depend on the mixture preparation and ignition process. In High Pressure Direct Injection (HPDI) dual fuel engine both diesel and natural gas are directly injected into the cylinder during combustion process [8] through a single injector. This concept requires design of combustion chamber optimized for HPDI operation and does not allow operation with pure diesel. It also requires special injectors currently not available on the market. In conventional dual fuel operation natural gas is port injected and ignited by a small amount of directly injected diesel fuel. The conventional dual fuel operation mode can be obtained by a relatively easy conversion of existing CI engines, which has a significant importance in bringing this technology to a market [9]. Also, conventional dual fuel operation allows easy switch between dual fuel and pure diesel operation which is important in the process of larger scale implementation of natural gas in transport when there is no dense network of natural gas refueling stations. The third operational mode is a dual fuel HCCI operation [10] which can be realized by both fuels being port injected, but can also be achieved in an engine prepared for conventional dual fuel operation. Because of the benefits of conventional dual fuel combustion it is expected that this combustion mode will lead a larger scale introduction of natural gas in transport sector.

Development of any type of engine or upgrades to the engine design requires a lots of experimental and simulation work to be carried out. In this process a number of different simulation models are used

ranging from complexed ones, e.g. 3D-CFD multi-phase simulation, to the real time simulations used for setting up of controls. The objective of this work are so-called cycle simulations which are, in terms of complexity, somewhere between 3D-CFD and real time simulations. Cycle simulation enables fast prediction of entire engine and vehicle performance with enough complexity that allows the use of the model for optimization of engine operating parameters that includes the limitation factors such as knock, turbocharger limits, misfires etc. In order to use cycle simulation of conventional dual fuel operation there is a need for predictive, reliable, physically based combustion model of conventional dual fuel combustion.

In [11], Papagiannakis et al. used a predictive 0-D dual fuel combustion model to study the effects of intake air preheating and pilot fuel quantity on the dual fuel combustion characteristics. In the presented model, the temperature and mixture homogeneity in the spray (burning zone) was assumed. Liquid fuel (diesel) and natural gas entrained in the spray zone burn in a mixing-controlled combustion mode, while the premixed mixture of air and natural gas burns due to the flame propagation through the combustion chamber. Flame surface has a conical shape, and only one flame propagates through the combustion chamber. The authors in [12] presented the development of a predictive 0-D dual fuel model, where spray was modeled through packet approach, while flame propagation was modeled through turbulent entrainment model. To account for the presence of multiple ignition sites and sources, an equation based on packet volume and packet burned mass fraction was used. In [13], Walther et al. presented the development of a predictive 0-D dual fuel model based on the 2-zone SI and pre-chamber gas engine combustion models. In order to include the effect of in-cylinder inhomogeneity on the ignition delay calculation, the diesel fuel spray is divided into a number of zones. It is assumed that the initial flame front consists of a truncated cone and a hemisphere, and as the flame propagates through the combustion chamber, the flame front becomes spherical. As long as the flame zone is smaller than the maximum spray region, liquid pilot fuel has an influence on the overall rate of heat release. In [14], Papagiannakis et al. used a predictive 0-D combustion model to study the effects of intake air preheating and exhaust gas recirculation (EGR) on the dual fuel combustion characteristics. Compared to the model presented in [11], in this model the flame surface is spherical. In [15], Eichmeier et al. presented the development of a predictive 0-D RCCI (Reactivity Controlled Compression Ignition) diesel-natural gas combustion model, where the diesel fuel spray is modeled using a Hiroyasu's multizone approach. In this model, the enhanced air entrainment after the end of injection as well as the effect of injection on the turbulent kinetic energy development is included. In [16], Mikulski et al. presented the development of an empirical 0-D dual fuel combustion model, where the rate of heat release is calculated with a Vibe function. In this way various physical phenomena are not included in the rate of heat release calculation, which means that it is necessary to adjust the combustion model parameters as the engine operating parameters change.

This paper presents the development of a predictive Dual Fuel Multi-Zone Combustion Model (DF-MZCM), which can be used for the simulation of combustion process in conventional dual fuel internal combustion engines. Spray process calculation is based on

the approach presented in [17], while the flame propagation calculation is based on the approach presented in [18, 19, 20]. Contrary to previously presented models, this model features a geometrical description of the effect of multiple ignition sources and multiple flames that propagate through the combustion chamber. Additionally, the effect of entrained methane is included in the calculation of ignition delay and spray burning rate. The developed model has been integrated within the commercial cycle-simulation software (AVL CruiseM) and validated with the experimental data that have been acquired at UC Berkeley. At the end of the paper a sensitivity analysis of the developed model on tuning parameters (turbulence and combustion) is presented.

DUAL FUEL COMBUSTION MODEL

Description of the Model

DF-MZCM is a multi-zone quasi-dimensional combustion model which can be used in cycle-simulation analyses of conventional dual fuel engines. The division of the in-cylinder content into a number of zones (multi-zone approach) enables description of in-cylinder heterogeneities (temperature and mixture composition), while the quasi-dimensional approach enables inclusion of influence of in-cylinder geometry, flame location and number of flames on the overall combustion rate. As natural gas is consisted primarily of methane, in this model natural gas is represented as pure methane. The presented combustion model is based on the existing combustion models which simulate the combustion processes in CI engines (AVL MZCM) and SI engines (fractal combustion model). The model is capable of appropriately describing all three combustion phases which occur in the conventional dual fuel engine, and it features:

- Multi-zone approach to combustion modeling.
- Description of the combustion chamber geometry.
- Description of the injector nozzle orientation and spray angle (injector data).
- Tracking of spray zone position (deflection of the chamber walls).
- In-cylinder turbulence modeling.
- Modeling of the spray processes (injection, charge entrainment, fuel evaporation, ignition and combustion).
- Calculation of the start of flame propagation condition & location of the ignition location.
- Flame propagation is calculated with a quasi-dimensional combustion model.
- Laminar flame surface is calculated with a newly developed multiple flame model.

Zone Formation and Evolution

Prior to direct injection of diesel fuel, the entire cylinder content is treated as a single zone; premixed homogeneous charge of methane, air and combustion products. Once the injection of diesel fuel starts a number of spray zones are created. During the injection process, for each time step a new parcel of zones is generated in the axial direction and this parcel is then further subdivided in the user-defined number of zones in radial direction (Figure 1, images on the right). During the spray evolution, fresh charge is entrained into every spray

packet (zone) from the unburned zone (UZ to SZ in Figure 1, image (a) on the left), liquid fuel is evaporated and combustible diesel fuel/methane/air mixture is created, and once the appropriate condition has been satisfied inside a given spray packet (ignition delay condition is satisfied), prepared mixture ignites. Mass, composition (equivalence ratio), temperature and mass burning rate are calculated for every individual spray packet (zone). The local equivalence ratio inside each spray zone is determined by the entrained air and methane mass as well as by the mass of evaporated diesel fuel.

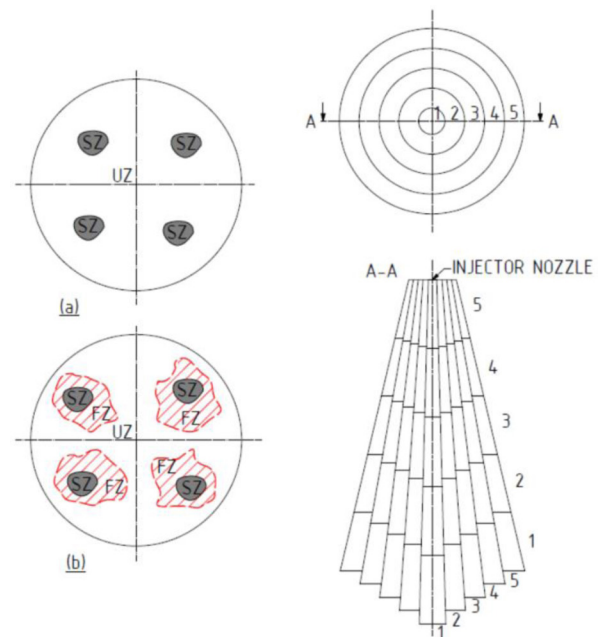


Figure 1. Schematic of zone interaction & spray zone formation

Once the ignition delay condition in a given spray zone has been satisfied, mixture ignites and burns in a stoichiometric way, which means that combustion in each spray zone is limited by either the amount of evaporated (Diesel) and entrained (methane) fuel or by the amount of entrained air. If there is a surplus of fuel inside the spray zone (rich mixture), the mass of fuel that burns equals the stoichiometric mass of fuel for a given mass of air inside the spray zone. Likewise, if there is a surplus of air inside the zone (lean mixture), the entire mass of prepared fuel burns; however, it burns in a stoichiometric way, which means that after the combustion is completed there is still a certain amount of air present in such zone. It is important to stress out that there is no immediate interaction between the spray zones (no heat or mass transfer between the zones). The equations that govern the spray processes (liquid fuel break-up, charge entrainment, droplet evaporation and spray combustion) will be presented in the following paragraphs.

Once the condition for the start of flame propagation has been satisfied, the flame propagation through the premixed mixture starts and the increase of burned zone is governed by both spray combustion and flame propagation. The presented model assumes that the flame propagation can only start if:

- Spray has ignited;
- Premixed mixture is within the flammability limits;

- There is sufficient amount of activation energy (sufficient amount of spray has burned and spray temperature is sufficiently high).

Flame is considered to have a spherical shape and it starts to propagate from the outer surface of the spray. Once the flame propagation has started, spray zones are engulfed with the propagating flame which means that new interactions between the zones are formed. There is an interaction between the unburned and burned (flame) zone which is governed by flame propagation, and an interaction between the burned (flame) and spray zones which is governed by the entrainment of new mass into the spray. Once the flame propagation starts the only mass that can be entrained into the spray zones is the burned mass that has been created as a result of flame propagation through the premixed mixture (FZ to SZ in [Figure 1](#), image (b) on the left). Spray combustion lasts until either the entire fuel mass inside the spray zone has been burned, or there is no more air mass inside the spray zone. This means that spray combustion and flame propagation can occur at the same time; actually there are cases where flame propagation has ended and there is still combustion going on inside the spray zones. The overall burning rate is a sum of the spray burning rate and the burning rate governed by the flame propagation through the premixed mixture.

Zonal Thermodynamics

In 0-D modeling approach the entire calculation domain is treated as one control volume without orientation and spatial discretization [20]; all dependent variables are solely a function of time. The 0-D models can generally be classified into two major groups: single zone and multizone models. In the multi-zone modeling approach the in-cylinder mass is divided into a number of zones, where every zone is essentially an open thermodynamic system for which two conservation equations (energy and mass) as well as gas equation are set and solved. For each zone, uniformity of composition and temperature is assumed, while the uniformity of pressure is assumed for the entire cylinder content. In IC engine simulations it is customary to use crank angle instead of time discretization. The equations for calculation of temperature and pressure derivatives are given in numerous reported studies [17, 20] and hence will not be specifically shown in this paper.

In-Cylinder Turbulence Modeling

In-cylinder flow structures of internal combustion engines are generated during the intake stroke when highly unstable recirculating flow occurs in the combustion chamber. The large scale flow structures are very dissipative due to viscous forces in the fluid, resulting with the generation of smaller scale structures that increase the in-cylinder turbulence level around TDC, which is further increased during the direct injection of diesel fuel. The level of in-cylinder turbulence is defined by the velocity fluctuation u' , usually called turbulence intensity. The geometry feature of turbulent eddies are described by the integral length scale L_1 representing the diameter of "spherical" shaped turbulent eddy. Both of these turbulence quantities influence the combustion process of internal combustion engines increasing the flame deformation, transfer of

momentum, heat and mass. Therefore, the correct prediction of turbulence quantities is very important for the calculation of combustion process in dual fuel engines.

Turbulence model used in this work is based on a 2-zone k-epsilon turbulence model presented in [19]. It includes two transport equations, one for turbulent kinetic energy k and the other for its dissipation rate ε . Under the assumption of isotropic and homogeneous turbulent flow field it is possible to define differential equations that can be applied within the 0-D modeling approach:

$$\frac{dk}{dt} = S_{in} \left(\frac{q_m^{in}}{m_c} U_{ives}^2 \right) + \frac{2}{3} \frac{k}{\rho} \frac{d\rho}{dt} + S_{inj} \left(\frac{q_m^{inj}}{m_c} U_{inj}^2 \right) - \frac{2}{3} \frac{k}{v} \frac{dv}{dt} - \varepsilon \quad (1)$$

$$\frac{d\varepsilon}{dt} = C_{in} \left(\frac{4}{3} \frac{q_m^{in}}{m_c} \varepsilon \right) + C_{\varepsilon} \left(\frac{4}{3} \frac{\varepsilon}{\rho} \frac{d\rho}{dt} \right) + C_{inj} \left(\frac{4}{3} \frac{q_m^{inj}}{m_c} \varepsilon \right) + \frac{5}{12} \frac{\varepsilon}{v} \frac{dv}{dt} - C_2 \frac{\varepsilon^2}{k} \quad (2)$$

In [equations \(1\) and \(2\)](#) the first terms of right hand side represent the source terms that describe the increase of k and ε in the cylinder during the intake stroke when the fresh air (or mixture) flows into the cylinder. The second terms describe the production of turbulence quantities during the high pressure cycle when the energy of large scale flow structures is transferred to the small turbulent eddies - rapid distortion theory [21]. The third terms are newly introduced terms that are used for calculating the effect of diesel fuel injection on the increase of turbulence quantities. The fourth terms are derived to capture diffusion effects, while the last terms represent destruction of both properties. During the fuel injection, the increase of turbulent kinetic energy occurs due to introduction of new kinetic energy with the spray and due to fuel spray interaction with the existing large flow structures in the cylinder that transfer energy to the turbulence level. The first effect is described by the applied turbulence equations while the spray interaction with the existing in-cylinder flow structures cannot be taken directly into account because 0-D approach is used. The fact that this effect is neglected can be compensated by the appropriate tuning of newly introduced user-defined constant S_{inj} and C_{inj} .

Physical properties of the unburned zone play the most important role in the combustion process that is governed by the flame propagation across the combustion chamber. Turbulent eddies in the fresh mixture increase fuel-air mixing while in the flame zone increase the entrainment of fresh mixture by wrinkling the flame front. Since the flame propagation is dominant combustion model in the dual fuel combustion progress, the two zone turbulence model was used in this study. This means that the turbulence of unburned zone was calculated and the quantities of the unburned zone were used to calculate the part of the burning rate caused by the flame front entrainment of the fresh mixture. The following k and ε differential equations were used for modeling of the unburned zone turbulence:

$$\frac{dk_{UZ}}{dt} = \frac{2}{3} \frac{k_{UZ}}{\rho_{UZ}} \frac{d\rho_{UZ}}{dt} - \frac{2}{3} \frac{k_{UZ}}{v_{UZ}} \frac{dv_{UZ}}{dt} - \varepsilon_{UZ} \quad (3)$$

$$\frac{d\varepsilon_{UZ}}{dt} = C_{\text{eps}}^{UZ} \cdot \left(\frac{4}{3} \frac{\varepsilon_{UZ}}{\rho_{UZ}} \frac{d\rho_{UZ}}{dt} \right) + \frac{5}{12} \frac{\varepsilon_{UZ}}{\nu_{UZ}} \frac{d\nu_{UZ}}{dt} - C_2 \frac{\varepsilon_{UZ}^2}{k_{UZ}} \quad (4)$$

where physical properties in both equations with index 'UZ' are related to the unburned zone (fresh mixture). The user-defined constant C_{eps}^{UZ} (-) defines the decrease of unburned zone turbulent kinetic energy compared to the evolution of total in-cylinder turbulent kinetic energy during the combustion process. More details about the applied two zone k-ε turbulence model can be found in [19, 20].

Also, the new feature of the turbulence model, compared to the one presented in [19, 20] is the introduction of controls for integral length scale size in the unburned zone, which improves the calculation of the final stage of flame propagation as it accounts for the geometry effects on the integral length scale. Integral length scale is calculated by the following expression:

$$L_1 = \frac{\sqrt{k^3}}{\varepsilon} \quad (5)$$

Under the assumption of isotropic and homogeneous turbulent flow field, Kolmogorov length scale can be expressed as:

$$l_k = \frac{L_1}{Re_T^{3/4}} \quad (6)$$

$$Re_T = \frac{u' L_1}{\nu_{UZ}} \quad (7)$$

$$u' = \sqrt{\frac{2k}{3}} \quad (8)$$

In the above equations ν_{UZ} (m²/s) is the unburned zone viscosity, while Re_T is the turbulent Reynolds number of the unburned zone. Geometrically allowed size of the integral length scale is calculated by the following expression:

$$L_{L,limit} = MIN \left[\left(2 \cdot \sqrt[3]{\frac{3 \cdot V_{UZ}}{4 \cdot \Pi}} \right), h_{PIS} \right] \quad (9)$$

$$L_{L,limit} = C_{limit} \cdot L_{L,limit} \quad (10)$$

In the above equations V_{UZ} (m³) is the unburned zone volume; h_{PIS} (m) is either the distance between piston top (in case of flat-flat geometry), or piston bowl bottom (in case of geometry with a bowl in piston) and cylinder head, while C_{limit} is the tuning parameter. Finally, the integral length scale is calculated as:

$$L_1 = MIN(L_1, L_{L,limit}) \quad (11)$$

The eddy turnover time, which is used in the calculation of the duration of transition from laminar to fully turbulent flame, is calculated from the following expression:

$$\tau_T = \frac{L_1}{u'} \quad (12)$$

The constants of k-ε turbulence model are determined using the previous experience with the application of turbulence model when the cycle-simulation results were compared with the available 3-D CFD results. Since the 3-D CFD results were not available in the present study, the turbulence constants were determined so that the level of turbulent kinetic energy at TDC is approximately 0.75 x mean piston speed [22].

Spray Combustion Model

Spray is modeled with a modified AVL MZCM [17] which is based on the packet approach first presented in [23], and which accounts for all physical processes relevant for spray development and combustion:

- Injection,
- Liquid fuel break-up,
- Charge entrainment,
- Evaporation,
- Combustion.

As was already mentioned, there is no interaction (heat and mass transfer) between the spray zones. Mass that is entrained in the spray is either from the unburned zone (before flame propagation starts), or from the flame zone (once the flame propagation through the premixed mixture has started), while the only heat transfer that is taken into account is the wall heat transfer. In this section, only the important equations that govern the reactive charge preparation and combustion process will be given, while the other AVL MZCM model equations and features can be found in [17]. As flow through the injector is assumed to be quasi-steady and incompressible [17], the injection velocity can be calculated from the Bernoulli's principle. The spray zone velocity is calculated according to a semi-empirical correlation given by Hiroaysu and Arai [23]. The effect of decrease of velocity in radial direction and slipstream effect are taken into account through correction functions which are given in [17]. The break-up moment is calculated assuming the equality of injection and zone penetration velocities through an equation given in [17]. In the break-up moment, liquid fuel is instantaneously split into droplets and the initial droplet diameter is calculated with the correlation given by Varde et al. [24]. There is no account for secondary breakup in this model; droplet diameter is further decreased through the process of droplet evaporation. Charge entrainment into the spray zones is calculated through the conservation of linear momentum principle:

$$m_{\text{entr},i} = C_{\text{entr}} \cdot m_{\text{inj},i} \left(\frac{v_{\text{inj}}}{v_i} - 1 \right) \quad (13)$$

In the equation (13) $m_{entr,i}$ is the charge mass entrained into the spray zone i , $m_{inj,i}$ is the fuel mass injected into the spray zone i , v_{inj} is the injection velocity, while v_i is the current zone velocity calculated from the correlation given in [20] (velocity of a spray zone i). C_{entr} is a user defined parameter which accounts for other physical mechanisms that decelerate the spray other than charge entrainment.

The process of liquid fuel evaporation is governed by simultaneous heat transfer from the surrounding charge to the droplet and mass transfer of the fuel from the droplet to the surrounding charge. The evaporation process is modeled with the equations taken from [25], while the equations for calculating the heating of the droplet and mass diffusion into the surrounding charge are given in [17]. In order to calibrate the evaporation model, evaporation rate is multiplied by a parameter C_{evap} .

In order to exactly track the position of each zone in the spray, which enables a precise calculation of the location of the propagating flame center, new features have been added to the spray model; spray angle and spray center calculations. Spray angle is calculated by the correlation given in [26]:

$$\tan\left(\frac{\varphi_{spray}}{2}\right) = C_{angle} \cdot \left[\left(\frac{\rho_{ch}}{\rho_{liq}}\right)^{0.19} - 0.0043 \cdot \left(\frac{\rho_{liq}}{\rho_{ch}}\right)^{0.5} \right] \quad (14)$$

In the equation (14), φ_{spray} ($^\circ$) is the calculated spray angle; ρ_{ch} (kg/m^3) is the charge density, while ρ_{liq} (kg/m^3) is the liquid density. C_{angle} (-) is the parameter which accounts for the injector geometry parameters and its value is given in the literature [26].

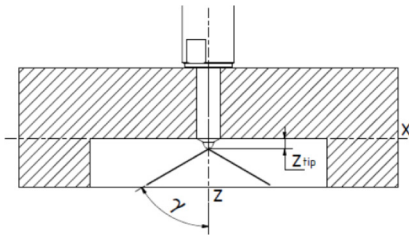


Figure 2. Schematic overview of the injector geometry

With this procedure it is possible to track the position of every zone more precisely and in the combination with more accurate representation of the cylinder geometry, more precisely calculate the moment when spray collides with the cylinder boundaries (walls and piston). Now, by accounting both injector geometry data (Figure 2), it is possible to calculate the exact position of the spray center:

$$R_{spray} = \frac{\sum m_i \cdot R_i}{m_{spray}} \quad (15)$$

$$R_{xyspray} = R_{spray} \cdot \sin \gamma \quad (16)$$

$$z_{spray} = (z_{spray} + z_{tip}) \cdot \cos \gamma \quad (17)$$

In the above equations, R_{spray} (m) is the location of the spray center in axial direction; $R_{xy,spray}$ (m) is the location of the spray center in the xy -plane of the cylinder, while z_{spray} (m) is the location of the spray center in the vertical plane of the cylinder.

Additional new features of the spray model are new methods of ignition delay and spray combustion calculation. Spray ignition is calculated with the appropriate ignition delay tables for n-heptane/methane/air/combustion products mixture, while the reaction rate in the spray zones is calculated through the specific reaction rate time scale which is taken from the look-up tables for n-heptane/methane/air/combustion products mixture. These tables were generated with an in-house code developed specifically for this purpose, which is based on the 0-D homogeneous constant volume reactor. Both tables were made as a function of 5 parameters:

- Temperature,
- Pressure,
- Fuel vapor mass fraction,
- Combustion products mass fraction,
- Mass fraction of methane in the n-heptane/methane fuel blend.

The temperature criterion is used to define the ignition delay moment; specifically, ignition delay moment is triggered when the second derivative of temperature curve equals zero [27]:

$$\text{sign}\left(\frac{d^2 T_i}{dt^2}\right)_t = -\text{sign}\left(\frac{d^2 T_i}{dt^2}\right)_{t-dt} \quad (18)$$

Spray combustion is initiated when the following term is satisfied:

$$\int_{t_{FC}}^t \frac{1}{C_{ID} \cdot \tau_{ID}(T_i, p, x_{FV,i}, x_{CP,i}, x_{met/FV,i})} \cdot dt \geq 1, \quad (19)$$

For each spray packet (zone), its temperature is used in both ignition delay and chemical reaction rate calculation. In the above equations τ_{ID} (s) is the ignition delay time, C_{ID} (-) is the ignition delay parameter, T_i (K) is the temperature of a spray zone i , p (bar) is the charge pressure, $x_{FV,i}$ (-) and $x_{CP,i}$ (-) are the fuel vapor and combustion products mass fractions of a spray zone i , while $x_{met/FV,i}$ (-) is the mass fraction of methane in fuel vapor of a spray zone i . The effect of entrained methane on n-heptane/methane fuel blend ignition delay is presented in the figure below.

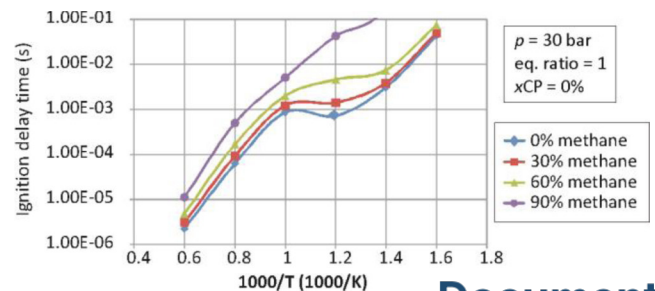


Figure 3. Effect of methane on n-heptane/methane ignition delay time